Mesoscale Modeling of Dynamic Fracture and Shock Compression in Quartzite and Sandstone

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Abstract

This doctoral thesis is part of the MEMIN (Multidisciplinary Experimental and Modeling Impact Research Network) project, which experimentally and numerically investigates the effects of meteorite impact on geological materials on a laboratory scale up to a natural scale.

The objective of this thesis is the development of mesoscale simulation models that represent the material behavior of quartzite and sandstone at load conditions typical for rocks in the vicinity of meteorite impacts. From these models, macroscale material properties are derived via homogenization. The latter are intended to provide a basis for the development of predictive macroscale material models that can be used to simulate impact cratering scenarios. The multitude and complexity of the physical phenomena occurring in meteorite impact scenarios necessitate the partitioning of all mechanisms into sub-processes that can be replicated in a mesoscale model. Two main mechanisms are modeled in this work, namely shock compression and dynamic fracture.

Shock compression is, in the case of meteorite impact, characterized by a primary shock wave that radially propagates from the impact point. This process is responsible for irreversible pore collapse and shock metamorphic effects in the quartz matrix. Two numerical models are proposed and investigated in order to build a comprehensive mesoscale model of compressive shock loading. Simulations with idealized geometries in planar symmetry are carried out using the meshfree Smoothed Particle Hydrodynamics (SPH) formulation. Using this approach, modeling aspects such as the choice for Equations of State and strength model are evaluated, as well as physical aspects such as the degree of water saturation. The effects of these different aspects on shock wave propagation and pore collapse mechanisms are investigated. The second model presented is a more detailed, three-dimensional Finite Element (FE) model. With this model, the effects of grain anisotropy and different types of strength on the macroscopic shock response are investigated. For both SPH and FE formulations, a parameter study is carried out in which the influence of the aforementioned parameters on macroscopic shock Hugoniots is quantified. In particular, relationships between particle
velocity and shock velocity, as well as between particle velocity and stress amplitude, are built up. Results from the models are compared to experimental reference literature. The FE model describes the low velocity regime (up to approximately 1000 m/s) well, while the SPH model is better-suited for higher velocities. A concept for a new mesoscale model is presented, in which features of the different modeling variants might be combined and a macroscale Equation of State might be derived from a series of simulations with one single model.

Dynamic fracture in impact cratering scenarios is characterized by crack patterns developing in the target that may induce spallation, i.e. the detachment and ejection of plates of the target material in the near-surface area. Based on a new mesoscale FE model, a novel methodology is developed to derive three-dimensional macroscale material data from one-dimensional dynamic fracture experiments, namely Split-Hopkinson-Bar experiments in spallation configuration. As a prerequisite, an improved cohesive zone formulation that models inter-granular failure using an energy-based approach is presented. In particular, improved stability and robustness of the numerical method are achieved. These improvements are particularly crucial to address multi-branched failure paths and prevent interpenetration between debonding grains. In the frame of a parameter study, mesoscopic failure parameters are indirectly calibrated to experimental data via the evaluation of equivalent macrosscopic failure quantities. The calibrated mesoscale model is then subjected to a set of multiaxial load cases. From the results, macroscopic yield and failure surfaces in the principal stress space are derived by using homogenization techniques. The results can be directly used to calibrate macroscale material models for dynamic fracture and thus improve the capabilities for predicting impact craters in geologic materials and, in particular, spallation effects.
Zusammenfassung


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Notation and abbreviations

Unless indicated otherwise, all vectors and tensors defined in this work implicitly refer to a three-dimensional vector space. Indicial notation on vectors and tensors will be implicitly adopted throughout this work. For example, let \( \mathbf{a} \) and \( \mathbf{c} \) be two vectors and \( \mathbf{B} \) a second-order tensor. The simple contraction of \( \mathbf{B} \) and \( \mathbf{a} \) gives \( \mathbf{c} \) and can be expressed by:

\[
\mathbf{c} = \mathbf{B} \cdot \mathbf{a} \iff c_i = B_{ij} a_j \iff c_i = \sum_{j=1}^{3} B_{ij} a_j
\]

**Stress description**

*Scalars*
- \( I_1, I_2, I_3 \)  Invariants of the stress tensor
- \( J_1, J_2, J_3 \)  Invariants of the deviatoric stress tensor
- \( P \)  Pressure
- \( \xi, \rho, \theta \)  Haigh-Westergaard stress coordinates
- \( \rho_T, \rho_C, \rho_S \)  Tensile, compressive and shear meridians
- \( \sigma_1, \sigma_{II}, \sigma_{III} \)  Principal stress components
- \( \sigma_L \)  Compressive longitudinal stress under 1D strain state
- \( \sigma_{vM} \)  von Mises stress
- \( \chi(\sigma) \)  Characteristic polynomial of the stress tensor

*Vectors*
- \( \mathbf{T} \)  Stress vector

*2nd order tensors*
- \( \mathbf{S} \)  Deviatoric stress tensor
- \( \mathbf{\sigma} \)  Cauchy stress tensor

**Strain description**

*Scalars*
- \( \varepsilon^{\text{pl}} \)  Infinitesimal effective plastic strain
- \( \zeta \)  Compressive volumetric strain: \( \zeta = -tr(\mathbf{\varepsilon}) \)
2nd order tensors
\( \bm{\varepsilon} \)  Infinitesimal strain tensor
\( \dot{\bm{\varepsilon}} \)  Infinitesimal strain rate tensor
\( \bm{\varepsilon}_{\text{dev}} \)  Infinitesimal deviatoric strain tensor
\( \bm{\varepsilon}_{\text{vol}} \)  Infinitesimal volumetric strain tensor
\( \bm{\varepsilon}^{\text{el}} \)  Infinitesimal elastic strain tensor
\( \bm{\varepsilon}^{\text{pl}} \)  Infinitesimal plastic strain tensor

Material constitutive description

Scalars
\( a, b \)  Drucker-Prager material parameters
\( c_V \)  Isochoric heat capacity
\( c \)  Cohesion
\( E \)  Isotropic Young's modulus
\( E_1, E_2, E_3 \)  Orthotropic Young's moduli
\( e_H \)  Hugoniot energy
\( \mathcal{F}_0(\bm{\sigma}) \)  Initial yield function
\( \mathcal{F}(\bm{\sigma}) \)  Yield function
\( \mathcal{F}(\bm{\sigma}, \bm{\varepsilon}^{\text{pl}}) \)  Hardening function
\( G \)  Isotropic shear modulus
\( G_{12, 13, 23} \)  Orthotropic shear moduli
\( G \)  Plastic potential
\( K \)  Isotropic bulk modulus
\( K_1, K_2, K_3, B_0, B_1 \)  Coefficients of the Polynomial Equation of State
\( P_H \)  Hugoniot pressure
\( P_{\text{min}} \)  Critical pressure
\( s \)  Linear coefficient of the \( U_s(U_1) \) relation
\( s_k \)  \( k \)-th polynomial coefficient of the \( U_s(U_1) \) relation
\( T_{\text{min}} \)  Critical compressive normal stress
\( T_n \)  Normal traction component
\( T_t \)  Tangential traction component
\( v \)  Mass-specific volume
\( Y \)  von Mises yield stress
\( \alpha(\varepsilon_{\text{eff}}^{\text{pl}}) \)  Isotropic hardening function
\( \alpha_p \)  Isobaric volumetric thermal expansion
\( \beta_T \)  Isothermal compressibility
\( \Gamma \)  Grüneisen coefficient
\( \eta \)  \( \eta = 1 - \rho_1/\rho_0 \)
κ Yield stress under pure shear loading
\(d\Lambda\) Flow rule factor
\(\lambda, \mu\) Lamé coefficients
\(\nu_{ij}, i, j = 1,2,3\) Orthotropic Poisson’s ratios
\(\rho\) Density
\(\rho_0\) Initial density
\(\phi\) Angle of internal friction

\(2^{nd}\)-order tensors
\(\sigma_\beta\) Kinematic hardening function

\(4^{th}\)-order tensors
\(\mathbb{C}\) Elastic stiffness tensor
\(\mathbb{S}\) Elastic compliance tensor

Wave mechanics description

Scalars
\(A\) Section of the shock tube
\(C_B\) Bulk sound speed
\(C_L\) Longitudinal sound speed
\(C_p\) Primary sound speed
\(C_s\) Shear sound speed
\(C_{A,B}\) Longitudinal sound speeds of media \(A\) and \(B\)
\(E_{\text{int}}\) Internal energy
\(E_{\text{kin}}\) Kinetic energy
\(e_0, e_1\) Mass-specific internal energies of non-shocked and shocked media
\(F\) External force
\(l_0, l_1\) Lengths of non-shocked and shocked regions at time \(t\)
\(l'_0, l'_1\) Lengths of non-shocked and shocked regions at time \(t'\)
\(m\) Mass
\(P_0, P_1\) Pressures in non-shocked and shocked media
\(t\) Time
\(U(x,t)\) Longitudinal velocity at position \(x\) and time \(t\)
\(U_0, U_1\) Longitudinal velocities of non-shocked and shocked media
\(U_{bc}(t)\) Velocity boundary condition prescribed over time
\(U_i, U_r, U_t\) Incident, reflected and transmitted velocities
\( U_s \) Longitudinal shock velocity
\( v_0, v_1 \) Mass-specific volumes in non-shocked and shocked media
\( W \) Work
\( x \) Longitudinal position
\( \rho_0, \rho_1 \) Densities of non-shocked and shocked media
\( \rho_{\mathcal{A}}, \rho_{\mathcal{B}} \) Densities of media \( \mathcal{A} \) and \( \mathcal{B} \)
\( \sigma(x, t) \) Longitudinal stress at position \( x \) and time \( t \)
\( \sigma_i, \sigma_r, \sigma_t \) Incident, reflected and transmitted stresses
\( \varphi, \psi \) Wave functions
\( \omega_i, \omega_r, \omega_t \) Incident, reflected and transmitted waves

**Kinematics description**

_Scalars_

\( x \) Longitudinal coordinate
\( \alpha, \theta \) Rotation angles

_Vectors_

\( \mathbf{F} \) Force
\( \mathbf{n} \) Surface normal unit vector
\( \mathbf{U} \) Velocity vector
\( \mathbf{u} \) Displacement vector
\( \mathbf{x} \) Position vector
\( \xi \) Elongation

_2nd-order tensors_

\( \mathcal{A} \) Orthogonal transformation matrix
\( \mathcal{K} \) Stiffness matrix

**Finite Element method description**

_Notions_

\( e \) Finite element
\( \mathcal{f} \) Facet
\( M \) Material point
\( \mathcal{N} \) Node
\( \Gamma \) Boundary of \( \Omega \)
\( \Gamma_e \) External boundary
\( \Gamma_{\mathcal{f}} \) Boundary associated to facet \( \mathcal{f} \)
\( \Gamma_{\text{int}} \) Internal boundary
\( \Gamma_T \) Traction-prescribed boundary
\( \Gamma_u \) Displacement-prescribed boundary
\( \Omega \) Volumetric body
\( \Omega_e \) Volumetric domain of finite element \( e \)

**Scalars**

- \( c_{\text{max}} \) Largest wave speed in the medium
- \( m_k \) Lumped mass of node \( N_k \)
- \( m_e^k \) Partial lumped mass of the element \( e \) connected to node \( N_k \)
- \( N_k(x) \) Shape function related to node \( N_k \)
- \( n_e \) Number of finite elements
- \( n_n \) Number of nodes
- \( dS \) Infinitesimal surface
- \( \Delta t_{\text{CFL}} \) Maximum admissible time step size in the medium
- \( \Delta t^{(n)} \) Size of the \( n \)-th time step
- \( dV \) Infinitesimal volume
- \( \Delta x_{\text{min}} \) Smallest finite element size in the medium
- \( \alpha^{(n)} \) Value of an arbitrary function \( \alpha \) at the \( n \)-th time step
- \( \beta \) Parameter for mixed formulation of forward and backward finite difference schemes
- \( \varphi^h(x, t) \) FE approximation of a function \( \varphi(x, t) \)
- \( \varphi_k(t) \) Interpolation value of \( \varphi \) at node \( N_k \)

**Vectors**

- \( b \) Body force
- \( f_{\text{ext}}^k \) External force at node \( N_k \)
- \( f_{\text{int}}^k \) Internal force at node \( N_k \)
- \( T^{bc} \) Traction prescribed on \( \Gamma_T \)
- \( u^{bc} \) Displacement prescribed on \( \Gamma_u \)
- \( \bar{\psi} \) Virtual displacement

**2nd-order tensors**

- \( M \) Mass matrix
- \( M^d \) Diagonalized mass matrix

**Smoothed Particle Hydrodynamics description**

**Notions**

- \( I, J \) Particles \( I \) and \( J \)
Scalars

$C$ Dimension-dependent parameter
$D$ Dimension of the problem
$E_i, E_j$ Young’s modulus of particles $i$ and $j$
$h$ Smoothing length
$2h$ Kernel radius
$r$ $r = ||x||$
$\Delta V_j$ Volume attributed to particle $J$
$W(x)$ Kernel function
$w(r/h)$ Mono-variable kernel function $w(r/h) = W(x)$
$\delta(x)$ Dirac function

Vectors

$f^{Hg}_i$ Hourglass corrective force on particle $i$
$X$ Position vector in the reference configuration
$X_{ij}$ Distance vector pointing from particle $i$ to particle $J$ in the reference configuration
$x_i, x_j$ Coordinates of particles $i$ and $j$
$x_{ij}$ Distance vector pointing from particle $i$ to particle $J$ in the deformed configuration
$\langle x_{ij} \rangle$ Theoretical distance vector pointing from particle $i$ to particle $J$ in the deformed configuration
$\langle x_{ij} \rangle^{sym}$ Symmetrized theoretical distance: $\langle x_{ij} \rangle^{sym} = \langle x_{ji} \rangle^{sym}$
$\varepsilon_{ij}$ Error vector $\langle x_{ij} \rangle^{sym} - x_{ij}$

$2^{nd}$-order tensors

$F$ Deformation gradient

Cohesive-Zone-Element description

Notions

$\mathcal{B}, \mathcal{B}_1, \mathcal{B}_2$ Body $\mathcal{B}$ and sub-bodies $\mathcal{B}_1$ and $\mathcal{B}_2$
$C_{12}$ Cohesive zone
$C^\#$ Cohesive zone element associated to facet $f$
$M, M_1, M_2$ Point $M$ and two new sub-points $M_1$ and $M_2$
$\varepsilon_0$ Half-spheroid of critical tractions

Scalars

$\mathcal{D}$ Damage value: $\mathcal{D} = \delta^{eff} / \delta^{crit}$
$\mathcal{D}_{stab}$ Threshold damage value for traction locking
$G^{crit}$ Fracture energy
$dS, dS_1, dS_2$  
Infinitesimal surface $dS$ and two infinitesimal 
subsurfaces $dS_1$ and $dS_2$

$S_\mathbf{f}$  
Surface of facet $\mathbf{f}$

$\mathbf{T}^{0}$  
Nominal traction

$\mathbf{T}^{eff}$  
Effective traction

$T_n$  
Normal component of the cohesive traction

$T_t$  
Tangential component of the cohesive traction

$\mathbf{T}^{crit}_n$  
Critical traction under pure normal loading

$\mathbf{T}^{crit}_t$  
Critical traction under pure tangential loading

$\mathbf{T}_n$  
Normal component of the internal traction

$\mathbf{T}_t$  
Tangential component of the internal traction

$t_{coh}$  
Activation time of the cohesive zone

$\beta$  
Coupling factor between sliding and normal opening 
displacements

$\gamma$  
Tangential-to-normal ratio of the opening vector $\langle \delta \rangle$

$\delta^{eff}$  
Effective opening

$\delta_n$  
Normal component of the separation vector

$\delta_t$  
Tangential component of the separation vector

$\delta^{crit}_n$  
Critical separation under pure normal loading

$\delta^{crit}_t$  
Critical separation under pure tangential loading

$\delta_n^{max}$  
Maximal separation along the reversible unloading-
reloading path under pure normal loading

$\delta_t^{max}$  
Maximal separation along the reversible unloading-
reloading path under pure tangential loading

$\varphi$  
Free energy potential

$\mathbf{f}^{coh}_{k1\rightarrow k2}$  
Cohesive force acting from node $N_{k2}$ to node $N_{k1}$

$\mathbf{f}^{f}_{k1\rightarrow k2}$  
Cohesive force relative to the cohesive zone element
$C^f$ and acting from node $N_{k2}$ to node $N_{k1}$

$n$  
Mid-surface normal unit vector

$n_{\mathbf{f}}$  
Normal unit vector of facet $\mathbf{f}$

$\mathbf{T}$  
Current cohesive traction

$T_\infty$  
Far-field loading traction

$\mathbf{T}^{avg}$  
Average traction of two elements sharing a common 
cohesive facet: $\mathbf{T}^{avg} = \sigma^{avg} \cdot n_{\mathbf{f}}$

$\mathbf{T}^{f}_{k1\rightarrow k2}$  
Cohesive traction relative to the cohesive zone
element $C^f$ and acting from node $N_{k2}$ to node $N_{k1}$

$\mathbf{T}^{init}$  
Initial cohesive traction

$\mathbf{F}$  
Internal traction
$t$  Unit vector projection of $\mathbf{T}$ on the mid-surface plane
$
\hat{u}_k^{ps-coh}$ Node acceleration contribution imparted on sub-node $\mathcal{N}_k$ from the other sub-nodes sharing the same primary node $\mathcal{N}_k$
$
\delta$ Separation vector joining $M_1$ to $M_2$
$
\dot{\delta}$ Separation velocity
$
\ddot{\delta}$ Separation acceleration
$
(\delta)$ Opening vector
$
\sigma_{avg}$ Average stress of both elements sharing a common cohesive facet
$
\sigma_{e}^{Gauss}$ Stress at the Gauss integration point of element $e$
$
\sigma_{avg}$ Average stress tensor at node $\mathcal{N}_k$ from weighted stresses of elements $e$ sharing $\mathcal{N}_k$
$
\sim$ accent Corrective term

**Split-Hopkinson-Bar-Test description**

**Scalars**

$C_{spe}, C_{alu}$ Longitudinal sound speed of the specimen and of aluminum

$D_k$ Damage of the $k$-th cohesive zone element

$E_{int}(t)$ Internal energy of the whole specimen at time $t$

$E_{kin}(t)$ Kinetic energy of the whole specimen at time $t$

$E_{spe}$ Young’s modulus of the specimen

$E_{tot}(t)$ Total energy of the whole specimen at time $t$

$e_{int}(x,t)$ Internal energy of an infinitesimal portion of the specimen at position $x$ and time $t$

$e_{kin}(x,t)$ Kinetic energy of an infinitesimal portion of the specimen at position $x$ and time $t$

$e_{tot}(x,t)$ Total energy of an infinitesimal portion of the specimen at position $x$ and time $t$

$E_{\text{failed}}(t_2)$ Actual total energy of the failed specimen at time $t_2$

$E_{\text{intact}}(t_2)$ Virtual total energy of an intact specimen at time $t_2$

$G_{crit}^{exp}$ Experimental dynamic fracture energy

$G_{crit}^{\sim}$ Average value of measured dynamic fracture energy values

$G_{\text{macro}}$ Macroscopic fracture energy

$G_{\text{meso}}$ Mesoscopic fracture energy
Theoretical fracture energy

Impulse transfer from the left fragment to the right fragment

Specimen length

RVE initial length

Masses of the left and right fragments

Mid-surface area of the $k$-th cohesive zone element

Cross-sectional area of the RVE

Average value of measured dynamic tensile strength values

Macroscopic tensile strength

Mesoscopic critical traction

Mesoscopic critical traction under pure normal loading

Mesoscopic critical traction under pure tangential loading

Failure initiation time: $t_1 = t_{fail}$

Time of full fragment separation

Back-and-forth wave propagation time in the specimen: $t_{delay} = 2L/C_{spe}$

Pull-back time

Longitudinal velocity at position $x$ and time $t$

Velocities of the left and right fragments

Longitudinal velocity at the free end of the specimen

Longitudinal velocity boundary condition

Longitudinal stress associated to $U_{bc}(t)$

Average stress in the RVE

Total stress or resulting stress resulting from wave superimposition: $\sigma_{tot} = \sigma_l + \sigma_r$
Compressive shock loading description

 Scalars

\( e \) Mass-specific internal energy
\( \tilde{\gamma} \) Helmholtz free energy
\( \tilde{G} \) Apparent shear modulus
\( K_{iso}^0, G_{iso}^0 \) Equivalent isotropic bulk and shear moduli at zero pressure
\( K_{iso}(P), G_{iso}(P) \) Pressure-dependent equivalent isotropic bulk and shear moduli
\( K_{Reuss}, G_{Reuss} \) Lower Reuss bound for equivalent isotropic bulk and shear moduli
\( K_{Voigt}, G_{Voigt} \) Higher Voigt bound for equivalent isotropic bulk and shear moduli
\( \bar{K}_{EOS} \) Apparent bulk modulus prescribed by the Equation of State
\( P_{EOS} \) Pressure prescribed by the Equation of State
\( P_T(\rho) \) Isotherm pressure lines over density
\( S \) Entropy
\( T \) Temperature
\( T_P(\rho) \) Isobar temperature lines over density
\( U_p \) Particle velocity
\( \bar{U}_p \) Average of longitudinal velocity over \( m_{ref} \)
\( \bar{U}_{p_voxel} \) Average of longitudinal velocity over \( m_{voxel} \)
\( U_s \) Shock velocity
\( V_{ref}, m_{ref} \) Reference volume and reference mass
\( V_{voxel}, m_{voxel} \) Voxel volume and voxel mass
\( \bar{\sigma}_L \) Average of longitudinal stress over \( V_{ref} \)
\( \bar{\sigma}_{L_voxel} \) Average of longitudinal stress over \( V_{voxel} \)

\( \text{hist} \) subscript Value of a variable evaluated at a history point

\( 2^{\text{nd}}\)-order tensors

\( A \) Coupling stiffness term between \( S \) and \( \zeta \)
\( B \) Coupling stiffness term between \( P \) and \( \epsilon_{dev} \)

\( 4^{\text{th}}\)-order tensors

\( C_{dev} \) Deviatoric stiffness tensor
RHT model description

Scalars

- $F_R$: Strain rate-dependent factor function
- $f_c$: Failure stress under 1D compressive stress state
- $f_s$: Failure stress under pure shear loading
- $f_t$: Failure stress under 1D tensile stress state
- $P_t$: Volumetric tensile limit
- $Q$: Failure function

Operators

- $Q(P^*) = R_3(P^*, \theta = 0)$
- $Q_1$: $f_s/Q_1$ is the shear failure stress on the compressive meridian
- $Q_2$: $f_t/Q_2$ is the tensile failure stress on the compressive meridian
- $R_3$: Lode angle-dependent factor function
- $\varepsilon^p$: Maximum allowable plastic strain
- $\dot{\varepsilon}_0$: Reference strain rate in the $F_R$ function
- $\dot{\varepsilon}_{limit}$: Intermediate strain rate in the $F_R$ function
- $\sigma_f$: Failure function
- $\sigma_Y$: Yield function

* superscript: Normalization of a quantity by $f_c$

Cos, sin, tan: Cosinus, sinus and tangent operators

det: Matrix determinant

ln: Natural logarithm

max: Maximum value of a set of variables

tr: Matrix trace

$o(X)$: Little-o of the function $X$

$\Delta X$: Variation of the function $X$

$dx$: Infinitesimal variation of the function $X$

$\partial X$: Partial derivative of the function $X$ with respect to $Y$

$\frac{\partial Y}{\partial X}$: Total derivative of the function $X$ with respect to $Y$

$X^T$: Transposition of the matrix $X$

$X(t) \equiv Y(t)$: Congruence relation for which two temporal signals $X(t)$ and $Y(t)$ are equal modulo a temporal shift
Macaulay operator on scalar: \( \langle X \rangle = \max(X, 0) \)

Macaulay operator on vector: \( \langle X \rangle = X_t t + \langle X_n \rangle n \)

Euclidian norm of the vector \( X \)

Difference of \( X \) values across a boundary

\( \{X_{i,n}\}_k \)

\( (X_{1,1}, \ldots, X_{1,k}, \ldots, X_{1,n}, X_{2,1}, \ldots, X_{2,k}, \ldots, X_{2,n}, X_{3,1}, \ldots, X_{3,k}, \ldots, X_{3,n}) \)

\( \nabla X \)

Gradient of the scalar \( X \)

\( \nabla . X \)

Divergence of the vector \( X \)

\( \nabla . X \)

Divergence of the 2\(^{\text{nd}}\) order tensor \( X \)

\( (\vec{X}, \vec{Y}) \)

Angle between the vectors \( X \) and \( Y \)

\( X \times Y \)

Vector product of the vectors \( X \) and \( Y \)

\( R_\alpha \)

Rotation matrix by an angle \( \alpha \)

\( R_{(\alpha, \Delta)} \)

Rotation matrix by an angle \( \alpha \) around the axis \( \Delta \)

\( 1 \)

Identity matrix

\( \forall \)

For all

\( \in \)

Set membership

\( \cup \)

Set union

\( \subset \)

Set inclusion

**Abbreviations**

ANEOS: Analytical Equation of State

CFL: Courant-Friedrichs-Lewy

DEM: Discrete Element Method

FE: Finite Element

FV: Finite Volume

HEL: Hugoniot Elastic Limit

MEMIN: Multidisciplinary Experimental and Modeling Impact Research Network

PDF: Planar Deformation Feature

RHT: Riedel-Hiermaier-Thoma

RVE: Representative Volume Element

SPH: Smoothed Particle Hydrodynamics
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1 Introduction

1.1 Motivation – From meteorite impacts to mesoscale models

Meteorite impact on Earth is a wide topic that has increasingly gained interest over the past years. Apart from the threat meteorites represent for human civilization, larger meteorites that collided with Earth up to several millions of years ago can be traced back via the crater morphology they left behind. From in-situ evidences on Earth, such as crater size and shape, faults or shock metamorphism in the surrounding crater area, the geoscience community has attempted not only to date back cratering events, but also to reconstruct the impact conditions that might have prevailed at the time of occurrence. Different branches of science accomplish this challenging work. On the basis of contemporary crater observations, geologists are able to assess the soil nature preceding impact by considering long-term stratification and erosion effects. Mineralogists survey shock metamorphic effects in rocks, thus giving clues about the rock composition and the loading, e.g. pressure, and investigate metallic inclusions to find out whether they have a meteoritic origin. Physicists and geophysicists set the focus on impact physics. Their purpose is to attempt, on the basis of in-situ observations such as crater size and shape, rock composition, porosity or water-saturation, to derive key parameters describing meteorite impact conditions, namely meteorite material, size, impact speed and incident angle. Naturally, all of these scientific branches are interrelated and cannot act separately in the process of understanding meteorite impact. An exhaustive description of meteorite impact processes from the point of view of geophysics can be found in [66][36]. The authors characterize the different stages of an impact, which are the contact and compression stage, the excavation stage and the modification stage. At the contact and compression stage, two shock waves arise at the contact interface and propagate into the impactor and the target, respectively. At the excavation stage, the shock-wave induced excavation flows into the target and forms a cavity, the maximum of which is called transient crater. At the modification stage, the transient crater is shaped into the so-called final crater, e.g. via spallation phenomena. Figure 1.1 exemplarily shows a photograph of a natural crater located in Arizona called Meteor Crater or Barringer Crater.
The crater rim has a quite circular shape and roughly amounts to 1200 m in diameter.

Figure 1.1: Photograph of the Meteor Crater (or Barringer Crater) in Arizona, USA. Image from Peter L. Kresan.

In order to address the impact cratering issue with the most comprehensive approach, the Multidisciplinary Experimental and Modeling Impact Research Network or MEMIN project is comprised of investigations in the areas of geoscience, material science and numerical modeling. From the experimental point of view, geologic materials are investigated on the laboratory scale through downscaled impacts of metallic spherical projectiles, up to one centimeter in diameter, onto quarried rock cubes of up to about half a meter edge length [47][55], see Figure 1.2 for illustration. From these experiments, e.g., morphometric properties and microstructural features of these laboratory craters can be identified and interpreted.
Figure 1.2: Snapshots of ejected material following a laboratory sphere impact on a sandstone block at four different instants of time [47]. The first image shows a hot central plume and the initial ejecta cone. In the second image, the expanding and then steepening trend of the ejecta cone results in a kink in the ejecta pattern. The cone eventually steepens to a tube (third image) and conveys large-sized spallation plates from the block subsurface (fourth image).

A further objective of the MEMIN project is to set up relevant principal relationships, such as the dependency of cratering efficiency on impactor velocity or target strength. On this basis, upscaling is used to extrapolate cratering experiments to natural cratering events on Earth [77]. The knowledge of the transient crater, which is formed as a result of shock-wave compression and subsequent wave rarefaction, is of high relevance as it is used as a basis for the development of scaling laws. Using scaling, small laboratory craters and large natural craters can be directly compared. In gravity-dominated natural craters, the transient crater is about ten to twenty times as large in diameter as the projectile and the final crater is, due to gravitational forces, filled with debris. Due to the high cratering efficiency, i.e. the ratio of transient crater mass to projectile mass, spallation zones may also exist in natural craters but are minimally significant [54]. In this regard, spallation phenomena in natural craters do not disturb the identification of the transient crater. In contrast, the impact craters generated in laboratory impact tests on rocks are strength-dominated. In that case, the cratering process is halted by the material strength and the transient crater diameter is only a few times larger than the projectile diameter. As a result, the final crater is substantially larger than the transient crater since chunks and plates spalling from the target subsurface amount to a large volume, see Figure 1.3.
For laboratory craters, it is essential to develop methods that allow for the quantification of spallation zones in order to determine the transient crater in the post-experimental crater analysis. Mathematical methods, such as parabolic fits, are generally employed to reconstruct the transient crater with good approximation [27]. Water-saturation is an important factor that enhances the shock wave propagation in granular rocks and reduces inter-granular fracture due to the cushioning effect acting between grains [54][96]. In contrast, dry pores may represent a barrier against shock wave propagation and stimulate pore crushing mechanisms. From a macroscale point of view, higher crater efficiencies are encountered in water-saturated materials than in dry ones.

Besides impact experiments and scaling laws, another important part of the MEMIN project, intended to support experimental investigations and in-situ observations, is the development of numerical models. This area is in the focus of this thesis. The continuous increase of computational power and the additional development of specific scientific software packages have enabled the numerical prediction of craters and impact-related features such as fracturing of grains or grain metamorphism. Macroscale models, which are based on continuum theory, offer the opportunity to compute cratering scenarios on large scales without resolving micromechanical details [22][76]. Cratering-related properties such as cracking and the ejection of spallation plates can be captured and compared to experimental data for a given impact scenario [93]. However, macroscale models can only predict craters if they are parameterized with realistic material data. In the case of shock loading, only a
few sources in the open literature provide substantial material data, and the generation of new data is expensive. The available data is mostly derived under simple one-dimensional loading conditions. For geologic materials, in particular, the variations of chemical composition, porosity, grain and pore size distributions, grain shapes, water saturation, pre-loading, etc. found in the field are very large, and it is not feasible to characterize the high rate behavior of each of these variants. For these reasons, mesoscale models can be very helpful and may improve macroscale material modeling. If the behavior of the constituents and their interaction is known and the model has been validated by comparison with experimental results, it can be modified and used to investigate the stress-strain relation for other material variants and for load cases which can hardly be generated experimentally, such as multiaxial dynamic loading. Following this approach, mesoscale models support the calibration of macroscale material models and improve the basis for extrapolations. Moreover, mesoscale modeling naturally supplies knowledge on shock wave effects on the microscale, such as planar deformation features, pore crushing, influence of crystal anisotropy or grain boundaries [38].

1.2 Status quo

1.2.1 Macroscale models of granular materials

Macroscale models are homogeneous material models that do not explicitly resolve mesoscopic heterogeneities, such as grain interfaces, pores or other inclusions, but summarize their local effects into macroscopic parameters. Thus, in the frame of a Finite Element discretization, the choice for the mesh resolution of a macroscopic geometry is not constrained by heterogeneities acting on the mesoscale. Instead, the resolution depends on the specific purposes of the macroscale problem. This way, the computational effort can be kept small and, in favor of a coarsened mesh, the computation of large macroscopic geometries is possible. For example, an intuitive and relevant meshing procedure, when applied to impact cratering simulations, consists of a mesh refinement near the impact point to better capture local deformation processes. A coarse mesh can then be used at far ranges as the shock wave attenuates. There, no attention has to be paid to microstructural features that would be encountered from a mesoscale modeling point of view.
Nevertheless, macroscale model formulations are sometimes inspired by phenomena acting on the mesoscale. This allows for a better material description based on physics and is expected to improve the capability to predict the material response. Porosity models, for example, can be based on the empirical assertion that porosity reduces macroscopic pressure. The most common one is the $P-\alpha$ model [20][44] which scales the pressure of the dense material, also called bulk pressure, by a macroscopic distension variable $\alpha$. The latter is described by a separate thermodynamic function dependent on pressure or, as alternatively proposed in the $\varepsilon-\alpha$ model [106], on the macroscopic compressive strain.

In general, porosity models only account for the amount of porosity and disregard other mesoscale features, such as pore size distribution and shape.

In addition, accurate modeling of inelastic deformation is of high relevance for porous materials on the macroscale. In contrast to metals, for which plasticity is observed in load cases with shear components only, porous materials may exhibit irreversible deformations due to pore crushing when subjected to volumetric compression. This localized effect, when homogenized to macroscale, is often represented using a plasticity model with a capped, ellipsoidal yield surface in the principal stress space. Indeed, the combined effects of shear and volumetric loading enhance irreversible pore compaction in comparison with pure volumetric load cases. This phenomenon, called shear-enhanced compaction, is described in [7][25][95]. A strain-rate dependent strength model, describing pore shrinking dynamics along with plastic hardening, is proposed in [3][17]. The post-yielding behavior is generally described by a macroscopic damage variable reflecting the growth and coalescence of microscopic cracks. A degraded stiffness model, characterized by an attenuation of the shear and bulk moduli as the damage parameter increases, is proposed in [39]. In the Johnson-Cook failure model [52], initially developed for metals, damage is accounted for as a cumulative plastic strain normalized by a critical failure strain beyond which the material shear resistance is annihilated. The Johnson-Holmquist model [53] describes gradual or sudden strength degradation with increasing damage while the O’Keefe model [73] additionally incorporates a dilatancy or bulking model. A review of these strength theories in the field of geologic rocks is given in [49].
1.2.2 Mesoscale modeling of dynamic loading in granular materials

Driven by the ongoing improvement of computational capabilities, mesoscale modeling has increasingly gained interest since the 1990s. In the literature, a variety of contributions address mesoscale simulations of granular materials under dynamic loading.

A considerable number of mesoscale investigations of tensile failure at high strain rates has been published for concrete [34][43][91][108]. By explicitly modeling mortar and aggregates in concrete, local inertial effects on the macroscopic concrete response can be assessed. As most mesoscale models address two-dimensional configurations and employ Cartesian grids, the geometric accuracy of material boundaries and the replication of inter-granular physics might be called into question. An innovative approach, in which the spallation behavior of a three-dimensional concrete mesoscopic structure with tetrahedral mesh is modeled by using an initially rigid cohesive zone formulation, is proposed in [60].

Mesoscale analysis of compressive shock loading is also addressed in the literature. For instance, relationships between phenomena resolved on the mesoscale and macroscopic material properties can be described for granular ceramics under planar compressive shock conditions [15][100]. After an initially rigid behavior dominated by grain contacting, an elastic-plastic behavior, characterized by granular compression and pore crushing, is adopted by the bulk material. Once porosity is removed, the macroscopic response stiffens and converges to the behavior of its non-porous counterpart. In addition to geometrical and grain strength effects, effects of crystal anisotropy on the macroscopic behavior may play an important role, as highlighted in [50] in the case of polycrystalline metals. Mesoscale modeling of the shock behavior of geologic rocks has also been addressed in the literature. Pore crushing and grain fracturing have been modeled in [96] using a hybrid Smoothed Particle Hydrodynamics (SPH) and Discrete Element Method (DEM) formulation. However, since a two-dimensional geometry model and a simple linear elastic model for quartz have been employed, only a qualitative analysis could be provided. Quartzite and sandstone with idealized pore shapes using a Finite Volume (FV) approach have been investigated in [42]. Local pressure concentrations with regard to pore crushing and quartz phase transition effects could be predicted and quantified. Due to the use of
idealized pore shapes, details such as grain shapes, grain boundaries and, in particular, crystallographic orientation, could not be explicitly modeled. Similar analyses have been conducted in [24] on generic granular materials.

1.2.3 Overview of rock properties

Quartz is the principal constituent of both quartzite and sandstone. An overview of its physical and geological properties is given before quartzite and sandstone are briefly introduced.

Quartz is a crystalline structure constituted of silica with the chemical formula SiO$_2$. Two quartz structures can be commonly encountered in nature: the high-temperature hexagonal $\beta$-quartz, and the low-temperature trigonal $\alpha$-quartz. The most common quartz crystal structure that can be observed in the Earth’s upper continental crust is the $\alpha$-trigonal form. When submitted to high confining pressures, the crystalline structure of quartz changes. Low pressure regimes generally give rise to the so-called Planar Deformation Features or PDFs. These are characterized by multiple sets of parallel thin lamellae. High pressure regimes produce amorphized phases of quartz such as diaplectic quartz glass [4] and polymorph phases of coesite and stishovite [61][62][94][101]. The following temperature-pressure phase diagram, see Figure 1.4, summarizes all possible phases quartz can adopt. As some phases only appear under stringent conditions, the interpretation of the quartz phase diagram has to be conducted with care. PDFs and diaplectic glass only appear under shock conditions involving short and steep pressure pulses (see the shock Hugoniot curve additionally plotted on the phase diagram). Besides, coesite and stishovite are almost only observable in impact craters since their formations are governed by quartz melting at extreme pressures beyond 50 GPa, followed by quartz recrystallization within their respective stability fields.
The quartzite type that has been investigated in the MEMIN project is Taunus quartzite from the Rhenish massif. This polycrystalline quartz-bearing sample has an extremely low porosity and contains quartz grains of size 100-200 µm with randomly distributed crystallographic orientations. A second quartzite variant that has been used in Split-Hopkinson-Bar-Tests is Wasa quartzite from Dalarna in Sweden. This quartzite variant has similar properties to the Taunus variant but possesses some more impurities. The sandstone type of investigation is called Seeberger sandstone and originates from Thuringia in Germany. It presents a fine granularity, i.e. an average grain size of about 100 µm, and a porosity of about 23%. The sandstone specimens dedicated to laboratory impact tests were quarried through a specific stratigraphic layer to ensure high quartz content and small grain sizes. Micrographs of Taunus quartzite, Wasa quartzite and Seeberger sandstone are shown in Figure 1.5.

Figure 1.4: Phase diagram of quartz with a shock Hugoniot curve (red), which is characterized by several phase changes (taken from [62] and [94] and extended).
Figure 1.5: Micrographs of Taunus quartzite (top left), Wasa quartzite (top right) and Seeberger sandstone (bottom).

1.3 Objectives and outline

The primary goals of this work are 1) the development of realistic mesoscale models for quartzite and sandstone, and 2) the derivation of homogenized relationships, capable of supporting the design of predictive macroscale models for these rocks. Since simulations of impact cratering scenarios are envisaged in the long term, the focus must be on specific loading configurations. In the scope of this work, two essential loading cases will be investigated, namely shock compression and dynamic fracture. The former essentially refers to the primary shock wave compression that radially extends from the impact point, while the latter is associated to dynamic spallation that takes place in the subsurface area in strength-dominated crater formations.
In order to capture the prominent features taking place in quartzite and sandstone at the microstructural level, Representative Volume Elements or RVEs are built up at the so-called mesoscale or grain scale. An RVE can be defined as the smallest volumetric extract of a macroscopic geometry that is capable of yielding representative quantities of the whole geometry. The optimal RVE size should ensure a sufficient representativeness of the macroscale geometry at minimum computational effort. The optimal RVE size is prescribed by the microstructure morphology, namely granularity, material contrasts or periodicity, and also by the macroscopic quantities of interest. A detailed introduction to the concept and validity range of RVEs is given in [13][26]. In this work, RVEs will be considered adequate if they are comprised of at least five quartz grains per RVE edge length. Since the quartz grains composing quartzite and sandstone have a diameter of 100 µm on average, RVEs of size 0.5 mm will be generated for each rock type.

Dynamic fracture is simulated using a Finite Element (FE) formulation. The models represent modified Split-Hopkinson-Bar-Tests in spallation configuration. Key parameters that can be derived from these experiments are the dynamic tensile strength and the dynamic fracture energy. A tailor-made mesoscale setup will be developed accordingly in order to reproduce the experimental geometry and loading conditions as realistically as possible. The objective is to derive, for each rock type, a set of mesoscale parameters, capable of reproducing the experimentally observable macroscopic behavior. In particular, modeling of inter-granular failure processes using an improved cohesive zone formulation is proposed.

The simulation of shock compression scenarios often calls the stability and robustness of computational schemes into question. In this respect, the meshfree Smoothed Particle Hydrodynamics (SPH) method, allowing for the use of idealized RVEs, is the method of choice to address this issue. Consolidated literature-based shock data on quartzite and sandstone will be used as an experimental reference. Here, the purpose of SPH simulations is to evaluate the pore collapse mechanisms taking place in sandstone and to derive macroscopic relationships comparable to literature data via homogenization methods. In particular, the effects of the quartz Equation of State and of different quartz strength hypotheses on the simulated macroscopic response will be assessed. Additional FE simulations, although more prone to numerical instabilities caused by
high mesh distortions, will be conducted in order to determine shock features in geometrically more realistic quartzite and sandstone RVEs. Mesoscale properties such as grain anisotropy, which cannot be represented in SPH models, will be investigated in combination with different quartz strength models, and their influence on the macroscopic shock response will be shown. Generally, only a partial investigation of mesoscale parameters is carried out by authors in the literature. The approach presented here is aimed at giving valuable clues for determining the set of mesoscale parameters for which the simulated macroscopic shock responses of quartzite and sandstone replicate literature shock data.

The final step of this work consists in enlarging the spectrum of homogenized relationships in view of the development of future macroscale material models. To achieve this, a multitude of multiaxial loads will be applied at different strain rates to quartzite and sandstone models. Macroscopic yield and failure states will be derived for quartzite and sandstone. A short review of the RHT material model will be given and will, on the basis of the observed homogenized results, illustrate the potential calibration procedure for macroscale parameters. In the literature, standard macroscale models for geologic materials assume a regular distribution of microstructural features such as porosity. By contrast, in this work, macroscale models will be derived that take into account local effects on the mesoscale via a proper homogenization process.

The outline of this work is sketched out in Figure 1.6, which points out the sequence of tasks to be addressed and interrelations between the different chapters. Two main directions of research, namely dynamic fracture and shock compression in quartzite and sandstone, constitute the core of this work. The starting point of the modeling approach is the generation of appropriate RVEs for quartzite and sandstone, see Chapter 3. Grain-resolved RVEs, dedicated to the FE formulation, are generated for the modeling of dynamic inter-granular fracture in rocks as well as for compressive shock loading. Idealized RVEs used in the SPH formulation are intended to provide deep insight about pore collapse dynamics. Chapter 4 describes the Cohesive-Zone-Element formulation, including a review of standard formulations, and presents new improvements achieved within this work. Chapter 5 is dedicated to the setup of a Split-Hopkinson-Bar simulation model in which the mesoscopic material failure parameters of quartzite and sandstone are indirectly calibrated to experimental data. Chapter 6 addresses the compressive shock behavior
in quartzite and sandstone. An extended parameter study, in which quartz strength, Equation of State, anisotropy degree and degree of saturation with water in pores are varied, is conducted in order to derive homogenized Hugoniot relationships and open avenues for improved modeling in the light of standard literature data. Chapter 7 reports on the derivation of homogenized yield and failure surfaces for quartzite and sandstone from parametric mesoscale simulations. The failure parameters used in these simulations are determined in Chapter 5 and a specific Equation of State adopted for quartz is described in Chapter 6. Analogies between the homogenized results and comprehensive macroscale models such as the RHT model are drawn and suggestions for future research with regard to macroscale modeling improvements are given at the end of Chapter 7.
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Figure 1.6: Schematic outline of this work consisting of two main courses: mesoscale simulation of dynamic fracture and shock compression in quartzite and sandstone.
2 Mechanical fundamentals

2.1 Isotropy vs. anisotropy

Before addressing some basics about material laws, the concept of isotropy will be outlined against anisotropy in the following, see also [63].

2.1.1 Physical background of isotropy

The concept of isotropy relates to the invariance of a given property with respect to the spatial orientation. In mechanics, a material admits an isotropic behavior if and only if its mechanical response to an arbitrary loading is independent of the loading direction. To take a concrete example, a two-dimensional body consisting, say, of shortpastry, is considered, see Figure 2.1. Within this pastry, two tensile specimen-like biscuits are punched out along two different directions.

Figure 2.1: Exemplary sketch of a two-dimensional pastry-like body, from which two tensile specimen-like biscuits of different orientations are punched out.

It is assumed here that the material law of specimen (1) is ruled by a constitutive relation of the following type:

$$F^{(1)} = \mathbf{K} \cdot \xi^{(1)} \quad \Leftrightarrow \quad F_i^{(1)} = K_{ij} \xi_j^{(1)} \quad \text{with} \quad i = 1 \text{ to } 2 \quad (2.1)$$
where \( F^{(1)} \) is the force in Newton applied on the specimen and \( \xi^{(1)} \) is its elongation in meter. \( K \) is a second-order material tensor called stiffness tensor. It linearly relates the specimen force and elongation and can be regarded as a generalization of the classical one-dimensional spring elongation law. A specific elongation \( \xi^{(1)} \) oriented along the longitudinal direction of specimen (1), here vertical, is prescribed on specimen (1) in the following. Let \( R_\alpha \) be a rotation matrix such that it rotates any vector around the out-of-plane axis by an angle \( \alpha \). The angle \( \alpha \) is such defined that it transforms, as sketched in Figure 2.1, the longitudinal direction of specimen (1) into that of specimen (2). Applying \( R_\alpha \) on \( \xi^{(1)} \) delivers a new elongation \( \xi^{(2)} \) of same amplitude and oriented along the longitudinal direction of specimen (2). To ensure isotropy, the stiffness tensor of specimen (2) must be such defined that the resulting force \( F^{(2)} \) directly derives from the application of the rotation matrix on \( F^{(1)} \).

Knowing that \( R_\alpha = R_\alpha^{-1} \), this mathematically requires that:

\[
F^{(2)} = K \cdot \xi^{(2)} \iff R_\alpha \cdot F^{(1)} = K \cdot R_\alpha \cdot \xi^{(1)} \iff K = R_\alpha^T \cdot K \cdot R_\alpha
\]

This way, the stiffness matrix \( K \) is mathematically constrained by \( n = 2 \) equations relating the stiffness coefficients with each other, where \( n \) is the dimension of the problem. Since this condition has to be met for any angle \( \alpha \), some stiffness coefficients are enforcedly zeroed and the resulting stiffness \( K \) matrix is sparse. In the more general three-dimensional case, the rotation matrix \( R_\alpha \) is generalized to an orthogonal transformation \( \mathcal{A} \) which conserves the scalar product of two vectors. In addition to rotations, reflections about planes can also be considered.

### 2.1.2 Different degrees of anisotropy in linear elasticity

The previous case can be extended to linear elasticity, where the problem is described in terms of second-order tensors. For the sake of clarity, the hypothesis of infinitesimal deformations will be adopted in the following. Accordingly, the infinitesimal strain tensor \( \varepsilon \) will be employed along with the Cauchy stress tensor \( \sigma \). The physical meaning of this mathematical concept will be sketched in more detail in section 2.2. The linear relation between the stress and strain tensors is given by Hooke’s law:
\[
\sigma = \mathbb{C} : \varepsilon \quad \Leftrightarrow \quad \sigma_{ij} = \mathbb{C}_{ijkl} \varepsilon_{kl} \quad \text{with} \quad i, j, k, l = 1 \text{ to } 3 \quad (2.3)
\]

where \( \mathbb{C} \) is the so-called elastic stiffness tensor. Due to the fourth-order nature of \( \mathbb{C} \), the number of stiffness coefficients amounts to \( 3^4 = 81 \). Owing to the symmetric nature of the stress and strain tensors, the maximal number of independent stiffness coefficients can be reduced to 21. Accordingly, the Voigt notation allows for a reduced matrix equation:

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{31}
\end{pmatrix} =
\begin{pmatrix}
\mathbb{C}_{11} & \mathbb{C}_{12} & \mathbb{C}_{13} & \mathbb{C}_{14} & \mathbb{C}_{15} & \mathbb{C}_{16} \\
\mathbb{C}_{12} & \mathbb{C}_{22} & \mathbb{C}_{23} & \mathbb{C}_{24} & \mathbb{C}_{25} & \mathbb{C}_{26} \\
\mathbb{C}_{13} & \mathbb{C}_{23} & \mathbb{C}_{33} & \mathbb{C}_{34} & \mathbb{C}_{35} & \mathbb{C}_{36} \\
\mathbb{C}_{14} & \mathbb{C}_{24} & \mathbb{C}_{34} & \mathbb{C}_{44} & \mathbb{C}_{45} & \mathbb{C}_{46} \\
\mathbb{C}_{15} & \mathbb{C}_{25} & \mathbb{C}_{35} & \mathbb{C}_{45} & \mathbb{C}_{55} & \mathbb{C}_{56} \\
\mathbb{C}_{16} & \mathbb{C}_{26} & \mathbb{C}_{36} & \mathbb{C}_{46} & \mathbb{C}_{56} & \mathbb{C}_{66}
\end{pmatrix}
\begin{pmatrix}
\epsilon_{11} \\
\epsilon_{22} \\
\epsilon_{33} \\
2\epsilon_{31} \\
2\epsilon_{12}
\end{pmatrix} \quad (2.4)
\]

The above symmetric stiffness matrix stands for general anisotropy, for which the 21 coefficients may be independent of each other. Nevertheless, some materials might, although not being fully isotropic, exhibit a reduced degree of anisotropy. In the following paragraphs, different degrees of anisotropy are briefly outlined. Deeper mathematical details can be found in [14].

2.1.2.1 Orthotropy
In orthotropic materials, material properties are invariant by reflection about three planes all orthogonal to each other. Typical orthotropic materials are wood or woven fabric composites. The abovementioned orthotropic properties can be transposed into equations to reduce the complexity of the stiffness tensor. In order to facilitate the mathematical description of orthotropy, a classical three-dimensional physical case, involving vector quantities such as the force \( \mathbf{F} \) and the elongation \( \xi \), is first considered. Moreover, the orthotropic axes are supposed to be aligned with the coordinate axes. Let \( \mathbf{A}_1 \) and \( \mathbf{A}_2 \) be reflections about the \( x_2x_3 \)-plane and the \( x_1x_3 \)-plane, respectively. They are expressed by the matrices:

\[
\mathbf{A}_1 = \begin{pmatrix}
-1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix} \quad \mathbf{A}_2 = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & 1
\end{pmatrix} \quad (2.5)
\]
Using the invariance property $\mathbf{K} = \mathbf{A}_1^T \mathbf{K} \mathbf{A}_1$ delivers:

$$\mathbf{K} = \begin{pmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{pmatrix} = \begin{pmatrix} K_{11} & -K_{12} & -K_{13} \\ -K_{21} & K_{22} & K_{23} \\ -K_{31} & K_{32} & K_{33} \end{pmatrix} \quad (2.6)$$

This implies that the coefficients $K_{12}$, $K_{21}$, $K_{13}$ and $K_{31}$ must be zeroed. Similarly, the invariance property $\mathbf{K} = \mathbf{A}_2^T \mathbf{K} \mathbf{A}_2$ delivers:

$$\mathbf{K} = \begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{22} & K_{23} \\ 0 & K_{32} & K_{33} \end{pmatrix} = \begin{pmatrix} K_{11} & 0 & 0 \\ 0 & K_{22} & -K_{23} \\ 0 & -K_{32} & K_{33} \end{pmatrix} \quad (2.7)$$

Similarly, the coefficients $K_{23}$ and $K_{32}$ must be zeroed. The resulting stiffness tensor $\mathbf{K}$ is diagonal and comprises three independent stiffness coefficients.

In linear elasticity, plane reflections must be replaced by their fourth-order counterparts. For the sake of conciseness, the calculation details will not be explicated and the resulting sparse stiffness tensor, see [2], is directly given in the Voigt notation by:

$$\mathbf{C} = \begin{pmatrix} \frac{1 - \nu_{32}v_{32}}{E_2E_3\Delta} & \frac{v_{23} + \nu_{31}v_{31}}{E_2E_3\Delta} & \frac{v_{31} + \nu_{21}v_{32}}{E_2E_3\Delta} & 0 & 0 & 0 \\ \frac{v_{21} + \nu_{31}v_{33}}{E_2E_3\Delta} & \frac{1 - \nu_{33}v_{33}}{E_1E_3\Delta} & \frac{v_{32} + \nu_{12}v_{33}}{E_1E_3\Delta} & 0 & 0 & 0 \\ \frac{v_{31} + \nu_{21}v_{32}}{E_2E_3\Delta} & \frac{v_{32} + \nu_{12}v_{31}}{E_1E_3\Delta} & \frac{1 - \nu_{12}v_{21}}{E_1E_2\Delta} & 0 & 0 & 0 \\ 0 & 0 & 0 & G_{23} & 0 & 0 \\ 0 & 0 & 0 & 0 & G_{13} & 0 \\ 0 & 0 & 0 & 0 & 0 & G_{12} \end{pmatrix} \quad (2.8)$$

where $\Delta = \frac{1 - \nu_{12}v_{21} - \nu_{23}v_{32} - \nu_{31}v_{13} - 2\nu_{21}v_{32}v_{13}}{E_1E_2E_3}$. 
Reversely, the compliance tensor \( S \), defined as the inverse of the stiffness tensor \( \mathbb{C} \), is expressed by:

\[
S = \begin{pmatrix}
\frac{1}{E_1} & -\frac{\nu_{12}}{E_2} & -\frac{\nu_{13}}{E_3} & 0 & 0 & 0 \\
-\frac{\nu_{21}}{E_1} & \frac{1}{E_2} & -\frac{\nu_{23}}{E_3} & 0 & 0 & 0 \\
-\frac{\nu_{31}}{E_1} & -\frac{\nu_{32}}{E_2} & \frac{1}{E_3} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{G_{23}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_{13}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{G_{12}}
\end{pmatrix}
\]

(2.9)

Both stiffness and compliance tensors reveal twelve material parameters, such as three directional Young's moduli \( E_i \), three directional shear moduli \( G_{ij}, \ i < j \) and six Poisson's ratios \( \nu_{ij}, \ i \neq j \). Owing to tensor symmetries, the following equalities are satisfied: \( \frac{\nu_{ij}}{E_i} = \frac{\nu_{ji}}{E_j} \) and the number of actual independent material parameters drops from twelve to nine.

### 2.1.2.2 Transverse isotropy

In transverse isotropic materials, material properties are symmetric about a particular axis. As a consequence, the isotropy condition is fully satisfied within the plane orthogonal to that axis, which is called plane of isotropy. Typical transverse isotropic materials include unidirectional fiber composite laminates. To ascertain the stiffness tensor sparseness in the transverse isotropic case, classical physics is again considered. By convention, the axis of symmetry is said to be aligned with the \( x_3 \)-coordinate axis. Let \( \mathcal{A}_\theta \) be a rotation about the \( x_3 \)-axis by an angle \( \theta \), for which the matrix expression is given by:

\[
\mathcal{A}_\theta = \begin{pmatrix}
\cos(\theta) & \sin(\theta) & 0 \\
-\sin(\theta) & \cos(\theta) & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

(2.10)
It can be easily demonstrated that the application of the invariance property $\mathbf{K} = \mathbf{A}_0^T \mathbf{K} \mathbf{A}_0$ annihilates, for $\theta = \pi$, the stiffness coefficients $\mathcal{K}_{13}$, $\mathcal{K}_{31}$, $\mathcal{K}_{23}$ and $\mathcal{K}_{32}$. Moreover, it turns out for $\theta = \frac{\pi}{2}$ that $\mathcal{K}_{11} = \mathcal{K}_{22}$ and $\mathcal{K}_{12} = -\mathcal{K}_{21}$. Since stiffness coefficients must be positive from a physical point of view, the coefficients $\mathcal{K}_{12}$ and $\mathcal{K}_{21}$ must be zeroed. It results from this analysis a diagonal stiffness tensor for which the diagonal terms are $(\mathcal{K}_{11}, \mathcal{K}_{11}, \mathcal{K}_{33})$.

In linear elasticity, a similar analysis delivers the following compliance tensor $\mathbf{S}$:

$$
\mathbf{S} = \begin{pmatrix}
\frac{1}{E_1} & -\frac{\nu_{21}}{E_1} & -\frac{\nu_{31}}{E_1} & 0 & 0 & 0 \\
-\frac{\nu_{12}}{E_1} & \frac{1}{E_1} & -\frac{\nu_{31}}{E_1} & 0 & 0 & 0 \\
-\frac{\nu_{13}}{E_1} & -\frac{\nu_{13}}{E_1} & \frac{1}{E_1} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{G_{23}} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{2(1 + \nu_{12})}{E_1}
\end{pmatrix}
$$

(2.11)

Analogously to the orthotropic case, tensor symmetries show that $\nu_{12} = \nu_{21}$ and $\frac{\nu_{13}}{E_1} = \frac{\nu_{31}}{E_1}$. As a consequence, only five independent coefficients are required to describe transverse isotropy. These are the Young’s modulus $E_1$ and the Poisson’s ratio $\nu_{12}$ in the isotropic plane, and the Young’s modulus $E_3$, the Poisson’s ratio $\nu_{13}$ and the shear modulus $G_{23}$ along the symmetry axis.

2.1.2.3 Pure isotropy

Pure isotropy can be regarded as a combination of three transverse isotropic models, the symmetry axes of which are the coordinate axes, respectively. This way, the isotropic compliance matrix $\mathbf{S}$ can be naturally derived:
There, only two independent coefficients are needed, namely the isotropic Young's modulus $E$ and the isotropic Poisson's ratio $\nu$.

### 2.2 Continuum mechanics, elasticity and plasticity

Introductive aspects about continuum mechanics [18][51], such as the definition of stress and strain tensors in the frame of small deformations, will be briefly introduced in the following subsection. In addition, the definition of tensor invariants and the essential mathematical properties they convey will be given. The concepts of elasticity and plasticity, corroborated by some examples, will be then addressed in the subsequent subsections.

#### 2.2.1 Some basics on continuum mechanics

Continuum mechanics is based on a fundamental hypothesis: two infinitely close material points in a deformable body remain, upon transformation of this body from a reference configuration to a deformed configuration, infinitely close. This postulate therefore underlies an appropriate mathematical description of physical quantities attached to deformable media for which continuity and differentiability conditions are satisfied. In order to describe the infinite spectrum of forces applicable on all possible oriented surfaces within a continuum medium in an affordable way, the definition of a second-order tensor, called Cauchy stress

$$\S = \begin{pmatrix}
\frac{1}{E} & -\nu & -\nu & 0 & 0 & 0 \\
-\nu & \frac{1}{E} & -\nu & 0 & 0 & 0 \\
-\nu & -\nu & \frac{1}{E} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{2(1 + \nu)}{E} & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{2(1 + \nu)}{E} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{2(1 + \nu)}{E}
\end{pmatrix}$$

(2.12)
Mechanical fundamentals

tensor $\sigma$, is of relevance. When considering any oriented surface, the projection of the stress tensor on the surface normal vector $n$ delivers the so-called stress vector $T$:

$$ T = \sigma \cdot n \quad \text{or} \quad T_i = \sigma_{ij} n_j $$

The stress vector can be regarded as the ratio of the force acting on the $n$–oriented surface in the current configuration to the surface area. In this respect, the definition of the Cauchy stress tensor is powerful since it is able to summarize an infinite palette of surficial forces into a single second-order tensor. Further stress measures, such as the first and second Piola-Kirchhoff stress tensors, can also be defined, see e.g. [45]. In so far as an updated Lagrange scheme, where the reference configuration is updated to the current configuration every time step, is used, see Chapter 3, the hypothesis of small deformations is met. Accordingly, the use of the Cauchy stress tensor is well-suited for the oncoming numerical models. It can be shown that the momentum equilibrium enforces the Cauchy stress tensor to be symmetric.

The strain tensor, as the dual quantity of the stress tensor, departs from the displacement field of a material point. The latter is defined as the difference of the position vectors of a material point between the current and reference configurations. In order to gauge the displacement field variation with respect to the spatial coordinates in a concise way, a second-order strain tensor is introduced. It is defined in its infinitesimal form by:

$$ \varepsilon = \frac{1}{2} (\nabla u + \nabla^T u) \quad \text{or} \quad \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) $$

Non-linearized strain definitions, such as the Green-Lagrangian strain tensor or the Hencky strain tensor, can be defined for larger deformations. As for the Cauchy stress tensor, the closeness of the reference and current configurations according to the updated Lagrange scheme makes the small deformation hypothesis applicable. Equation (2.14) trivially shows that the infinitesimal strain tensor is, like the Cauchy stress tensor, symmetric.
Due to their symmetric nature, stress and strain tensors offer a variety of interesting mathematical properties that can be exploited for the comprehension and development of material models. In particular, these tensors are diagonalizable and can thence be represented by three eigenvalues associated to three eigenvectors.

As far as the stress tensor is concerned, the three eigenvalues are called principal stresses while the three eigenvectors are called principal stress directions. Accordingly, the stress tensor can be reduced to a pseudo-stress vector, the representation of which is given in the so-called principal stress space. Alternatively, symmetric tensors can be described by $n = 3$ invariants, where $n$ is the space dimension. These invariants are the coefficients of the characteristic polynomial of the stress tensor, as evidenced by Equation (2.15):

$$\chi(\sigma) = \det(\sigma - \lambda 1) = \lambda^3 - I_1\lambda^2 - I_2\lambda - I_3$$  \hspace{1cm} \text{(2.15)}$$

In the following, the Arabic numerals will be associated with the stress tensor coefficients and the Roman numerals with the principal stress values. Equations (2.16) give an explicit formula for the three invariants, which are here expressed in terms of principal stress values:

$$I_1 = tr(\sigma) = \sigma_I + \sigma_{II} + \sigma_{III}$$ \hspace{1cm} \text{(2.16a)}$$

$$I_2 = \sigma_I\sigma_{II} + \sigma_{II}\sigma_{III} + \sigma_{III}\sigma_I$$ \hspace{1cm} \text{(2.16b)}$$

$$I_3 = \det(\sigma) = \sigma_I\sigma_{II}\sigma_{III}$$ \hspace{1cm} \text{(2.16c)}$$

Since any tensor can be decomposed into a deviatoric component and a volumetric component, the following expression can be derived for the stress tensor:

$$\sigma = S - P 1$$ \hspace{1cm} \text{(2.17)}$$

where $S$ is the deviatoric stress tensor and $P = -\frac{1}{3}I_1$ is the pressure term. Similarly, invariants of the deviatoric stress tensor can be defined:
\[ J_1 = tr(S) = 0 \quad (2.18a) \]
\[ J_2 = \frac{1}{2} S_{ij} S_{ij} \quad (2.18b) \]
\[ J_3 = \frac{1}{3} S_{ij} S_{jk} S_{ki} \quad (2.18c) \]

An alternative coordinate system, namely the Haigh-Westergaard coordinate system, is also defined to impart a geometrical interpretation of the stress invariants in the principal stress space. The Haigh-Westergaard coordinates are defined by:

\[ \xi = \frac{1}{\sqrt{3}} I_1 = -\sqrt{3} P \quad (2.19a) \]
\[ \rho = \sqrt{2 J_2} \quad (2.19b) \]
\[ \cos(3\theta) = \frac{3\sqrt{3}}{2} \frac{J_3}{J_2^{\frac{3}{2}}} \quad (2.19c) \]

The \( \xi \) variable depicts the projected length of the stress point on the \((1,1,1)\)-oriented hydrostatic axis. The \( \rho \) variable stands for the distance between the stress point and the hydrostatic axis. The so-called Lode angle \( \theta \) represents the angle in the so-called deviatoric plane between the stress point and the nearest principal stress axis, see Figure 2.2.
When studying plasticity of materials, the principal stress space representation is well-suited since yield surfaces, the expansions of which are governed by hardening laws, can be easily tracked, see subsection 2.2.3.

2.2.2 Elasticity theory

Elasticity denotes the ability of a solid material to change its shape under the application of a force and to recover its original shape upon force removal. In continuum mechanics, two types of elasticity are commonly addressed: hyperelasticity and linear elasticity. Hyperelasticity applies to materials that reversibly deform up to very large strains, such as rubbers, see e.g. [71]. Linear elasticity covers materials having a reversible behavior at small strains, such that the stress-strain relationship can be linearized in this range. Linear elasticity will be adopted in the course of this work. The associated linear stress-strain relationship has already been exposed in Equation (2.4) as the different concepts of anisotropy were introduced in subsection 2.1.2. A short review of the elastic stiffness coefficients in the isotropic case and their physical meaning is given in the following. The
compliance tensor as expressed by Equation (2.12) highlights two independent stiffness coefficients: the Young's modulus $E$ and the Poisson's ratio $\nu$. In the case of a one-dimensional stress state, i.e. $\sigma_{11} \neq 0$ and $\sigma_{ij} = 0$ otherwise, the stress-strain relationship reduces to:

$$\sigma_{11} = E\varepsilon_{11} \tag{2.20a}$$
$$\varepsilon_{22} = \varepsilon_{33} = -\nu\varepsilon_{11} \tag{2.20b}$$

The Young’s modulus stands for the material stiffness that proportionally relates the longitudinal stress to the longitudinal strain in the case of a one-dimensional stress state. The Poisson’s ratio $\nu$ represents the opposite of the ratio of any of the two transverse strains with respect to the longitudinal strain. According to physics, $\nu$ has to range between -1 and 0.5. In general, it is positive since elongation in the longitudinal direction naturally results in contraction in the transverse directions. If $\nu = 0.5$, the material volume remains constant under uniaxial tensile loading. The Poisson’s ratio might get negative in more exotic materials such as foams. A common description of linear elasticity is given by rewriting the Hooke’s law in the isotropic case as follows:

$$\sigma = \lambda \text{tr}(\varepsilon)\mathbf{1} + 2\mu \varepsilon \tag{2.21}$$

where $\lambda$ and $\mu$ are the so-called Lamé coefficients. A decomposition of the strain tensor into volumetric and deviatoric contributions leads to the following alternative formulation:

$$\sigma = \left(\lambda + \frac{2}{3}\mu\right) \varepsilon_{\text{vol}} + 2\mu \varepsilon_{\text{dev}} = K \varepsilon_{\text{vol}} + 2G \varepsilon_{\text{dev}} \tag{2.22}$$

where $\varepsilon_{\text{vol}} = \text{tr}(\varepsilon)\mathbf{1}$ and $\varepsilon_{\text{dev}} = \varepsilon - \frac{1}{3} \varepsilon_{\text{vol}}$

The stiffness coefficient $K$ is called the bulk modulus and proportionally relates $P$ to $-\text{tr}(\varepsilon)$. The stiffness coefficient $G$ is called the shear modulus and proportionally relates $S$ to $2\varepsilon_{\text{dev}}$. A considerable advantage offered by isotropic elastic materials is that the volumetric and deviatoric stress-strain relationships can be determined independently from each other. In
the case of anisotropy, though, coupling terms have to be dealt with, see Chapter 6 for more details.

2.2.3 Plasticity theory

A material attains plasticity if, after load application, its removal results in permanent, non-reversible deformations in the material. Two underlying aspects of plasticity are described in the following paragraphs, namely yielding and flowing.

2.2.3.1 Yielding

Yielding corresponds to the stress state at which the material begins to undergo plasticity. A variety of yielding criteria exist, which are generally described by a yield function dependent on the principal stress values for isotropic materials, or alternatively on the stress invariants or the Haigh-Westergaard coordinates. Usually, a yield function of type $\mathcal{F}(I_1, J_2, J_3)$ is defined and discriminates non-yielded states from yielded states via the following inequations:

\[
\mathcal{F} < 0 \iff \text{no yielding} \quad (2.23a) \\
\mathcal{F} \geq 0 \iff \text{yielding} \quad (2.23b)
\]

Theoretically, the greater-than-or-equal sign should be strictly replaced by an equal sign, since the yield function represents a limiting envelope the stress tensor cannot trespass. However, this criterion is enlarged for numerical purposes since the evaluation of the yield function may result in slightly positive values at yield initiation.

Four usual yield criteria are briefly exposed in the following. The von Mises yield criterion is the most common one and suitably applies for ductile materials, such as metals. The yield function is given by:

\[
\mathcal{F}(I_1, J_2, J_3) = \mathcal{F}(J_2) = \sqrt{J_2} - \kappa 
\]

where $\kappa$ is the so-called yield stress under pure shear loading. The yield function solely depends on the second invariant of the deviatoric stress
tensor, or, in the Haigh-Westergaard coordinate system, on the $\rho$ variable. Accordingly, the graphical representation of the von Mises yield surface in the principal stress space is a circular cylinder with the hydrostatic axis as symmetry axis and a radius $r = \sqrt{2} \kappa$ according to Equation (2.19b). Furthermore, the von Mises stress or effective stress is defined as $\sigma_{vM} = \sqrt{3 J_2}$ and equals the uniaxial stress in the case of a one-dimensional stress state. A three-dimensional representation of the von Mises cylinder in the principal stress space and a projection thereof on the deviatoric plane are given in Figure 2.3.

![Figure 2.3](image_url)

**Figure 2.3:** Left: Three-dimensional representation of the von Mises and Tresca yield surfaces in the principal stress space. Right: projection of the left diagram on the deviatoric plane.

The dependency of the von Mises yield criterion on the sole $J_2$ variable implies that the application of any confining pressure is ineffective regarding plasticity. In addition, the von Mises yield criterion is invariant by rotation about the hydrostatic axis.

The Tresca yield criterion, based on the maximum shear stress theory, is defined in terms of principal stresses by:

$$
\mathcal{F}(\sigma_I, \sigma_{II}, \sigma_{III}) = \frac{1}{2} \max (|\sigma_I - \sigma_{II}|, |\sigma_I - \sigma_{III}|, |\sigma_{II} - \sigma_{III}|) - \kappa
$$

(2.25)

where $J_t$ denotes the tangential stress on an arbitrary oriented surface, i.e. the stress vector component in the plane orthogonal to the normal
vector of that surface. Physically, plastic yielding is initiated once the highest shear stress, i.e. half of the highest difference between two principal stresses, reaches the critical shear value $\kappa$. Graphically, the Tresca yield surface is a prismatic, hexagonal cylinder inscribed into a circular cylinder of radius $r = \sqrt{2} \kappa$. The latter corresponds to the von Mises yield surface if the same $\kappa$ value is assumed for both yield criteria. As opposed to the von Mises yield surface, the Tresca yield surface shows, in addition to the $J_2$-dependence, a dependence on the Lode angle or the third stress invariant $J_3$.

The Drucker-Prager yield criterion is, as opposed to the von Mises and Tresca yield criteria, pressure-dependent. Pressure-dependent yield criteria are well-suited to describe the behavior of porous and geologic materials. In particular, the pre-application of a confining pressure, tantamount to a given pore compaction, tends to delay the onset of plastic yielding. The Drucker-Prager yield function is expressed as follows:

$$F(l_1, l_2, l_3) = F(l_1, l_2) = \sqrt{J_2} + a l_1 - b$$ (2.26)

where $a$ and $b$ are material parameters.

The Drucker-Prager yield surface is, as the von Mises yield surface, invariant by rotation about the hydrostatic axis. In contrast, it does not describe a cylinder with constant radius but a cone, expanding towards negative stresses. The cone origin is symbolized by the critical negative pressure $P_{\text{min}} = -\frac{b}{3a}$ for which no elastic shear deformations can be carried out.

Analogously, the Mohr-Coulomb yield criterion can be defined as a combination of the Drucker-Prager yield criterion and the Tresca yield criterion [102]. The underlying idea of the Mohr-Coulomb yield criterion is the so-called Coulomb's law of shear strength, which stipulates that for any oriented surface, the tangential stress $T_t$ shall not exceed a function of the compressive normal stress $T_n$, as given by:

$$T_t \leq T_n \tan(\phi) + c$$ (2.27)
where $\phi$ is called angle of internal friction and $c$ the cohesion. The compressive normal stress $T_n$ stands for the opposite of the stress vector component along the normal vector. For $T_n$ values ranging underneath the critical value $T_{\text{min}} = -\frac{c}{\tan(\phi)}$, shear deformations are only governed by plasticity. In terms of the yield function, Coulomb’s law of shear strength can be rewritten as:

$$F(T_t, T_n) = T_t - T_n \tan(\phi) - c$$  \hspace{1cm} (2.28)

The Mohr-Coulomb yield surface exhibits a hexagonal shape in all deviatoric planes. It can be demonstrated that both Mohr-Coulomb and Drucker-Prager yield surfaces are geometrically linked to each other if the following relationship between the $a, b$ coefficients and the $\phi, c$ coefficients is established:

$$a = \frac{2 \sin(\phi)}{\sqrt{3} (3 \mp \sin(\phi))}, \quad b = \frac{6 \cos(\phi)}{\sqrt{3} (3 \mp \sin(\phi))}$$  \hspace{1cm} (2.29)

where, in the denominator, the minus sign (resp. plus sign) denotes that the Drucker-Prager yield surface circumscribes (resp. inscribes) the Mohr-Coulomb yield surface. A graphical representation of the Drucker-Prager and Mohr-Coulomb yield surfaces in the principal stress space, where the former here circumscribes the latter, and of the Coulomb’s law of shear strength is given in Figure 2.4. Attention must be paid that, for graphical purposes, the principal stress axes have been reversed.
2.2.3.2 Plastic flowing

Plastic flowing corresponds to the accumulation of irreversible, plastic deformations upon fulfillment of a yield criterion. Plastic strain denotes the amount of permanent strain that still exists after removal of a stress loading. Accordingly, the strain tensor $\varepsilon$ is decomposable into an elastic strain $\varepsilon^{el}$ and a plastic strain $\varepsilon^{pl}$:

$$\varepsilon = \varepsilon^{el} + \varepsilon^{pl} \tag{2.30}$$

The example of a one-dimensional stress state in an elastic-perfect plastic material is first considered, as illustrated by the stress-strain diagram in Figure 2.5. During the elastic loading phase, the uniaxial stress is proportional to the total, elastic strain via the Young’s modulus $E$. Upon plastic yielding, the uniaxial stress level is kept constant at the $Y$ value while the material plastically flows. As the stress gets removed, the material elastically unloads with the same stiffness as during the elastic loading.
In this example, it geometrically turns out that all tensile strain increments carried out by the material from the yielding point are purely plastic. The flatness of the stress level is responsible for this so-called perfect plastic behavior. In the more general case, the stress level is not constant in the plastic regime but is monitored by a so-called flow rule. This consists in incorporating a plastic strain dependency into the yield function description, thus resulting in a hardening function of type $\mathcal{F}(\sigma, \varepsilon^{pl})$. Hardening must be understood in the sense that the yield stress increases with increasing plastic strain. Two types of hardening are commonly encountered.

Isotropic hardening corresponds to a radial expansion of the yield surface with respect to the hydrostatic axis and is typically expressed by:

$$\mathcal{F}(\sigma, \varepsilon^{pl}) = \mathcal{F}_0(\sigma) - \alpha(\varepsilon^{pl}_{eff})$$

(2.31)

where $\mathcal{F}_0$ is the initial yield function and $\alpha$ is a growing function of the effective plastic strain which is, analogously to the von Mises stress, defined by $\varepsilon^{pl}_{eff} = \sqrt{\frac{2}{3} \varepsilon^{pl}_{ij} \varepsilon^{pl}_{ij}}$. 

Figure 2.5: Stress-strain ($\sigma_{11}, \varepsilon_{11}$) diagram of an elastic-perfect plastic material under a one-dimensional stress state. After a first elastic loading phase, the stress is kept constant at $Y$ while plastic strain is accumulated. In the stress unloading phase, the elastic energy stored during the elastic loading phase is released. The residual strain after total stress removal is entirely plastic.
Kinematic hardening assumes a translation of the yield surface while the plastic strain increases and is given by:

\[
\mathcal{F}(\sigma, \varepsilon_{\text{eff}}^{\text{pl}}) = \mathcal{F}_0 \left( \sigma - \sigma_\beta(\varepsilon^{\text{pl}}) \right)
\]  

(2.32)

where \(\sigma_\beta\) is a reference stress, the components of which are growing functions of the attendant plastic strain components.

Another important aspect in plasticity theory is the associated or non-associated nature of the flow rule. In the case of associated plasticity, the plastic strain increment tensor is oriented along the gradient of the yield surface, which results in the following relationship:

\[
d\varepsilon^{\text{pl}} = d\Lambda \frac{\partial \mathcal{F}}{\partial \sigma}
\]

(2.33)

where \(d\Lambda\) is a scalar factor. If the flow rule is non-associative, the yield function is replaced by an arbitrary function \(\mathcal{G}\) called plastic potential:

\[
d\varepsilon^{\text{pl}} = d\Lambda \frac{\partial \mathcal{G}}{\partial \sigma}
\]

(2.34)

2.3 Elastic wave theory

In order to better apprehend the relationships existing between physical quantities in wave propagation media, some basics on elastic wave theory are briefly explored in the following subsection. A comprehensive presentation of the theory can be found in [45] and [68].

2.3.1 Wave equation

The propagation of a longitudinal elastic wave in an infinitely thin rod of density \(\rho\) and longitudinal sound speed \(C_L\) is considered. The rod slender-ness makes lateral stresses negligible and a one-dimensional stress state can be postulated. To determine the longitudinal sound speed \(C_L\), an infinitesimal cube of volume \(dx_1dx_2dx_3\) is considered, see Figure 2.6.
Figure 2.6: Representation of an infinitesimal cube of density $\rho$ experiencing a displacement field $\mathbf{u}$ under a one-dimensional stress state.

The left side of the cube is submitted to the longitudinal stress $\sigma_{11}$, while the right side thereof undergoes the longitudinal stress $(\sigma_{11} + \frac{\partial \sigma_{11}}{\partial x_1} dx_1)$. The associated forces are derived by multiplying the local stresses by the cross-sectional area $dx_2 dx_3$. The longitudinal displacement of the cube is expressed by the lower-case variable $u_1$, and its velocity by the upper-case variable $U_1$. By applying the second Newton’s principle to the infinitesimal cube, the following equation can be set up:

$$
\left(\sigma_{11} + \frac{\partial \sigma_{11}}{\partial x_1} dx_1\right) dx_2 dx_3 - \sigma_{11} dx_2 dx_3 = \rho \ dx_1 dx_2 dx_3 \ \frac{d^2 u_1}{dt^2}
$$

(2.35)

In the following, the longitudinal coordinate $x_1$ will be simplified to $x$ and the associated longitudinal quantities $u_1$ and $U_1$ to $u$ and $U$, respectively.

Due to the one-dimensional stress state, Hooke’s law reduces to the constitutive relationship $\sigma_{11} = E \ \varepsilon_{11}$. By using the strain definition $\varepsilon_{11} = \frac{\partial u}{\partial x}$, Equation (2.35) can be simplified to the following wave equation with respect to the longitudinal displacement $u$:

$$
\frac{\partial^2 u}{\partial x^2} = \frac{\rho}{E} \frac{d^2 u}{dt^2} = \frac{1}{C_L^2} \frac{d^2 u}{dt^2}
$$

(2.36)

where the longitudinal wave speed is identified as $C_L = \sqrt{\frac{E}{\rho}}$. Owing to differentiability and linearity of longitudinal quantities with respect to
each other, it can be easily shown that the wave equation is invariably satisfied for the longitudinal strain $\varepsilon_{11}$, the longitudinal stress $\sigma_{11}$ and the longitudinal velocity $U$. A solution of the differential equation is given by the expression:

$$u(x,t) = \varphi \left( t - \frac{x}{C_L} \right) + \psi \left( t + \frac{x}{C_L} \right)$$

(2.37)

where $\varphi$ is a right-traveling function and $\psi$ a left-traveling function of $x$ and $t$. Here, right-traveling means traveling in the $x$-direction, left-traveling denotes traveling in the $-x$-direction. In the present case, only right-traveling waves are considered and the function $\psi$ can thus be removed. Owing to the strain definition and derivative rules, a strain-velocity relationship can be set up by the use of the wave equation:

$$\varepsilon_{11}(x,t) = \frac{\partial u \left( t - \frac{x}{C_L} \right)}{\partial x} = - \frac{1}{C_L} \frac{\partial u \left( t - \frac{x}{C_L} \right)}{\partial t} = - \frac{U(x,t)}{C_L}$$

(2.38)

Accordingly, the longitudinal stress $\sigma_{11}$ is, according to the assumed linear elastic constitutive law, related to the longitudinal velocity $U$ via the following expression:

$$\sigma_{11}(x,t) = E \varepsilon_{11}(x,t) = \rho C_L^2 \varepsilon_{11}(x,t) = - \rho C_L U(x,t)$$

(2.39)

If an unbounded medium is now considered, no lateral strains are expected to occur and a one-dimensional strain state can be assumed. This way, the longitudinal wave speed is dictated by the constitutive relation $\sigma_{11} = \left( K + \frac{4}{3} G \right) \varepsilon_{11}$ and is commonly called primary sound speed $C_p$:

$$C_p = \sqrt{\frac{K + \frac{4}{3} G}{\rho}}$$

(2.40)

Furthermore, wave theory shows that the primary sound speed also governs the three-dimensional propagation of pressure waves or dilatancy waves, see [68].
In fluids or in solids deprived of shear strength, i.e. $G = 0$, stress waves, and by extension, pressure waves, propagate at the so-called bulk sound speed $C_B$:

$$C_B = \sqrt{\frac{K}{\rho}} \quad (2.41)$$

More generally, in the case of nonlinear elastic laws, one-dimensional longitudinal waves propagate at:

$$C_L = \sqrt{\frac{\partial \sigma_{11}}{\partial \varepsilon_{11}}} \quad (2.42)$$

In the case of materials for which the Equation of State is nonlinear but of the general thermodynamic form $P = P(\rho, e)$, where $e$ is the mass-specific energy, the bulk sound speed is directly related to the partial derivatives of $P$ with respect to $\rho$ and $e$. By assuming an isentropic loading, the following expression can be easily derived:

$$\frac{\partial P}{\partial \zeta} = \frac{\partial P}{\partial \rho} \frac{\partial \rho}{\partial \zeta} = \frac{\partial P}{\partial \rho} \left( \frac{d\ln \left( \frac{\rho}{\rho_0} \right)}{d\rho} \right)^{-1} = \rho \frac{\partial P}{\partial \rho} \bigg|_S = -\nu \frac{\partial P}{\partial v} \bigg|_S \quad (2.43)$$

where $\zeta = -tr(e) = -(\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}) = \ln \left( \frac{\rho}{\rho_0} \right)$ is the compressive volumetric strain, $\rho_0$ is the initial density, $\nu$ is the mass-specific volume and $S$ is the mass-specific entropy.

By using the first thermodynamic identity: $de = TdS - Pdv$, where $e$ is the mass-specific internal energy and $T$ the temperature, the bulk sound speed under thermodynamic pressure conditions is thence given by:

$$C_B = \sqrt{\frac{\partial P}{\partial \zeta} \bigg|_{\rho}} = \sqrt{\frac{\partial P}{\partial \rho} \bigg|_{e} \frac{P}{\rho^2} \frac{\partial P}{\partial e} \bigg|_{\rho}} \quad (2.44)$$
Other wave types, such as shear waves, can also be addressed. If a pure shear loading, e.g. described by a relationship of type $\sigma_{12} = 2G \varepsilon_{12}$, is applied on the cube, a transverse shear wave is initiated. As opposed to longitudinal waves, transverse waves are characterized by a particle motion orthogonal to the longitudinal wave propagation direction. It is demonstrated in [68] that the shear sound speed is, in the case of linear elasticity, given by:

$$C_s = \sqrt{\frac{G}{\rho}}$$

(2.45)

It can be noticed that $C_p^2 = C_s^2 + \frac{4}{3} C_B^2$.

2.3.2 Reflection, transmission, superposition of waves

In the following, all subscripts relative to the longitudinal direction will be removed and a one-dimensional stress state will be implicitly adopted.

Two media $\mathcal{A}$ and $\mathcal{B}$ with densities $\rho_A$ and $\rho_B$ and sound speeds $C_A$ and $C_B$ are now considered. A velocity function $U_{bc}(t)$ is prescribed at the left free end of $\mathcal{A}$. Accordingly, an elastic wave $\omega_l$ arises and propagates into $\mathcal{A}$. Upon arrival at the $\mathcal{A} - \mathcal{B}$ interface, the incident wave $\omega_l$ gets decomposed into a reflected wave $\omega_r$, propagating backward into $\mathcal{A}$, and a transmitted wave $\omega_t$, propagating forward into $\mathcal{B}$. Stress equilibrium at the $\mathcal{A} - \mathcal{B}$ interface requires that:

$$\sigma_l + \sigma_r = \sigma_t$$

(2.46)

Moreover, material continuity at the $\mathcal{A} - \mathcal{B}$ interface postulates a similar condition on the particle velocities:

$$U_l + U_r = U_t$$

(2.47)

Inserting (2.39) into alternatively (2.46) and (2.47) provides the two following equations:
\[
\frac{\sigma_i}{\rho_A c_A} - \frac{\sigma_r}{\rho_A c_A} = \frac{\sigma_t}{\rho_B c_B}
\]  
\(2.48\)

\[
\rho_A c_A U_i - \rho_A c_A U_r = \rho_B c_B U_t
\]  
\(2.49\)

It should be remarked that a minus sign is adjoined to the reflected term since the reflected wave propagates backwards. A combination of Equations (2.46) and (2.48) delivers the ratios of the reflected and transmitted stresses to the incident stress:

\[
\begin{cases}
\frac{\sigma_r}{\sigma_i} = \frac{\rho_B c_B - \rho_A c_A}{\rho_A c_A + \rho_B c_B} \\
\frac{\sigma_t}{\sigma_i} = \frac{2\rho_B c_B}{\rho_A c_A + \rho_B c_B}
\end{cases}
\]  
\(2.50\)

Similarly, particle velocity ratios can be obtained by combining (2.47) and (2.49):

\[
\begin{cases}
\frac{U_r}{U_i} = \frac{\rho_A c_A - \rho_B c_B}{\rho_A c_A + \rho_B c_B} \\
\frac{U_t}{U_i} = \frac{2\rho_A c_A}{\rho_A c_A + \rho_B c_B}
\end{cases}
\]  
\(2.51\)

Equations (2.50) and (2.51) naturally lead to the definition of material impedance, which is the product \(\rho c\). At a material interface, the ratio of the velocity and stress amplitudes of transmitted and reflected waves to those of the incident wave is fully governed by the impedance ratio of the two involved materials. From this observation, it turns out that the amplitudes of reflected and transmitted waves can be completely determined if the incident quantities \(\sigma_i\) or \(U_i\) and the material impedances are known.

In order to better illustrate the physical meaning conveyed by Equations (2.50) and (2.51), two idealized cases for medium \(\mathcal{B}\) are considered: a free surface, i.e. \(\rho_B = 0\), leading to a zero impedance \(\rho_B c_B\), and a rigid surface, i.e. \(c_B \to \infty\), making the impedance \(\rho_B c_B\) infinite. In the free surface case, stress and velocity ratios are given by:
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\[
\begin{align*}
\frac{\sigma_r}{\sigma_i} &= -1 \quad \frac{\sigma_l}{\sigma_i} = 0 \\
\frac{U_r}{U_i} &= 1 \quad \frac{U_l}{U_i} = 2
\end{align*}
\] (2.52)

This means that a tensile wave is, at a free surface, reflected in a compressive wave of the same amplitude, and reversely. The reflected and incident velocities are identical. In the rigid surface case, the ratios are given by:

\[
\begin{align*}
\frac{\sigma_r}{\sigma_i} &= 1 \quad \frac{\sigma_l}{\sigma_i} = 2 \\
\frac{U_r}{U_i} &= -1 \quad \frac{U_l}{U_i} = 0
\end{align*}
\] (2.53)

As can be expected, the reflected velocity has the opposite direction of the incident velocity.

In view of application of elastic wave theory to the geometrical setup addressed in the simulated Split-Hopkinson-Bar-Tests (see Chapter 5), a medium $\mathcal{M}$ of length $L$, sandwiched between two infinitely long media $\mathcal{A}$ (left) and $\mathcal{B}$ (right), is considered, see Figure 2.7.

![Figure 2.7](image_url)

Figure 2.7: Schematic representation of a medium $\mathcal{M}$ of length $L$ sandwiched between two media $\mathcal{A}$ (left) and $\mathcal{B}$ (right). Each medium has a specific density and sound speed.

A velocity boundary condition $U_{bc}(t)$ is prescribed at the $\mathcal{A} - \mathcal{M}$ interface, which is located at $x = 0$. A right-traveling wave is thus initiated in $\mathcal{M}$. Accordingly, any point belonging to $\mathcal{M}$ adopts the velocity $U(x,t) = U_{bc}\left(t - \frac{x}{C_M}\right)$ before any subsequent wave reflection occurs.
The incident wave then repeatedly reflects at the $M - B$ and $A - M$ interfaces successively. By applying the rule of elastic wave superimposition, a general mathematical expression for the velocity $U$ and the stress $\sigma$ at any position $x$ and time $t$ can be established:

$$U(x, t) = \sum_{k=0}^{\infty} \left( \alpha_A^k \alpha_B^k U_{bc} \left( t - \frac{2kL + x}{C_M} \right) \right)$$

$$+ \sum_{k=0}^{\infty} \left( \alpha_A^k \alpha_B^{k+1} U_{bc} \left( t - \frac{2(k + 1)L - x}{C_M} \right) \right)$$

(2.54a)

$$\sigma(x, t) = -\rho_M C_M \sum_{k=0}^{\infty} \left( \alpha_A^k \alpha_B^k U_{bc} \left( t - \frac{2kL + x}{C_M} \right) \right)$$

$$+ \rho_M C_M \sum_{k=0}^{\infty} \left( \alpha_A^k \alpha_B^{k+1} U_{bc} \left( t - \frac{2(k + 1)L - x}{C_M} \right) \right)$$

(2.54b)

where: $\alpha_A = \frac{\rho_M C_M - \rho_A C_A}{\rho_M C_M + \rho_A C_A}$ and $\alpha_B = \frac{\rho_M C_M - \rho_B C_B}{\rho_M C_M + \rho_B C_B}$

The $k$–th term of the first summand stands for the velocity pertaining to right-traveling waves after $2k$ reflections of the incident wave. Similarly, the $k$–th term of the second summand represents the velocity pertaining to left-traveling waves after $2k + 1$ reflections of the incident wave. By using the convention $U_{bc}(t) = 0$ if $t < 0$, the run of the summation index up to infinity is legitimate since, upon $n$ reflections of the incident wave, the summation terms all fall to zero for $k > n/2$.

2.4 Shock wave theory

2.4.1 Shock wave formation

Two distinct mechanisms in physics may engender a shock wave. The most common one is encountered in aeronautics, where a flying object moves faster than the acoustic wave speed it emits, thus breaking the sonic barrier. Accordingly, a characteristic bang testifies to the emergence of a shock wave and to the transition to the supersonic regime. The other possible mechanism takes place inside deformable matter. Upon com-
pressive loading, deformation waves are initiated, their propagation speeds are governed by the instantaneous stiffness exhibited by the material. During compression, the material stiffness might increase, thus raising the wave propagation speed. If the loading rate is fast enough, newly formed waves are prone to catch up to their slower precursors. In the latter case, the superposition of traveling wavelets builds up a steep front and a shock wave forms.

The latter mechanism will be explicated in the following, see also [12][45][66][82]. In Figure 2.8-left, a typical pressure-density $P-\rho$ diagram for porous materials is sketched. The first branch corresponds to a reversible elastic behavior. Physically, this means that grains are slightly brought into contact while pores are not substantially crushed. The second branch is associated with pore collapsing. The observable drastic curve flattening is attributed to high energy dissipation since the pore space irremediably gets filled by solid matter. The last branch mirrors a compact material behavior in which porosity is suppressed. These phenomena are also described for granular ceramics in [15].

![Figure 2.8: Left: pressure-density diagram for an exemplary porous material. The elastic, crushing and compact branches are visible. Right: Spatial representation of the resulting wave profile at three instants of time. The high-compressive plastic waves eventually catch up to the elastic precursor and merge into a shock wave front.](image)

As the compaction process proceeds, such materials exhibit a non-constant acoustic sound speed, which is defined as the slope of the $P-\rho$ curve according to Equation (2.44). As outlined in the introduction of this subsection, wave mechanics are particularly affected by this non-constant stiffness behavior. Figure 2.8-right gives an illustration of the resulting wave structure at three different instants of time. In this
example, the loading has been applied up to the high-compressive compact branch. A constant, moderate strain rate was such chosen that a two-wave structure develops. As the spatial plateau exhibited by the wave structure at $t_1$ shows, it turns out that the so-called elastic precursor travels faster than the subsequent plastic wavelets. At $t_2$, high-compressive waves tend to catch up to the slower traveling wavelets. As a result, the wave structure steepens in the plastic regime and the gap with the elastic precursor is attenuated. Ultimately, the plastic front catches up the elastic front at $t_3$ and a unique, steep wave front arises. The latter time point indicates the formation of a shock wave. Physical properties associated to shock waves are provided in the next subsection.

2.4.2 Rankine-Hugoniot equations

A typical illustrative case of shock conditions is the shock tube problem or Riemann problem, see Figure 2.9. There, a laterally-confined long tube, filled with a compressible fluid, is considered. A longitudinal, planar shock wave propagates through the tube. It is characterized by a right-traveling shock front of speed $U_s$. By considering two instants of time $t$ and $t'$, the evolution of the shock front and the newly shocked matter within the time span $\Delta t = t' - t$ are highlighted.
Physical quantities considered in the fluid medium are the density $\rho$, longitudinal velocity $U$, pressure $P$ and mass-specific internal energy $e$. Quantities attached to non-shocked fluid particles, i.e. rightward the shock front, are attributed the subscript 0. Those attached to shocked fluid particles leftward the shock front are attributed the subscript 1. In the following, the three fundamental conservation equations will be exploited in order to establish relationships between physical quantities in shocked and non-shocked states, namely the Rankine-Hugoniot equations.

2.4.2.1 Mass conservation
To express mass conservation, a mass balance of the total fluid system is operated between $t$ and $t'$, see Figure 2.9. Since the shock front acts like a moving diaphragm, the volume repartition between non-shocked and shocked fluid is altered over time. Let $A$ be the section of the shock tube and $l_0$ and $l_1$ (resp. $l_0'$ and $l_1'$) be the respective lengths of the
non-shocked and shocked regions at \( t \) (resp. \( t' \)). Mass conservation during \( \Delta t \) results in the following equation:

\[
\rho_0 l_0 A + \rho_1 l_1 A = \rho_0 l_0' A + \rho_1 l_1' A \tag{2.55}
\]

By taking the flowing left and right ends of the shock tube into account, in addition to the running shock wave, the updated lengths are given by \( l_0' = l_0 + (U_0 - U_s)\Delta t \) and \( l_1' = l_1 + (U_s - U_1)\Delta t \). Substituting these expressions into Equation (2.55) results, after some simplifications and term annihilation, into the mass conservation equation across a shock wave:

\[
\rho_0 (U_s - U_0) = \rho_1 (U_s - U_1) \tag{2.56}
\]

2.4.2.2 Momentum conservation

According to Newton’s second principle, the time derivative of the linear momentum \( mU \) of a system equals the sum of external forces \( F_{\text{tot}} \) applied on this system. In other words, the variation of linear momentum corresponds to the integration of force over time:

\[
\frac{d(mU)}{dt} = F_{\text{tot}} \quad \Rightarrow \quad (mU)_{t'} - (mU)_t = \int_t^{t'} F_{\text{tot}} dt \tag{2.57}
\]

In the shock tube, the applied external forces are located at both free ends. \( P_0 \) and \( P_1 \) stand for the pressures applied on the non-shocked and shocked areas, respectively. Owing to the highly compressive state prevailing in the shocked area, the inequation \( P_1 > P_0 \) is obviously satisfied. Since the applied pressures are constant over time, momentum conservation is, owing to Equation (2.57), expressed by:

\[
\rho_0 l_0' U_0 A + \rho_1 l_1' U_1 A - \rho_0 l_0 U_0 A - \rho_1 l_1 U_1 A = (P_1 - P_0) A \Delta t \tag{2.58}
\]

Inserting the expressions of \( l_0' \) and \( l_1' \) and substituting the mass conservation equation (2.56) into (2.58) provides, after some mathematical rearrangement, the following momentum conservation equation:
\[ P_1 - P_0 = \rho_0 (U_s - U_o)(U_1 - U_0) \] (2.59)

2.4.2.3 Energy conservation

During the time span \( \Delta t \), the work \( W \) supplied to the shock tube system by external pressures is entirely converted into a variation of the system energy. The latter can be split up into the variation of internal energy \( \Delta E_{\text{int}} \) and of kinetic energy \( \Delta E_{\text{kin}} \). The expressions of \( \Delta E_{\text{int}}, \Delta E_{\text{kin}} \) and \( W \) are given by:

\[
\Delta E_{\text{int}} = \rho_0 l'_e e_0 A + \rho_1 l'_1 e_1 A - \rho_0 l_0 e_0 A - \rho_1 l_1 e_1 A \\
\Delta E_{\text{kin}} = \frac{1}{2} \rho_0 l'_0 U_0^2 A + \frac{1}{2} \rho_1 l'_1 U_1^2 A - \frac{1}{2} \rho_0 l_0 U_0^2 A - \frac{1}{2} \rho_1 l_1 U_1^2 A \\
W = (P_1 U_1 - P_0 U_0) A \Delta t
\] (2.60a, 2.60b, 2.60c)

By inserting Equations (2.60) into the equation \( \Delta E_{\text{int}} + \Delta E_{\text{kin}} = W \), the energy conservation equation can be derived:

\[
\rho_0 (U_s - U_o)(e_1 - e_0) + \frac{1}{2} \rho_0 (U_s - U_o)(U_1^2 - U_o^2) = P_1 U_1 - P_0 U_0
\] (2.61)

A combination of the three conservation equations (2.56), (2.59) and (2.61) furthermore allows for a simplified relationship between internal energies, pressures and densities without the involvement of velocity terms. It is given by:

\[
e_1 - e_0 = \frac{1}{2} (P_0 + P_1) \left( \frac{1}{\rho_0} - \frac{1}{\rho_1} \right)
\] (2.62)

If the non-shocked medium is assumed to be at rest, which implies that the particle velocity \( U_o \) is annihilated, Equations (2.56), (2.59) and (2.61) can be simplified to the so-called Rankine-Hugoniot equations:

\[
\rho_0 U_s = \rho_1 (U_s - U_1) \\
P_1 - P_0 = \rho_0 U_s U_1 \\
\rho_0 U_s (e_1 - e_0) + \frac{1}{2} \rho_0 U_s U_1^2 = P_1 U_1
\] (2.63a, 2.63b, 2.63c)
The Rankine-Hugoniot equations are still available in the case of $U_0 \neq 0$ provided that the frame of reference moves with the non-shocked medium. In such a case, the velocities $U_1$ and $U_s$ involved in the Rankine-Hugoniot equations must be replaced by relative velocities $U'_1 = U_1 - U_0$ and $U'_s = U_s - U_0$, respectively.

2.4.3 Hugoniot curve

For convenience, the non-shocked medium will be assumed to be at rest in the following.

2.4.3.1 Resolvability of the Rankine-Hugoniot equations

As the above-presented Rankine-Hugoniot equations show, physical quantities in the shocked medium are unequivocally related to those in the non-shocked medium. However, the knowledge of the shock velocity $U_s$ is required and requires knowledge about the material constitutive law. To resolve this issue, the relationship between the shock velocity $U_s$ and the particle velocity $U_1$ in the shocked medium can be ascertained from characterization experiments, such as Planar-Plate-Impact tests. It is commonly acknowledged that the function $U_s(U_1)$ is, based on empirical observations, of polynomial nature:

$$U_s = C_B + \sum_{k=1}^{n} s_k U_1^k$$  \hspace{1cm} (2.64)

where $C_B$ is the bulk sound speed of the material and $s_k$ are polynomial coefficients. For solids, it can be reasonably assumed that this function reduces to a linear function expressed by:

$$U_s = C_B + s U_1$$  \hspace{1cm} (2.65)

Departing from the knowledge of $\rho_0$ and $U_1$, the combination of the three Rankine-Hugoniot equations and of the function $U_s(U_1)$ allows for a thorough determination of the shock state $(\rho_1, P_1, e_1)$, also called Hugoniot state. Under the linearity hypothesis expressed by Equation (2.65),
the substitution of the latter for $U_s$ in Equations (2.63) provides direct expressions for the shock-related variables:

\[
\rho_1 = \frac{\rho_0 + sU_1}{\rho_0 + U_1(s - 1)} \quad (2.66a)
\]

\[
P_1 = P_0 + \rho_0 c_B^2 \frac{\eta}{(1 - s\eta)^2} \quad (2.66b)
\]

\[
e_1 = e_0 + \frac{\eta}{\rho_0} P_1 - \frac{\eta^2}{2} \frac{c_B^2}{(1 - s\eta)^2} \quad (2.66c)
\]

where $\eta = 1 - \frac{\rho_0}{\rho_1}$

2.4.3.2 Graphical representation of a Hugoniot curve
In the light of the previously established equations, all Hugoniot states $(\rho_1, P_1, e_1)$ that may be achieved from a non-shocked state $(\rho_0, P_0, e_0)$ can be represented in a thermodynamic diagram. Figure 2.10 gives, from two different points of view, a three-dimensional representation $(v, e, P)$ of an exemplary Mie-Grüneisen Equation of State in which the Hugoniot curve is embedded. The variable $v = 1/\rho$ stands for the mass-specific volume. Mathematical aspects concerning the Mie-Grüneisen Equation of State will be outlined in the next paragraph. The reference non-shocked state, with subscript 0, and an exemplary final shock state, with subscript 1, are connected by the so-called Rayleigh line. Two isentropes, a compressive one starting from the reference state $(P_0, v_0)$ and a release one starting from the shocked state $(P_1, v_1)$, are also depicted.
Figure 2.10: Three-dimensional representation of a Mie-Grüneisen Equation of State in the \((v, e, P)\) space. The Hugoniot curve (red solid line) relies upon the depicted reference state (subscript 0). The Rayleigh line (dotted line) symbolizes the thermodynamic shock path between the reference non-shocked state and an exemplary final shock state (subscript 1). Isentropes (blue solid lines) are also represented.

The concatenation of all potential Hugoniot states builds up the so-called Hugoniot curve. It must be strongly emphasized that the Hugoniot curve does not represent a collection of intermediate transformations which the material passes through, but only a series of final shock states related to individual shock events. To ensure further disambiguation about the meaning of the Hugoniot curve, the definition of the Rayleigh line is of particular relevance. This straight line runs directly from the reference state to the final shock state and portrays the sudden state jump undergone by the material as a result of shock. Owing to the convex shape of the Equation of State surface, the straightness of the Rayleigh line demonstrates that shock transformations are located off the Equation of State surface, i.e. are highly transient processes. Final shock states, though, exhibit a thermodynamic equilibrium and thus justify the inclusion property of the Hugoniot curve within the Equation of State surface. In this respect, Hugoniot curves offer a good fundament to devise purposeful shock-related Equations of State. A common procedure may consist in extrapolating one-dimensional Hugoniot curves to two-dimensional Equation of State surfaces, e.g. by using the Mie-Grüneisen theory, see next paragraph.
Figure 2.11 shows a projection of the Hugoniot curve, both isentropes and the Rayleigh line on the $P - v$ plane. This two-dimensional representation allows for an eased geometrical interpretation of the shock-related quantities.

From Equation (2.62), it can be ascertained that the energy stored by the material during the shock event is given by the surface located below the Rayleigh line between $v_1$ and $v_0$. If the material subsequently releases from state 1 along the decompression isentrope $(P_1, v_1)$, the release energy, defined as the surface below that isentrope, underrates the shock energy. As a result, shock waves produce an irreversible amount of energy in the material as opposed to isentropic transformations. With a similar argumentation, the energy stored during isentropic compression from $v_0$ to $v_1$ largely undervalues the energy produced by a shock of same volumetric compression.

A geometrical interpretation of the particle velocity and the shock velocity can also be carried out. For this purpose, a re-arrangement of the Rankine-Hugoniot expressions allows for the following expressions:
\[ U_1 = \sqrt{(P_1 - P_0)(v_0 - v_1)} \]  
(2.67a)

\[ U_s = v_0 \frac{(P_1 - P_0)}{(v_0 - v_1)} \]  
(2.67b)

Accordingly, the particle velocity is proportional to the square root of the area of a rectangle for which the diagonal is the Rayleigh line. The shock velocity is proportional to the square root of the Rayleigh line slope.

2.4.3.3 Shock-related Equations of State
A very common Equation of State especially devised for shock states is the Mie-Grüneisen Equation of State. The underlying physics base on the Grüneisen theory [40], in which crystals are regarded as harmonic oscillators storing thermal energy. A dimensionless material parameter, called Grüneisen parameter \( \Gamma \), standing for the variation of vibrational frequencies with respect to volume variation, is also introduced. Via the use of a statistical mechanics-based approach, the Mie-Grüneisen Equation of State is expressed by:

\[ P(v, e) = P_H + \frac{\Gamma(v)}{v} (e - e_H) \]  
(2.68)

where \( P_H \) and \( e_H \) are the Hugoniot-related variables as exemplarily given by Equations (2.66) if a linear function \( U_s(U_1) \) is assumed. This way, any thermodynamic state can be decomposed into a pure shock Hugoniot contribution and an energy-based contribution. The latter involves the Grüneisen coefficient and is proportional to the difference between the actual energy and the Hugoniot-related energy. In practice, the \( U_s(U_1) \) relation can be derived from experimental tests, such as Planar-Plate-Impact tests, and the ratio \( \frac{\Gamma(v)}{v} \) is often approximated as a constant parameter defined by:

\[ \frac{\Gamma(v)}{v} = \frac{3\alpha_P}{c_V \beta_T} \]  
(2.69)

where \( \alpha_P \) is the isobaric volumetric thermal expansion, \( c_V \) is the isochoric heat capacity and \( \beta_T \) is the isothermal compressibility.
Alternative shock-related Equations of State can be used, such as the Polynomial Equation of State, which is defined by:

\[ P = K_1 \zeta + K_2 \zeta^2 + K_3 \zeta^3 + (B_0 + B_1 \zeta) \rho_0 e \]  \hspace{1cm} (2.70)

Phase changes under shock conditions can be appropriately modeled by the analytical Tillotson Equation of State or by tabular Equations of State, see [45]. In the frame of compressive shock simulations that will be addressed in Chapter 6, the ANEOS or Analytical Equation of State, especially devised for quartzite, will be introduced in paragraph 6.2.3.1 and employed in the simulation model.

2.4.4 Shear enhancement of shock waves

The shock wave theory addressed in the previous subsections bases on pure hydrodynamic materials, i.e. materials deprived of shear strength. In this subsection, a generalization of the shock wave theory in regard to shear-resistant materials is proposed. The most suitable way to achieve experimental shock conditions is the application of a planar wave on a specimen. Lateral deformations are generally prevented by a large width-to-length ratio, as is typically encountered in Planar-Plate-Impact tests, or by the use of a confining matrix. Under such loading conditions, the stress and strain states of the material are kept under control. Accordingly, experimental data can be easily correlated to material properties by the help of Hugoniot theory. Fundamentally, the conservation equations, and by extension, the Rankine-Hugoniot equations, must be rewritten by replacing the pressure term \( P \) by the longitudinal compressive stress \( \sigma_L \). The latter is here conventionally defined to be positive if the stress is compressive.

In order to show how far the Hugoniot curve is affected by the shear stiffness, an analogy can be drawn with linear elastic waves. For a one-dimensional strain state, it has been shown in section 2.2 that the longitudinal stress \( \sigma_L \) can be decomposed as follows:

\[ \sigma_L = -\sigma_{11} = -s_{11} + P = -\left(\frac{4}{3}G + K\right) \varepsilon_{11} = \left(\frac{4}{3}G + K\right) \zeta \]  \hspace{1cm} (2.71)
The corresponding sound speed is given by Equation (2.40) and can be reformulated as:

\[ C_p = \sqrt{\frac{4}{3} C_s^2 + C_B^2} = \sqrt{\frac{4}{3} \frac{G + K}{\rho}} = v \sqrt{-\frac{\partial s_{11}}{\partial v} + \frac{\partial P}{\partial v}} = v \sqrt{-\frac{\partial \sigma_L}{\partial v}} \]  \hspace{1cm} (2.72)

Equations (2.43), (2.44) and (2.67b) show that the pressure derivative with respect to volume which is involved in the bulk sound speed definition turns, under shock conditions, into a ratio of pressure difference over volume difference:

\[ C_B = v \sqrt{-\frac{\partial P}{\partial v}} \Rightarrow U_s = v_0 \sqrt{-\frac{\Delta P}{\Delta v}} \]  \hspace{1cm} (2.73)

Following the same argumentation, the primary sound speed \( C_p \) given by Equation (2.72) can be identically transposed to shock conditions:

\[ C_p = v \sqrt{-\frac{\partial s_{11}}{\partial v} + \frac{\partial P}{\partial v}} \Rightarrow U_s = v_0 \sqrt{-\frac{\Delta s_{11}}{\Delta v} + \frac{\Delta P}{\Delta v}} = v_0 \sqrt{-\frac{\Delta \sigma_L}{\Delta v}} \]  \hspace{1cm} (2.74)

Upon knowledge of the shear strength law, the shock velocity of the shear-resistant material can be unequivocally determined from Equation (2.74). By using the geometric properties of the Rayleigh line as described by Equations (2.67), the shock pressures and the particle velocities of the shear-resistant material can be easily derived. A graphical illustration of Hugoniot curves in the \( \sigma_L - \nu \) space and in the \( U_s - U_1 \) space is given in Figure 2.12 for both pure hydrodynamic and shear-enhanced material models. There, a linear \( U_s(U_1) \) relation has been assumed and the shock parameters \( C_B = 3775 \text{ m/s} \) and \( s = 1.695 \) are extracted from the Mie-Grüneisen model for quartz as will be addressed in Chapter 6. The deviatoric contribution has been modeled by elasticity, perfect plasticity, assuming a shear modulus \( G = 42.6 \text{ GPa} \) and a yield strength \( Y = 2.5 \text{ GPa} \). From the yield point, the tangent shear modulus or instantaneous shear modulus drops to zero, see again Figure 2.5. Accordingly, the apparent shear modulus \( \tilde{G} \), defined as the ratio of the total deviatoric stress to the total deviatoric strain, rapidly declines. This quantity is, in the case of a one-dimensional compressive strain state,
equal to the ratio $\frac{\Delta \varepsilon_{11}}{\Delta \varepsilon}$. As Equation (2.74) shows, the shear-resisting term therefore contributes to the shear-enhancing effect on shock velocities and, concomitantly, on shock-related compressive stresses.

![Graph](image)

Figure 2.12: Representation of Hugoniot curves for a shear-enhanced model and a pure hydrodynamic model in terms of $\sigma_L(GPa)$ curve (top) and $U_s(m/s)$ curve (bottom).

It can be observed in Figure 2.12 how far the shear-enhanced shock stress and velocity overrun their hydrodynamic counterparts. Due to shock conditions, from the yield point, called Hugoniot Elastic Limit (HEL), the decline of the apparent shear modulus attenuates the shock stress ascent and abruptly diminishes the shock velocity. At advanced compressive shock states, the shear resistance gets negligible and both models converge.
3 Numerical fundamentals

Whenever a physical problem cannot be solved analytically or is too complex to be tackled in a reasonable work schedule, numerical methods can be put forward. From the large palette of existing numerical methods, two standard discretization methods will be shortly outlined in the following sections. These are the Finite Element (FE) Method and the Smoothed Particle Hydrodynamics Method (SPH). Both methods will essentially support the numerical modeling developed within the scope of this work.

3.1 Finite Element method

The Finite Element method is introduced in the following and bases upon an updated Lagrangian formulation. Owing to this, the last achieved configuration is permanently set as the new reference configuration. The advantage offered thereby is that the computation of integrals can be conducted in Eulerian form, i.e. over the current deformed configuration. This is of particular relevance in dynamic processes since a material body may undergo severe deformations, thence accompanied by substantial reorientations of material boundaries or internal interfaces.

3.1.1 Discrete equation of linear momentum conservation

The Finite Element method departs from the equation of linear momentum conservation, for which the virtual work principle is applied, see [10] for a detailed description of the methodology. Let \( \Omega \) be a volumetric body, consisting of an internal boundary \( \Gamma_{int} \) and of an external boundary \( \Gamma_e \). The external boundary \( \Gamma_e \) can be decomposed into a displacement-prescribed boundary \( \Gamma_u \) and a traction-prescribed boundary \( \Gamma_T \), see Figure 3.1.
Figure 3.1: Sketch of a body $\Omega$ with internal and external boundaries. Displacement or traction boundary conditions are applied on the external boundary.

Let $\mathbf{u}$ be the displacement of a material point $M \in \Omega$ of density $\rho$ in the current configuration, and $\mathbf{\sigma}$ and $\mathbf{b}$ be the Cauchy stress and body forces, respectively, acting on it. The first of the three following relations is the equation of linear momentum conservation. This is expressed component-wise, for any point $M$ outside $\Gamma_u$, by:

$$\rho \ddot{u}_i - \frac{\partial \sigma_{ij}}{\partial x_j} - \rho b_i = 0 \quad \forall M \in \Omega \setminus \Gamma_u$$  \hfill (3.1a)

The second relation is given for points $M$ submitted to traction boundary conditions on $\Gamma_T$ with outward-pointing normal vector $\mathbf{n}$:

$$\sigma_{ij} n_j = T_i^{bc} \quad \forall M \in \Gamma_T$$  \hfill (3.1b)

The third relation makes use of Newton’s Third Law. This means that two material sides across an internal surface act on each other with forces of same amplitude but opposite direction. Since the normal vectors of both sides are opposite to each other, it follows that the projection of the Cauchy stress tensor on the normal vector $\mathbf{n}$ across internal boundaries $\Gamma_{int}$ must be continuous:

$$\left[ \sigma_{ij} n_j \right] = 0 \quad \forall M \in \Gamma_{int}$$  \hfill (3.1c)
A discretization of this problem can be achieved by using a weak formulation of the equation of linear momentum conservation (3.1a). For this purpose, the virtual work principle is applied and considers a field of admissible virtual displacements $\vec{\varphi}$. To be admissible, a virtual displacement $\vec{v}$ must be a continuous function of the space coordinate components $x_i$ and must vanish on $\Gamma_u$. This way, $\vec{v}$ is not conditioned by the boundary displacement conditions prescribed on the medium. The weak form of Equations (3.1a), (3.1b) and (3.1c) is obtained by multiplying Equation (3.1a) by $\tilde{v}_i$:

$$
\int_{\Omega} \tilde{v}_i \left( \rho \ddot{u}_i - \frac{\partial \sigma_{ij}}{\partial x_j} - \rho b_i \right) dV = 0 \quad (3.2)
$$

Using Gauss’s theorem, Equation (3.2) turns into:

$$
\int_{\Omega} \tilde{v}_i \rho (\ddot{u}_i - b_i) dV + \int_{\Omega} \frac{\partial \tilde{v}_i}{\partial x_j} \sigma_{ij} dV - \int_{\Gamma_r \cup \Gamma_u \cup \Gamma_{int}} \tilde{v}_i \sigma_{ij} n_j dS = 0 \quad (3.3)
$$

The last integral covers a priori the whole set of boundaries $\Gamma_r \cup \Gamma_u \cup \Gamma_{int}$ comprised in the body $\Omega$. Nevertheless, $\vec{v}$ was chosen to vanish on $\Gamma_u$. Moreover, integrals over internal boundaries are always calculated two-fold in order to encompass each material side, but with normal vectors pointing to opposite directions, respectively. Due to the continuity of $\sigma \cdot n$ and $\vec{v}$ across internal boundaries, integrals over $\Gamma_{int}$ ultimately compensate each other. In the present work, no body forces are exerted inside the material volume, therefore $b$ can be neglected. With these hypotheses and inserting (3.1b) into (3.1a), the weak form can be simplified to:

$$
\int_{\Omega} \tilde{v}_i \rho \ddot{u}_i dV + \int_{\Omega} \frac{\partial \tilde{v}_i}{\partial x_j} \sigma_{ij} dV - \int_{\Gamma_r} \tilde{v}_i T^{bc}_i dS = 0 \quad (3.4)
$$

The next step follows the so-called Bubnov-Galerkin procedure, in which shape functions are introduced. For this purpose, a discretization of the body $\Omega$ into a mesh of $n_e$ elements $e$ and $n_n$ nodes $\mathcal{N}$ is considered. The underlying idea of the Bubnov-Galerkin procedure is that any function $\phi$ dependent on the space coordinates $\mathbf{x}$ and time $t$ can be approximated using the following discretization scheme:
\[ \varphi(x, t) \approx \varphi^h(x, t) = \sum_{k=1}^{n_n} N_k(x) \varphi_k(t) \]  

(3.5)

where \( N_k \) is the \( k \)-th shape function and \( \varphi_k \) is the interpolation value of \( \varphi \) at the node \( \mathcal{N}_k \). For a given \( k \) value, the shape function \( N_k \) must equal unity when evaluated at the node \( \mathcal{N}_k \) and zero at any other node. Moreover, the sum of all shape functions must equal unity all over the volumetric domain \( \Omega \). This discretization scheme, applied to displacements and their temporal derivatives, provides the following discretized form of Equation (3.4):

\[
\sum_{k=1}^{n_n} (\tilde{\varphi}_i)_k \left( \sum_{p=1}^{n_n} \int_{\Omega} N_k \rho N_p (\ddot{u}_i)_p \, dV + \int_{\Omega} \frac{\partial N_k}{\partial x_j} \sigma_{ij} \, dV - \int_{\Gamma_T} N_k T_{bc}^i \, dS \right) = 0 \quad (3.6)
\]

This equality is valid for any continuous function \( \tilde{\varphi}_i \) that vanishes on \( \Gamma_u \). It can be mathematically proven that this condition is strong enough to claim that each \( k \)-th component in brackets must vanish to satisfy Equation (3.6). Since the shape function \( N_k \) is identically zero except within finite elements directly connected to the node \( \mathcal{N}_k \), each \( k \)-th component in brackets in Equation (3.6) can be rewritten as:

\[
\left( \sum_{p=1}^{n_n} M_{kp} (\ddot{u}_i)_p \right)_k = \sum_{p=1}^{n_n} \left( \sum_e \int_{\Omega_e} N_k \rho N_p \, dV \right) (\ddot{u}_i)_p \quad (3.7a)
\]

\[
(f_i^{int})_k = \sum_{e|\mathcal{N}_k \in \Omega_e} \int_{\Omega_e} \frac{\partial N_k}{\partial x_j} \sigma_{ij} \, dV \quad (3.7b)
\]

\[
(f_i^{ext})_k = \sum_{\mathcal{F}_k \in \Gamma_f} \int_{\Gamma_f} N_k T_{bc}^i \, dS \quad (3.7c)
\]

where \( e \) is an index running over finite elements of volumes \( \Omega_e \) and \( \mathcal{F} \) is an index running over element facets of boundaries \( \Gamma_\mathcal{F} \). The matrix \( M \) is called the mass matrix and the vectors \( f_k^{int} \) and \( f_k^{ext} \) are called the internal and external forces at the node \( \mathcal{N}_k \), respectively.
As Equation (3.7a) suggests, the mass matrix $M$ is sparse. Non-zero coefficients arise only at specific $p$-values for which the nodes $N_p$ and $N_k$ share common finite elements. Mass lumping is usually employed to facilitate the determination of the array of nodal accelerations $\{\ddot{u}_i\}_k$. In order to achieve this, the mass matrix $M$ is transformed into a diagonal matrix $M^d$. Each diagonal term $M^d_{kk}$ is defined as the sum of all coefficients of the $k$-th row of the original mass matrix $M$:

$$M^d_{kk} = \sum_{p=1}^{n} M_{kp} = \sum_{p=1}^{n} \sum_{e} \int_{\Omega_e} N_k \rho N_p dV$$

(3.8a)

The lumped mass $m_k = M^d_{kk}$ of the node $N_k$ can be rewritten as the sum of partial lumped masses $m^e_k$ of all elements connected to $N_k$:

$$m_k = \sum_{e|N_k \in \Omega_e} \sum_{p|N_p \in \Omega_e} \frac{\int_{\Omega_e} N_k \rho N_p dV}{m^e_k}$$

(3.8b)

Through the use of lumped masses, the acceleration vector of $N_k$ can be explicitly calculated:

$$\ddot{u}_k = \frac{1}{m_k} (f^e_k - f^i_k)$$

(3.9)

Equation (3.9) is called the discrete equation of linear momentum conservation.

In order to ease the calculation of integrals over finite element volumes $\Omega_e$, respectively their outer faces $\Gamma_e$, a numerical integration scheme is adopted. A common scheme is the one-point Gauss quadrature rule. When tetrahedral finite elements are involved, the volume or surface integral of a function is represented by an integration point located in the centroid of the tetrahedron or of the triangular facet, respectively. The integral is approximated by the function value at the integration point, weighted by the tetrahedral volume or the triangular area. With this quadrature rule, and assuming linear shape functions, linear polynomials are exactly integrated. Higher-order polynomials, such as the quadratic polynomial represented by the integrand of $m_k$, see Equation (3.8b), are
however, under-integrated. Another numerical quadrature scheme, namely the Lobatto quadrature rule, will be adopted concomitantly with the use of cohesive zone elements, see section 4.4.

### 3.1.2 Time integration

Different time integration schemes might be used to successfully calculate a nodal velocity from the nodal acceleration and a nodal displacement from the nodal velocity. They generally are based on a finite difference scheme of the following type:

\[ \alpha^{(n+1)} = \alpha^{(n)} + \Delta t^{(n)} \left( \beta \dot{\alpha}^{(n)} + (1 - \beta) \ddot{\alpha}^{(n+1)} \right) \]  

(3.10)

for an arbitrary function \( \alpha \). The parameter \( \beta \) ranges from 0 to 1 and allows for a mixed formulation of forward and backward finite difference schemes. If \( \beta = 1 \), Equation (3.10) simplifies to a forward difference scheme for which the evaluation of \( \alpha \) at \( t^{(n+1)} \) only depends on functions evaluated at \( t^{(n)} \). The discretization scheme is said explicit. If \( \beta = 0 \), Equation (3.10) simplifies to a backward difference scheme. There, the evaluation of \( \alpha \) at \( t^{(n+1)} \) depends on the evaluation of \( \dot{\alpha} \) at \( t^{(n+1)} \) and the resolution cannot be conducted explicitly. The discretization scheme is said implicit. The disadvantage of the forward and backward discretization schemes is that they exhibit only a first-order accuracy, owing to the Taylor development of a function:

\[ \alpha^{(n+1)} = \alpha^{(n)} + \Delta t^{(n)} \dot{\alpha}^{(n)} + o(\Delta t) \]  

(3.11a)

\[ \alpha^{(n)} = \alpha^{(n+1)} - \Delta t^{(n)} \ddot{\alpha}^{(n+1)} + o(\Delta t) \]  

(3.11b)

If, on the contrary, \( \beta \) is set to 0.5, a second-order accuracy of the finite difference scheme, said central, is achieved. To prove it, an intermediate time step \( t^{(n+1/2)} \) is inserted at the middle of \( t^{(n)} \) and \( t^{(n+1)} \) and a twofold Taylor development is performed:
\begin{align*}
\alpha^{(n+1)} &= \alpha^{(n+\frac{1}{2})} + \frac{\Delta t^{(n+\frac{1}{2})}}{2} \dot{\alpha}^{(n+\frac{1}{2})} + \left( \frac{\Delta t^{(n+\frac{1}{2})}}{2} \right)^2 \ddot{\alpha}^{(n+\frac{1}{2})} + o(\Delta t^2) \quad (3.12a) \\
\alpha^{(n)} &= \alpha^{(n+\frac{1}{2})} - \frac{\Delta t^{(n+\frac{1}{2})}}{2} \dot{\alpha}^{(n+\frac{1}{2})} + \left( \frac{\Delta t^{(n+\frac{1}{2})}}{2} \right)^2 \ddot{\alpha}^{(n+\frac{1}{2})} + o(\Delta t^2) \quad (3.12b)
\end{align*}

Subtracting (3.12b) from (3.12a) results in:

\[ \alpha^{(n+1)} - \alpha^{(n)} = \Delta t^{(n+\frac{1}{2})} \ddot{\alpha}^{(n+\frac{1}{2})} + o(\Delta t^2) \quad (3.13) \]

Since, owing to linear interpolation properties, \( \dot{\alpha}^{(n+\frac{1}{2})} = \frac{1}{2} \left( \dot{\alpha}^{(n)} + \dot{\alpha}^{(n+1)} \right) \), Equation (3.13) can be identified to Equation (3.10) for \( \beta = 0.5 \). This demonstrates the second-order accuracy of the central finite difference scheme. The application of this scheme to the acceleration double integration in regard to the displacement derivation is called leapfrog integration. The corresponding algorithm is given by:

\begin{align*}
\dot{u}_k^{(n+\frac{1}{2})} &= \dot{u}_k^{(n-\frac{1}{2})} + \Delta t^{(n)} \ddot{u}_k^{(n)} \\
\ddot{u}_k^{(n+1)} &= \ddot{u}_k^{(n)} + \Delta t^{(n+\frac{1}{2})} \dddot{u}_k^{(n+\frac{1}{2})} \quad (3.14a) \\
u_k^{(n+1)} &= u_k^{(n)} + \Delta t^{(n+\frac{1}{2})} \dot{u}_k^{(n+\frac{1}{2})} \quad (3.14b)
\end{align*}

Since the leapfrog integration scheme is of explicit nature, it enables a straightforward calculation of nodal displacements via the use of lumped masses. However, it is, unlike implicit integration schemes, conditionally stable since the time step cannot exceed a certain threshold value. The so-called Courant-Friedrichs-Lewy (CFL) condition [23] postulates that the maximum admissible time step size \( \Delta t_{CFL} \) to ensure a stable solution is given by the ratio of the smallest element size \( \Delta x_{min} \) to the maximum propagation wave speed \( C_{\text{max}} \) in the medium. It is mathematically expressed by:

\[ \Delta t_{CFL} = \frac{\Delta x_{min}}{C_{\text{max}}} \quad (3.15) \]

Other aspects treated in FE methods, such as artificial viscosity, hourglass issues or contact laws, will not be addressed in this work but can be found in [10] for further details.
3.2 Smoothed Particle Hydrodynamics Method

The Smoothed Particle Hydrodynamics method or SPH method is, as the FE method, a Lagrangian method for which integration points are not fixed in space but move along with the medium. As opposed to the FE method, the SPH method is a meshfree method, the integration points of which are represented by particles. The outcome of this is that a specific neighborhood around a given particle is not necessarily fixed over time but may be repeatedly renewed during a loading process. An undeniable advantage offered by the SPH method is the possibility of simulating high dynamic processes without having to deal with extreme mesh distortions as would occur in FE simulations. An overview of the SPH method is given in [65][99], the implementation specifically used in this work can be found in [86][87].

3.2.1 Kernel approximation

The SPH formulation departs from the sifting property of the Dirac function which postulates that the convolution of any integrable function $f$ with the Dirac function $\delta$ conserves the function $f$. Mathematically, this is expressed, for an arbitrary function $f$ defined over a domain $\Omega$, by:

$$ f(x) = \int_{\Omega} f(x')\delta(x - x')dV $$  \hspace{1cm} (3.16)

where $\delta(x - x') = 1$ for $x = x'$ and 0 otherwise. As the non-continuous nature of the Dirac function is not suitable for numerical computations, the use of a so-called kernel function $W(x)$, used to smooth out the Dirac function over a compact domain, is proposed. In the context of a SPH particle distribution over a domain $\Omega$, the evaluation of a function $f$ at a given particle $i$ of coordinates $x_i$ can be approximated by the following expression:

$$ f(x_i) = \int_{\Omega} f(x)W(x - x_i)dV $$  \hspace{1cm} (3.17)
To be consistent, the kernel function $W$ must fulfill a certain number of properties. Firstly, it must have a compact support, i.e. the kernel function is identically equal to zero except on a compact domain centered on the origin. In a two-dimensional case, the support domain describes a circle centered on the origin while, in the three-dimensional case, it describes a sphere. The kernel radius is denoted by $2h$, where $h$ is called the smoothing length. Secondly, the normality condition must be met:

$$
\int_{\Omega} W(x - x_i) dV = 1 \quad (3.18)
$$

This condition ensures that a constant function is exactly approximated by the SPH method. Thirdly, the following symmetry condition must be met:

$$
W(x_j - x_i) = W(x_i - x_j) \quad (3.19)
$$

for any pair of particles $I$ and $J$ of respective coordinates $x_i$ and $x_j$. The fourth condition is a monotonic decrease of the kernel function when the norm or Euclidian distance of its argument increases. The last condition is the convergence of the kernel function to the Dirac function as the support domain radius tends to zero. This last condition is, to some extent, redundant due to the fulfillment of (3.18). In practice, the kernel function solely depends on the Euclidian distance of its argument and can be described by a mono-variable function of type $W(x) = w(r/h)$, where $r = \|x\|$. The most common kernel function is the cubic spline and is defined by:

$$
w\left(\frac{r}{h}\right) = \begin{cases} 
\frac{C}{h^3} \left(1 - \frac{3}{2} \frac{r}{h} \right)^2 + \frac{3}{4} \left(\frac{r}{h}\right)^3 & \text{if } 0 \leq \frac{r}{h} < 1 \\
\frac{C}{4h^3} \left(2 - \frac{r}{h}\right)^3 & \text{if } 1 \leq \frac{r}{h} \leq 2 \\
0 & \text{if } \frac{r}{h} > 2 
\end{cases} \quad (3.20)
$$
where $D$ is the dimension of the problem and $C$ is a dimension-dependent parameter:

$$C = \begin{cases} 
\frac{2}{3} & \text{if } D = 1 \\
\frac{10}{7\pi} & \text{if } D = 2 \\
\frac{1}{\pi} & \text{if } D = 3 
\end{cases}$$

(3.21)

Figure 3.2 gives a graphical representation of the cubic spline in two dimensions. The kernel function is centered on an arbitrary particle $I$ and its compact support of radius $2h$ encompasses a set of SPH particles in its direct neighborhood.

![Graphical representation of the cubic spline](image)

Figure 3.2: Graphical representation of the cubic spline in two dimensions. It is centered on a particle $I$ and its compact support of radius $2h$ encompasses a set of SPH particles labeled by $J$ around the particle $I$.

Analogously to the FE method, the integral as given in Equation (3.17) is not analytically calculated but approximated by a discrete sum over the SPH particles or integration points:
where $\Delta V_j$ is a volume attributed to each particle $j$ and depends on the SPH particle concentration in space. Due to the decreasing nature of the kernel function with increasing radius, it becomes intuitive that the influence of a remote particle with respect to the central particle $i$ is slighter than the influence of a closer one. A great advantage offered by the cubic spline is that, provided that the SPH particles are all regularly distributed, it approximates linear functions exactly.

Besides, the approximation of function gradients can be straightforwardly derived from the original function. To achieve this, the divergence theorem is applied to the integral form of the gradient of an arbitrary function $f$:

$$
\nabla f(x_i) = \int_\Omega \nabla f(x) W(x - x_i) dV \\
= \int_\Omega f(x) W(x - x_i) dV - \int_\Gamma f(x) \nabla W(x - x_i) n dS
$$

(3.23)

where $\mathbf{n}$ is the unit normal vector of a local surface belonging to the boundary $\Gamma$ of the volumetric domain $\Omega$. Aside from border effects for which a separate treatment is required, the kernel support relative to an inner SPH particle is fully included in the volumetric domain $\Omega$. Accordingly, the surface integral vanishes and the gradient operator is transferred to the kernel function in the integral, see Equation (3.24):

$$
\nabla f(x_i) = - \int_\Omega f(x) \nabla W(x - x_i) dV \approx - \sum_{j=1}^n f(x_j) \nabla W(x_j - x_i) \Delta V_j
$$

(3.24)

### 3.2.2 Standard improvements of the SPH method

Equations (3.22) and (3.24) represent the discretized approximations of a function and of its gradient in the frame of a SPH formulation. In order to
ensure an exact approximation of constant functions, also called completeness of zeroth order, the following system of equations must be evidently satisfied:

\[
\begin{align*}
\sum_{j=1}^{n} W(x_j - x_i) \Delta V_j &= 1 \\
\sum_{j=1}^{n} \nabla W(x_j - x_i) \Delta V_j &= 0
\end{align*}
\] (3.25)

3.2.2.1 SPH symmetrization

The fulfillment of Equations (3.25) may yet be questioned if the SPH particles are irregularly distributed or located in the vicinity of external boundaries. To address this issue, a symmetrization of the gradient is proposed in [9] via the use of an additional term:

\[
\nabla f(x_i) = - \sum_{j=1}^{n} f(x_j) \nabla W(x_j - x_i) \Delta V_j + f(x_i) \sum_{j=1}^{n} \nabla W(x_j - x_i) \Delta V_j = - \sum_{j=1}^{n} (f(x_j) - f(x_i)) \nabla W(x_j - x_i) \Delta V_j
\] (3.26)

The new additional term, since it is supposed to vanish in the case of exactly approximated functions, does not degrade the approximation scheme of these functions. Even more, it ensures an exact approximation of any constant function even for border particles and regardless of the particle distribution.

3.2.2.2 SPH normalization

An alternative way to achieve completeness of zeroth order, regardless of the boundary nature or distribution regularity of SPH particles, is proposed in [79] and consists in normalizing the function \( f \) by the first equation of (3.25). This provides the new approximation equation:

\[
f(x_i) = \frac{\sum_{j=1}^{n} f(x_j) W(x_j - x_i) \Delta V_j}{\sum_{j=1}^{n} W(x_j - x_i) \Delta V_j}
\] (3.27)
In addition, an upgrade of zeroth order-completeness to first order-completeness, for which linear functions are exactly approximated, can be achieved with the SPH normalization technique. In practice, the function gradient approximation of Equation (3.24) is extended to the following form:

$$\nabla f(x_i) = \left( -\sum_{j=1}^{n} \left( f(x_j) - f(x_i) \right) \nabla W(x_j - x_i) \Delta V_j \right) \cdot B$$

where $B = \left( -\sum_{j=1}^{n} (x_j - x_i) \times \nabla W(x_j - x_i) \Delta V_j \right)^{-1}$

(3.28)

3.2.2.3 SPH hourglass control

Hourglass mode issues, as can be commonly encountered in classical FE problems, see [8], can be removed in SPH formulations owing to a recent improvement in [37]. In the FE method, hourglass modes generally occur when under-integrated elements are used. Indeed, a single integration point, to which stress and strain values are attached, is representative for each finite element and thus assumes constant stress and strain fields over the entire element. By spatial integration, it turns out that only linear displacement and velocity fields can be exactly modeled when under-integrated elements are involved. Accordingly, nodal displacements need to be described with exactness by the deformation gradient $F$, which linearly transforms the distance vector $X_{ij} = X_j - X_i$ between two material points $I$ and $J$ in the reference configuration to the distance vector $x_{ij} = x_j - x_i$ between them in the deformed configuration, such that $x_{ij} = FX_{ij}$.

An hourglass analogy can be drawn with the SPH method since any SPH particle assumes mean stress and strain fields in its neighborhood. The following argumentation is conducted for a total Lagrangian SPH formulation, in which physical quantities are not functions of the current coordinates $x$ but of the reference coordinates $X$. To remedy hourglass issues, an error vector $E_{ij}$, defined as the difference between the theoretical distance vector $(x_{ij})$ between a central particle $I$ and any neighbor particle $J$ and the actual distance vector $x_{ij}$ is defined. By applying the
SPH discretization scheme on \( \langle x_{ij} \rangle \) and by symmetrizing mutual interactions of particles \( I \) and \( J \), the error vector is expressed as:

\[
\mathcal{E}_{ij} = (x_{ij})^{sym} - x_{ij} = \frac{1}{2} (F_i + F_j) x_{ij} - x_{ij}
\]  

(3.29)

The hourglass correction then consists in applying a spring-like repulsive force \( f_i^{HG} \) on the particle \( I \) such that \( f_i^{HG} \) is collinear to the actual distance vector \( x_{ij} \) and proportional to the projection of the error vector \( \mathcal{E}_{ij} \) on \( x_{ij} \). The repulsive force \( f_i^{HG} \) is given by the following expression:

\[
f_i^{HG} = -\alpha \sum_{j=1}^{n} \Delta V_i \Delta V_j W(x_{ij}) \frac{1}{2} (E_i + E_j) \frac{\mathcal{E}_{ij} \cdot x_{ij}}{\|x_{ij}\|^3} \frac{x_{ij}}{\|x_{ij}\|}
\]  

(3.30)

where \( \alpha \) is an amplitude scaling factor and \( E_i \) and \( E_j \) are the Young’s moduli attached to particles \( I \) and \( J \), respectively.

A powerful application of hourglass control is the removal of tensile instabilities which represent usual pitfalls in SPH formulations.

### 3.3 Computational cycle in a Hydrocode

In the course of this work, the hydrocode SOPHIA has been employed. A brief overview of the algorithmic sequence conducted within a computational cycle is schematically provided in Figure 3.3.
3.4 RVE model setup

Methodologic aspects regarding the setup of Representative Volume Elements or RVEs for quartzite and sandstone are shortly outlined in the following.

In the quest of the generation of realistic RVEs, microstructural analyses, which provide informative statistics about grain sizes and shapes, can be conducted. Microscope imaging, as a classical method, requires that samples be casted into an epoxy matrix and polished. Accordingly, microstructures may get altered by this preparation. Moreover, the construction of a three-dimensional structure on the basis of 2D statistics may be far from reality. Instead, a particle sizing instrument can be employed. This fully non-invasive technique bases upon laser diffraction and yields particle sizes ranging from 0.02 to 2000 micrometers. When a particle encounters a laser ray, the light gets deviated in an angle that directly correlates with the particle size. Smaller particle sizes are associated to higher deviation angles and lower light intensity. Upon analysis of deviating light patterns, the grain size distribution can be...
reconstructed. The grain size distribution obtained with this technique is provided for a Seeberger sandstone sample in Figure 3.4-left in the form of a histogram. Each rectangle is associated to an average grain equivalent diameter and a corresponding frequency. The diameter ranges from about 60 nanometers to about 222 micrometers.

![Histogram of grain sizes](image)

Figure 3.4: Left: grain equivalent diameter distribution in a small-sized Seeberger sandstone sample delivered by a particle sizing instrument. Middle: seeded grains into a cubic box. Right: sandstone RVE with tetrahedral mesh.

The statistical grain size distribution is then used as an input for the structure generator GEOSTAT which delivers an aggregate of ellipsoid-shaped quartz grains with a target porosity of about 23%, see Figure 3.4-middle. The different algorithmic steps conducted in GEOSTAT, in particular the seeding of ellipsoidal grains as inspired from [33] and extended, are detailed in the appendix of this work, see Chapter 11. Eventually, a tetrahedral mesh is generated from the resulting structure by the help of the commercial SIMPLEWARE program, see Figure 3.4-right. As a result, a sandstone RVE with an edge size of about half a millimeter is obtained.

For quartzite, the use of the GEOSTAT program is inappropriate as it fails in generating compact structures with zero porosity. To remedy this issue, the construction of a Voronoi diagram [35], based on the random distribution of points in a cubic box, has been opted for, see Figure 3.5. Accordingly, polygonal quartz grains with clearly-resolved grain boundaries can be aggregated to a compact structure. Tetrahedral meshing has been performed by the open-source program TETGEN. The half millimeter-sized quartzite RVE has been such constructed that quartz grain equivalent diameters amount in average to 100 µm, as is also observable.
in common quartzite structures. Uncertainties related to the topology and orientation of quartz grains in the quartzite RVE, when compared to the sandstone RVE, are acceptable since quartzite does not involve contact laws and thus does not require an accurate geometric modeling of contact surfaces.

Figure 3.5: Left: randomly seeded points into a cubic box. Middle: resulting quartzite RVE with grain boundaries on the basis of a Voronoi diagram. Right: quartzite RVE with tetrahedral mesh.
4  Cohesive-Zone-Element formulation: standards and new improvements

4.1  Failure process: from physics to modeling

Cohesive-Zone-Element formulations date back to the 1960s, when Dugdale [28] and Barenblatt [6] described fracture as a separation process localized at a crack tip. The background idea developed in these references bases on the existence of a process zone in the forefront of a progressing crack tip, in which irreversible damage and deformations occur, as exemplarily sketched in Figure 4.1.

![Figure 4.1: Crack tip progressing perpendicularly to an applied far-field loading $T_\infty$. The ready-to-fail forefront of the crack tip is depicted as a process zone.](image)

The generation of a process zone generally results from the excess of a critical traction. From a modeling point of view, a process zone can be represented by the cohesive zone concept. Conditions for emergence and evolution of a cohesive zone are explained in the following and illustrated in Figure 4.2.

Let $\mathcal{B}$ be a body and $\mathcal{B}_1$ and $\mathcal{B}_2$ two sub-bodies such that $\mathcal{B} = \mathcal{B}_1 \cup \mathcal{B}_2$. Let $M$ be a material point located at the interface of $\mathcal{B}_1$ and $\mathcal{B}_2$, and let $dS$ be an infinitesimal internal surface centered on $M$. If $T$ is the internal traction acting on $M$ and $T^{\text{init}}$ a critical traction, the failure initiation
The relationship \( T = T(\delta) \) is called the traction-separation law or cohesive law and fully governs the behavior of the cohesive zone. Depending on the mathematical description of the traction-separation law, \( T \) and \( \delta \) do not necessarily point in the same direction. However, both vectors are contained in the quadrant \((\mathbf{t}, \mathbf{n})\) of the plane defined by the projections of \( T \) on and orthogonally to the mid-surface plane, see Figure 4.2. This vector property merely connotes that a positive elongation, respectively a shear displacement, is necessarily associated to a positive normal cohesive traction, respectively tangential cohesive traction in the shear direction.

In addition to the activation threshold \( T^{\text{init}} = T(\mathbf{0}) \), the cohesive law \( T = T(\delta) \) monitors the subsequent irreversible softening of the cohesive zone, namely the decohesion process. When a critical separation \( \delta^{\text{crit}} \), in norm, is achieved, the crack is fully opened. Accordingly, the so-called fracture energy \( G^{\text{crit}} \), as an energy per surface, is completely dissipated and the cohesive zone can be deleted. In the light of the aforementioned properties, the cohesive zone formulation constitutes an elegant baseline in an effort to replicate the physics of crack nucleation, propagation and coalescence in a realistic way, see [6] and [28].
The cohesive zone formulation is used to represent mode I failure as well as mode II and mode III failure. Moreover, if the separation proceeds either purely orthogonally to the mid-surface \( dS \) (mode I) or purely tangentially to \( dS \) (mode II and III), the cohesive law \( T(\delta) \), including activation threshold, may be governed by two independent equations. When combining normal failure and tangential failure, i.e. a mixed mode, a coupling of normal and tangential cohesive laws can be performed, see section 4.3.

### 4.2 Cohesive law for single-mode failure

For single mode I failure, let \( T_n \) and \( \delta_n \) be the respective single components of \( T \) and \( \delta \) with respect to \( n \). For single mode II-III failure, \( T_t \) and \( \delta_t \) are the respective single, positive components of the projection of \( T \) and \( \delta \) in the plane orthogonal to \( n \). For the sake of convenience, only single mode I failure will be addressed in this section. The argumentation can be transposed to single-mode II-III failure by replacing the subscript \( n \) by the subscript \( t \). In either case, the vectorial traction-separation function can be simplified to a scalar relation.

Two standard categories of cohesive laws can be distinguished: the initially elastic or intrinsic cohesive law and the initially rigid or extrinsic cohesive law. Their respective underlying traction-separation curves \( T_n = T_n(\delta_n) \) are plotted for the case of linear softening in Figure 4.3.
In the following argumentation, linear traction-separation relationships are considered and are based upon the work of [19] and [74]. The intrinsic approach presupposes the pre-existence of a cohesive zone even if the material is not loaded. An initial reversible elastic branch exists and can be compared to a spring behavior. Once $T_n$ reaches $T_n^{crit}$, the decohesion process is initiated and $T_n$ linearly decreases with increasing separation $\delta_n$ along the so-called decohesion path. The maximum current separation is denoted by $\delta_n^{max}$. If, during the decohesion process, the separation $\delta_n$ reversely goes below $\delta_n^{max}$, the cohesive traction accordingly decreases proportionally to $\delta_n$ and may even get zero. The interpenetration case, for which $\delta_n$ becomes negative, needs to be appropriately handled, e.g. with a contact repulsive law. Contact issues pertaining to cohesive zones will be addressed at the end of this chapter in subsection 4.5.2. For any subsequent increase of $\delta_n$, i.e. reloading, the cohesive traction follows the reversible branch upwards until the decohesion branch is recovered. The more advanced the decohesion process is, the more compliant is the unloading behavior of the cohesive zone, the more the cohesive zone is damaged. This corroborates the physical intuition that a process zone gradually softens as it opens.

The extrinsic approach deviates from the intrinsic one in that no initial elasticity precedes the decohesion process. Instead, the internal traction $T_n$ must first override the critical traction $T_n^{crit}$. Unloading and reloading processes are modeled as in the intrinsic approach. As a linear traction-separation relationship is assumed, the cohesive traction obeys the following system of equations:
Cohesive-Zone-Element formulation: standards and new improvements

\[
\begin{align*}
T_n &= T_n^{\text{crit}} \left(1 - \frac{\delta_n}{\delta_n^{\text{crit}}}\right) & \text{if } \delta_n = \delta_n^{\text{max}} \\
T_n &= T_n^{\text{crit}} \left(1 - \frac{\delta_n^{\text{max}}}{\delta_n^{\text{crit}}}\right) \cdot \frac{\delta_n}{\delta_n^{\text{max}}} & \text{if } \delta_n \leq \delta_n^{\text{max}}
\end{align*}
\]

where \( \delta_n^{\text{crit}} = \frac{2G_n^{\text{crit}}}{t_n^{\text{crit}}} \). The first equation points to the decohesion path while the second one describes the reversible unloading-reloading path.

Equations (4.1) can be transposed to pure tangential loading by replacing the subscript \( n \) by the subscript \( t \). Further mathematical functions for \( T_n \) can be addressed. For instance, [107] use two independent exponential laws to describe the reversible and decohesion branches, respectively.

When applying the cohesive zone formulation to Finite Element methods, the use of an extrinsic approach, since granular materials are modeled, is of relevance. This way, any spurious elastic stresses that may propagate through the material will be invisible to extrinsic cohesive zone elements, whereas intrinsic cohesive zone elements get elastically pre-loaded. Accordingly, the intrinsic approach induces stiffness discontinuities between bulk elements and cohesive zone elements and may alter the global material behavior, even prior to the actual failure initiation. In this respect, only the extrinsic approach will be addressed in the rest of this chapter. The intrinsic approach, though, can be relevantly employed when modeling e.g. composites [21] or bonded joints [72], for which delamination or debonding processes along a well-known failure path are sought. The interest of the intrinsic approach for such materials can be intuitively seized in that the initial elastic elongation of a cohesive zone element presumably prompts a chain reaction over its neighbors, and so on.

4.3 Cohesive law for mixed-mode failure

When mode I failure and mode II-III failure are superimposed, a coupling of both single-mode failure types for the cohesive law is required. The cohesive zone approach presented here is essentially inspired by literature references [19][74][75][92] and is also used in a similar form in [59].
4.3.1 Cohesive zone activation

When mixed-mode failure is involved, the three-dimensional critical failure traction is determined using a mixed formulation. Let the Macaulay brackets $\langle \cdot \rangle$ be defined as follows:

$$\langle \Phi \rangle = \begin{cases} \Phi & \text{if } \Phi > 0 \\ 0 & \text{if } \Phi \leq 0 \end{cases}$$

if $\Phi$ is a scalar \hspace{1cm} (4.2a)

$$\langle \Psi \rangle = \Psi t + \langle \Psi_n \rangle n$$

if $\Psi$ is a vector \hspace{1cm} (4.2b)

As only tensile tractions are accounted for in failure mode I, the compressive tractions being related to contact which is not considered in this section, the Macaulay brackets are solely intended to eliminate negative normal components of the cohesive traction and separation vectors. Assuming a quadratic interaction, upon activation of a cohesive zone, the internal traction, denoted by $\vec{T} = \vec{T}_t t + \vec{T}_n n$ at $t_{coh}$, must fulfill Inequality (4.3):

$$\left( \frac{T_t}{T_t^{crit}} \right)^2 + \left( \frac{T_n}{T_n^{crit}} \right)^2 \geq 1$$

The unit vector $t$ indicates the direction of the cohesive traction projection on the tangential plane. The initial cohesive traction is accordingly given by $T^{init} = \langle \vec{T} \rangle$. Discontinuities between $T^{init}$ and $\vec{T}$ arise if negative normal tractions are involved. To circumvent this issue, as mentioned above, an appropriate repulsive contact law must be combined with the cohesive law. During the decohesion process, the cohesive traction can be likewise decomposed: $T = T_t t + T_n n$. The reference system $(t, n)$ is not fixed in space but depends on potential rotations of the cohesive zone and of the cohesive traction $T$.

The graphical representation of the failure initiation criterion is twofold. If positive normal tractions are involved, i.e. $\langle T_n \rangle = \bar{T}_n > 0$, the limiting envelope is a half-spheroid $\mathcal{E}_0$, characterized by two identical semi-axes of length $T_t^{crit}$ and a third one of length $T_n^{crit}$. If negative tractions are encountered, i.e. $\langle T_n \rangle = 0 > \bar{T}_n$, the half-spheroid is prolonged by a circular cylinder of radius $T_t^{crit}$ stretching towards negative tractions. The limiting envelope is invariant by rotation about the third semi-axis $n$. Accordingly, the graphical representation of the limiting envelope can be
reduced to a two-dimensional cross-sectional curve in the \((t,n)\) plane, see Figure 4.4. Due to time discretization pertaining to numerical schemes, the internal traction vector \(\mathbf{T}\) may exceed the limiting envelope within one time step, but generally does not coincide with it. To conform to the model assumptions, \(\mathbf{T}\) is, immediately upon fulfillment of (4.3), pushed back onto the failure initiation envelope. An analogy between cohesive zone activation and classical yielding in elastic-plastic materials can be drawn. In both cases, the internal traction vector and the stress tensor, respectively, are confined within a limiting envelope and obey a push-back routine once the envelope is transgressed. The direction of the push-back traction is provided by the traction increment that is responsible for envelope transgression.

Figure 4.4: Limiting envelope for the internal traction of an emerging cohesive zone. Any internal traction exceeding the failure criterion is pushed back on the envelope. The cohesive traction disregards any negative normal component of the internal traction.
4.3.2 Decohesion law

4.3.2.1 Mathematical description

In the literature, various contributions address decohension law models involving mixed-mode failure [59][74][92]. The underlying hypothesis to most of cohesive zone formulations is that the cohesive traction $T$ can be derived from differentiation of a free energy potential $\varphi$ with respect to the separation vector $\delta$, see Equation (4.4):

$$T = \frac{\partial \varphi}{\partial \delta_t} t + \left( \frac{\partial \varphi}{\partial \delta_n} \right) n$$  \hspace{1cm} (4.4)

A further assumption consists in reducing the dependency of $\varphi$ on $\delta_n$ and $\delta_t$ to a dependency on the scalar effective opening $\delta^{eff}$, defined by:

$$\delta^{eff} = \sqrt{\beta^2 \delta_t^2 + (\delta_n)^2}$$  \hspace{1cm} (4.5)

where $\beta$ is a coupling factor between sliding and normal opening displacements. The physical meaning of $\beta$ will be outlined in the following. Let the effective traction $T^{eff}$ be defined as the total derivative of $\varphi$ with respect to $\delta^{eff}$:

$$T^{eff} = \frac{d \varphi}{d \delta^{eff}}$$  \hspace{1cm} (4.6)

Using the chain rule delivers the modified expression of the cohesive traction $T$:

$$T = \frac{d \varphi}{d \delta^{eff}} \frac{\partial \delta^{eff}}{\partial \delta_t} t + \frac{d \varphi}{d \delta^{eff}} \left( \frac{\partial \delta^{eff}}{\partial \delta_n} \right) n$$  \hspace{1cm} (4.7)

Embedding Equations (4.5) and (4.6) into Equation (4.7) and conducting some derivative calculation leads to the final expression of $T$:

$$T = T^{eff} \frac{\delta^{eff}}{\delta^{eff}} (\beta^2 \delta_t t + (\delta_n) n)$$  \hspace{1cm} (4.8)

The effective traction $T^{eff}$ can be seen as the actual decohesion function that decreases as the effective opening $\delta^{eff}$ grows. It must be empha-
sized that even if $T^{eff}$ does not depend on the individual components of the so-called opening vector $\langle \delta \rangle$, the actual cohesive traction components $T_n = T \cdot n$ and $T_t = T \cdot t$ do. It can be derived from Equation (4.8) that the tangential-to-normal ratios of $\langle \delta \rangle$ and $T$ are proportional to each other:

$$\frac{T_t}{T_n} = \beta^2 \frac{\delta_t}{\langle \delta_n \rangle} = \beta^2 \gamma \quad (4.9)$$

where $\gamma = \frac{\delta_t}{\langle \delta_n \rangle}$ and is called the tangential-to-normal ratio of the opening vector $\langle \delta \rangle$. If the starting hypothesis is the linearity of the decohesion law for single-mode failure, as addressed in section 4.2, the free energy from which $T^{eff}$ is differentiated must be a second-order polynomial in $\delta^{eff}$:

$$\varphi = T^0 \delta^{eff} \left(1 - \frac{\delta^{eff}}{2\delta^{crit}}\right) \quad (4.10)$$

where $T^0$ is a nominal traction and $\delta^{crit}$ is the critical separation. The explicit linear expression for $T^{eff}$ can thus be derived:

$$T^{eff} = T^0 \left(1 - \frac{\delta^{eff}}{2\delta^{crit}}\right) \quad \text{if } \delta^{eff} = \delta^{max} \quad (4.11a)$$

$$T^{eff} = T^0 \left(1 - \frac{\delta^{max}}{\delta^{crit}}\right) \cdot \frac{\delta^{eff}}{\delta^{max}} \quad \text{if } \delta^{eff} \leq \delta^{max} \quad (4.11b)$$

Depending on the mixed-mode models that are addressed in the literature, different definitions for the coupling factor, the nominal traction and the critical separation can be given. Here, the coupling factor $\beta$ is set to unity and thence ensures that the cohesive traction and the opening vector are collinear. Furthermore, the nominal stress is set equal to the norm of the initial cohesive traction $\|T^{init}\|$. At failure initiation, Equation (4.11a) shows that $T^{eff}$ and $T^0$ are equal. Accordingly, the elliptical condition given by Equation (4.3) and Equation (4.8) can be rewritten into the following system of equations:

$$\begin{align*}
\left\{ \begin{array}{l}
\left(\frac{T^{init}_t}{T^{crit}_t}\right)^2 + \left(\frac{T^{init}_n}{T^{crit}_n}\right)^2 = 1 \\
\|T^{init}\|^2 = (T^{init}_t)^2 + (T^{init}_n)^2 = (T^0)^2
\end{array} \right. \quad (4.12)
\end{align*}$$
By inserting Equation (4.9) into Equations (4.12), a general expression for the nominal traction can be established, knowing that $\beta = 1$:

$$
T^0 = T_n^{\text{crit}} T_t^{\text{crit}} \sqrt{\frac{1 + \gamma^2}{(T_t^{\text{crit}})^2 + \gamma^2 (T_n^{\text{crit}})^2}}
$$

(4.13)

The critical separation is accordingly given by $\delta^{\text{crit}} = \frac{2\sigma^{\text{crit}}}{T^0}$. The underlying motivation of these assumptions follows the development made in [59] in that a constant fracture energy amount must be dissipated during the decohesion process, regardless of the opening direction considered. From Equations (4.8), (4.11a) and (4.13), an elliptical equation, valid along the decohesion path for any effective opening $\delta^{\text{eff}}$, can be derived:

$$
\left(\frac{T_t}{T_t^{\text{crit}}}\right)^2 + \left(\frac{T_n}{T_n^{\text{crit}}}\right)^2 = \left(1 - \frac{\delta^{\text{eff}}}{\delta^{\text{crit}}}\right)^2
$$

(4.14)

At failure initiation, i.e. $\delta^{\text{eff}} = 0$, the cohesive traction $T$ is located on the half-spheroid $\mathcal{E}_0$ as depicted in Figure 4.4. At constant values of $\delta^{\text{eff}}$, the right member of (4.14) demonstrates that $T$ moves on a set of half-spheroids homothetic to $\mathcal{E}_0$ that shrink towards the origin as $\delta^{\text{eff}}$ increases. The consistency of Equation (4.14) with the single-mode decohesion law, see Equations (4.1), can be easily verified. In the very first time steps after failure initiation, the direction of the cohesive traction vector $T$ is very sensitive to the tangential-to-normal ratio of $\langle \delta \rangle$. This sensitivity originates from the discontinuous nature of $T$ when the effective opening $\delta^{\text{eff}}$ tends to zero. This feature can be evidenced by reformulating Equation (4.8) when $\langle \delta_n \rangle$ and $\delta_t$ tend to zero:

$$
\lim_{\|\delta\| \to 0} T = T_n^{\text{crit}} \gamma t + T_n^{\text{crit}} n \text{ if } \langle \delta_n \rangle \neq 0
$$

$$
\lim_{\|\delta\| \to 0} T = T_t^{\text{crit}} t + \frac{T_t^{\text{crit}}}{\gamma} n \text{ if } \langle \delta_n \rangle = 0
$$

(4.15)

If $\gamma$ is fixed during the decohesion process, the traction $T$ as expressed in Equation (4.8) is linear with respect to $\delta^{\text{eff}}$. 
4.3.2.2 Graphical representation
In the light of the previous mathematical description, a graphical representation of the decohesion law in mixed-mode failure is provided in Figure 4.5. Normalized tractions \( \left( \frac{T_n}{T_n^{\text{crit}}}, \frac{T_t}{T_t^{\text{crit}}} \right) \) are plotted over normalized openings \( \left( \frac{\delta_n}{\delta_n^{\text{crit}}}, \frac{\delta_t}{\delta_t^{\text{crit}}} \right) \), where \( \delta_n^{\text{crit}} = \frac{2G_n^{\text{crit}}}{T_n^{\text{crit}}} \) and \( \delta_t^{\text{crit}} = \frac{2G_t^{\text{crit}}}{T_t^{\text{crit}}} \) as the critical normal and tangential separations, respectively. The upper diagrams reflect a normal-to-tangential critical traction ratio of one half while the lower diagrams base upon identical normal and tangential critical traction values.
4.3.2.3 Traction locking method at small openings

The mathematical discontinuity of the cohesive traction when the effective opening $\delta^{\text{eff}}$ is close to zero, see again Equations (4.15), can be slightly discerned on the 3D plots of Figure 4.5 by following different oriented decohesion paths from the origin. As a result, variations of $\gamma$ at small openings may induce spurious oscillations of the cohesive traction $\mathbf{T}$. In order to avoid this issue, [59] proposes a traction locking method which applies from failure initiation up to the achievement of a threshold damage value $D^{\text{stab}}$. The damage $D$ is defined by the ratio of the effective opening $\delta^{\text{eff}}$ to the critical opening $\delta^{\text{crit}}$. The underlying...
principle is that the cohesive traction, instead of following the high directional oscillations of the opening vector in the very first decohesion steps, tends to stay aligned with the initial cohesive traction vector $T^{\text{init}}$. In order to ensure a smooth transition from the direction $T^{\text{init}}$ at failure initiation to the direction of $\langle \delta \rangle$ at $D^{\text{stab}}$, the cohesive traction $T$ gets smoothly rotated from $T^{\text{init}}$ to $\langle \delta \rangle$ during the stabilization process. If $D$ is the current damage, the cohesive traction is then oriented along the following vector:

$$\frac{T}{\|T\|} = R_{\alpha \Delta} \frac{T^{\text{init}}}{\|T^{\text{init}}\|}$$

(4.16)

where $\alpha = \frac{D}{D^{\text{stab}}} (T^{\text{init}}, \langle \delta \rangle)$, i.e. the opening angle $(T^{\text{init}}, \langle \delta \rangle)$ scaled by the ratio of instantaneous damage $D$ to the threshold damage $D^{\text{stab}}$. The vector $\Delta$ corresponds to the vector product $T^{\text{init}} \times \langle \delta \rangle$. Accordingly, $R_{\alpha \Delta}$ is the rotation matrix describing a rotation by an angle $\alpha$ around the axis defined by the vector $\Delta$. As $\langle \delta \rangle$ varies over time, the rotation must be continuously updated. A graphical representation is given in Figure 4.6. The smaller the transitional damage is, the more representative is the decohesion process, but the likelier are spurious oscillations to arise. An optimum value for $D^{\text{stab}}$ is achieved when non-physics and spurious oscillations are held at a minor level. The optimal transitional damage value generally depends on the physical problem considered and cannot be evaluated deterministically.
Figure 4.6: Stabilization process at different decohesion steps. The failure initiation envelope is denoted by the dashed blue curve. The time-dependent, maximum admissible traction curve is denoted by the solid red curve. At $t_0$, the critical traction is achieved. In the subsequent time steps, from $t_1$ to $t_3$, the direction $\langle \delta \rangle$ strongly oscillates. In this time span, the cohesive traction $T$ is incrementally rotated in order to tend to the orientation of $\langle \delta \rangle$. As the threshold damage value $D_{\text{stab}}$ is achieved at $t_4$, the directions of $T$ and $\langle \delta \rangle$ coincide back. At $t_5$, $T$ further decreases in norm while $\langle \delta \rangle$ increases along the direction of $T$. 
4.4 Standard discretization of cohesive zones using the FE method

In this section, the applicability of the cohesive zone formulation to the FE scheme is explained in detail.

As already suggested in section 3.1, the Lobatto quadrature rule is substituted for the standard one-point Gauss quadrature rule. This choice is motivated by the facilitated computation of external forces, and by extension, to cohesive forces in the FE discretization scheme. Instead of defining one integration point at the centroid of a finite element, an integration point is defined for each node of the element. A similar argumentation can be conducted for element boundaries in case of surface integrals. These integration points are said to be conjugated to the mesh nodes because they share the same spatial locus but are of different nature. The weighting factor is constant for all integration points and amounts, in the case of tetrahedral meshes, to one fourth for volume integrals and one third for surface integrals. A considerable advantage offered by the Lobatto rule when compared to the Gauss rule is that \( \hat{\mathbf{f}} \) does not depend on the external forces acting on adjacent nodes of \( \mathcal{N}_k \), but only on those acting on \( \mathcal{N}_k \) directly. Therefore, \( \hat{\mathbf{f}} \) is composed of additive facet-wise boundary traction contributions over all facets \( \hat{\mathbf{f}} \) adjacent to \( \mathcal{N}_k \), provided that \( \Gamma_f \subset \Gamma_{\mathcal{F}} \):

\[
\hat{\mathbf{f}}_k^{\text{ext}} = \sum_{p=0}^{n_n} \sum_{k \in \Gamma_{\hat{\mathbf{f}}}} N_k \mathbf{T}^{bc} dS = \sum_{\hat{\mathbf{f}} | \mathcal{N}_k \in \Gamma_{\hat{\mathbf{f}}}} \frac{T^{bc}_{\hat{\mathbf{f}}} dS_{\hat{\mathbf{f}}}}{3} \quad (4.17)
\]

4.4.1 Partially-activated cohesive zone elements

Owing to the Lobatto quadrature rule, cohesive zone elements can be partially activated, i.e. each node can be individually split. In this respect, it will be demonstrated in this subsection that the direct nodal relations between external tractions and external forces can be transferred to cohesive zone elements as well. A physical body \( \mathcal{B} \), constituted of two sub-bodies \( \mathcal{B}_1 \) and \( \mathcal{B}_2 \) separated by an internal facet \( \Gamma_{\text{int}} \), is considered in the following. An inner crack is assumed to arise at some location in \( \Gamma_{\text{int}} \). Accordingly, cohesive zones emerge and internal surfaces are replaced by

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cohesive surfaces or pseudo-external surfaces. Like internal surfaces, cohesive surfaces are submitted to opposite and mutually acting traction vectors according to Newton’s Third Law. Though, in contrast to internal surfaces, cohesive surfaces allow in essence for a displacement discontinuity or gap $\delta$. From the numerical point of view, the birth of cohesive zone elements is associated with the duplication of at least one node. Figure 4.7 schematizes in 2D the node duplication and the emergence of cohesive zone elements as a result of the inner crack formation.

![Figure 4.7: Finite Element discretization of a body $B$ undergoing the formation of an inner crack formation. Left: configuration just before node duplication. Right: configuration just after node duplication.](image)

The left-hand side of Figure 4.7 illustrates a set of finite elements connected to the node $N_k$. The depicted facets $f_I$ and $f_{II}$ have reached the critical traction and are about to fail. On the right hand of Figure 4.7, the cohesive process has just set in. This is characterized by a node duplication of $N_k$ into $N_{k1}$ and $N_{k2}$, and by the birth of two new cohesive zones $C^{f_I}$ and $C^{f_{II}}$. Upon failure, the internal facet $f_I \cup f_{II}$ of the body $B$ becomes, from the point of view of each sub-body $B_1$ and $B_2$, respectively, a local cohesive facet or local pseudo-external facet. Accordingly, the sub-nodes $N_{k1}$ and $N_{k2}$ are submitted to so-called cohesive forces $f_{k1-k2}^{coh}$ and $f_{k2-k1}^{coh}$, respectively. These cohesive forces can be regarded as pseudo-external forces and obey the same discretization scheme as external forces $f_k^{ext}$. Thus, their expressions are, in the spirit of Equation (4.17), given by:
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\[
f_{k1\leftarrow k2}^{\text{coh}} = \sum_{\dot{\mathcal{f}} \mid \mathcal{N}_k \in \Gamma_{\dot{\mathcal{f}}}} f_{k1\leftarrow k2}^{\dot{\mathcal{f}}} = \sum_{\dot{\mathcal{f}} \mid \mathcal{N}_k \in \Gamma_{\dot{\mathcal{f}}}} \frac{T_{k1\leftarrow k2}^{\dot{\mathcal{f}}} dS}{3} = -f_{k2\leftarrow k1}^{\text{coh}} \tag{4.18}
\]

where \(\dot{\mathcal{f}}\) is the index running over all cohesive facets attached to \(\mathcal{N}_k\), \(T_{k1\leftarrow k2}^{\dot{\mathcal{f}}}\) is the cohesive traction relative to the cohesive zone element \(\mathcal{C}^{\dot{\mathcal{f}}}\) and defined as acting from \(\mathcal{N}_k\) to \(\mathcal{N}_1\), and \(f_{k1\leftarrow k2}^{\dot{\mathcal{f}}}\) is its associated force. The cohesive forces \(f_{k1\leftarrow k2}^{\text{coh}}\) and \(f_{k2\leftarrow k1}^{\text{coh}}\) have the same absolute value but opposite directions, in accordance with Newton’s Third Law. The traction \(T_{k1\leftarrow k2}^{\dot{\mathcal{f}}}\) suggests that a cohesive traction is associated to a facet-node pair. More generally, a cohesive zone element \(\mathcal{C}^{\dot{\mathcal{f}}}\) is governed by as many traction-separation laws \(T_{p1\leftarrow p2}^{\dot{\mathcal{f}}} (\delta)\) as nodes \(\mathcal{N}_p \in \dot{\mathcal{f}}\) subjected to duplication. A cohesive zone element is said to be fully activated if all nodes sharing \(\dot{\mathcal{f}}\) are duplicated. If at least one but not all of its nodes are duplicated, the cohesive zone element is said to be partially activated. Another situation can be encountered when considering a body \(\mathcal{B}\) in which a crack tip propagates, as illustrated by Figure 4.1. The corresponding discretized 2D scenario is depicted in Figure 4.8.

Figure 4.8: Finite Element discretization of a body \(\mathcal{B}\) in which a crack tip propagates. Left: configuration just before node duplication. Right: configuration just after node duplication.

In this scenario, the left-hand cohesive zone \(\mathcal{C}^{\dot{\mathcal{f}}_I}\), which was already partially activated, gets fully activated while the right-hand cohesive zone \(\mathcal{C}^{\dot{\mathcal{f}}_II}\) newly emerges and gets partially activated.
4.4.2 Forces induced by cohesive surfaces for standard cohesive zone formulations

Adopting the notations of section 3.1, Equation (3.9) can be extended, for standard node duplication, to the form:

\[
\begin{align*}
\ddot{u}_{k1} &= \frac{1}{m_{k1}} \left( f_{k1}^{\text{ext}} + f_{k1\rightarrow k2}^{\text{coh}} - f_{k1}^{\text{int}} \right) \\
\ddot{u}_{k2} &= \frac{1}{m_{k2}} \left( f_{k2}^{\text{ext}} + f_{k2\rightarrow k1}^{\text{coh}} - f_{k2}^{\text{int}} \right)
\end{align*}
\] (4.19)

At failure initiation, the initial cohesive tractions \( T_{k1\rightarrow k2}^{\text{init}} \) are assumed to have a unique common value \( T_{k1\rightarrow k2}^{\text{init}} \). With this assumption, a direct relation between \( f_{k1\rightarrow k2}^{\text{coh init}} \) and \( T_{k1\rightarrow k2}^{\text{init}} \) can be established:

\[
\begin{align*}
f_{k1\rightarrow k2}^{\text{coh init}} &= \left( \sum_{\mathcal{N}_k \in \Gamma_{\mathcal{N}_k}} \frac{1}{3} \mathbb{S}_{\mathcal{B}} \right) \cdot T_{k1\rightarrow k2}^{\text{init}} = -f_{k2\rightarrow k1}^{\text{coh init}}
\end{align*}
\] (4.20)

Adopting this hypothesis is particularly intuitive when all cohesive surfaces are coplanar, i.e. oriented along the same normal vector. As the initial cohesive tractions intrinsically account for the facet orientation they refer to, Equation (4.20) can be satisfactorily extended to nodes \( \mathcal{N}_k \) for which the adjacent cohesive surfaces are not coplanar. An explicit expression for \( f_{k1\rightarrow k2}^{\text{coh init}} \), and consequently for \( T_{k1\rightarrow k2}^{\text{init}} \), can be obtained by setting up the discrete equation of linear momentum conservation at two instants of time, namely immediately prior to failure and upon failure. It is assumed that no external forces \( f_k^{\text{ext}} \) are being prescribed on \( \mathcal{N}_k \). Prior to failure:

\[
\dot{u}_k = -\frac{f_k^{\text{int}}}{m_k} = -\frac{f_{k1}^{\text{int}} + f_{k2}^{\text{int}}}{m_{k1} + m_{k2}}
\] (4.21a)

Upon failure:

\[
\dot{u}_{k1} = \frac{f_{k1\rightarrow k2}^{\text{cohinit}} - f_{k1}^{\text{int}}}{m_{k1}}
\] (4.21b)
A condition that unifies the three latter equations is time continuity of the acceleration of $N_k$ during the failure transition, see [59][75]:

$$\ddot{u}_k = \ddot{u}_{k1} = \ddot{u}_{k2}$$ \hspace{1cm} (4.21d)

In general, time discontinuity in nodal accelerations may be caused by time discontinuities in internal forces or potential external forces. While time continuity is not guaranteed for accelerations, it is automatically fulfilled for velocity and displacements vectors since they result from explicit time integration of the acceleration vector. Accordingly, strain and stress tensors are time continuous. Nevertheless, cohesive zones are per nature very sensitive to fluctuations in nodal accelerations, especially at small openings for which a traction locking algorithm is needed, see again paragraph 4.3.2.3. Moreover, jumps in nodal accelerations may induce over-estimated internal forces and lead to the undesired activation of cohesive zones in the immediate vicinity of existing cohesive zones. This is especially true when a node, located at the intersection of several failure paths, is likely to undergo successive duplications. Using the four Equations (4.21), basic calculation delivers key expressions for the cohesive forces:

$$f_{k2\leftarrow k1}^{\text{coh init}} = -f_{k1\leftarrow k2}^{\text{coh init}}$$ \hspace{1cm} (4.22a)

$$f_{k1\leftarrow k2}^{\text{coh init}} = \frac{m_{k2}f_{k1}^{\text{int}} - m_{k1}f_{k2}^{\text{int}}}{m_{k1} + m_{k2}}$$ \hspace{1cm} (4.22b)

Evidently, the cohesive tractions are given by:

$$T_{k1\leftarrow k2}^{\text{init}} = -T_{k2\leftarrow k1}^{\text{init}}$$ \hspace{1cm} (4.23a)

$$T_{k1\leftarrow k2}^{\text{init}} = \frac{3}{(\sum_{\phi}|N_k\in\Gamma_k\hat{f}_\phi|)} \cdot \frac{m_{k2}f_{k1}^{\text{int}} - m_{k1}f_{k2}^{\text{int}}}{m_{k1} + m_{k2}}$$ \hspace{1cm} (4.23b)

Equations (4.22a) and (4.23a) confirm that Newton’s Third Law is not violated. Equation (4.22b) shows that the cohesive forces consist of a mass weighting of the internal forces. Here, potential secondary node
duplications based on the sub-nodes $N_{k1}$ and $N_{k2}$ have been discarded. The case of multiple, simultaneous node split around a master node has been addressed in [59] and [75]. Since a system of $n$ equations, where $n$ is the number of created sub-nodes, needs to be solved, this standard approach will be put aside in this work in favor of a novel and computational effort-saving methodology, see subsection 4.5.1.

4.4.3 Standard cohesive zone activation criteria

In the literature, different methods assessing activation criteria for cohesive zones can be found. Generally, a purely mechanically-based criterion, e.g. the excess of a critical traction at an internal surface, might not be sufficient to activate a cohesive element. A geometrically-based criterion often needs to be additionally achieved. The latter criterion ensures that a failure path, which locally separates two elemental partitions, can develop. Mechanically-based criteria will be detailed in the next three paragraphs before the geometrical criterion is explained.

4.4.3.1 Top-bottom stress activation
For each inactive cohesive facet $f$, the top-bottom stress method calculates the average stress tensor of both adjacent elements sharing that surface. The resulting stress tensor $\sigma^{avg}$ is contracted with the normal vector $n_f$ of the facet to deliver an average traction vector $T^{avg}$. Normal and tangential projections of $T^{avg}$ with respect to $n$ and the tangential plane, respectively, are then evaluated in the spheroid criterion, see Inequation (4.3). If the criterion is fulfilled, the cohesive facet is marked as failed. An example of this methodology can be found in [85].

4.4.3.2 Cauchy's theorem method
In the Cauchy’s theorem method, a node-wise stress tensor is evaluated for each interfacial node, and is given by:

$$
\sigma_k^{avg} = \frac{\sum_{e|N_k \in \Omega_e} \left( \frac{1}{m_e} \cdot \sigma_e^{gauss} \right)}{\sum_{e|N_k \in \Omega_e} \left( \frac{1}{m_e} \right)}
$$

(4.24)
where \( m_k^e \) are the lumped mass contributions to node \( N_k \) of all elements \( e \) sharing \( N_k \), and \( \sigma^e_{Gauss} \) is the stress tensor value at the centroid or Gauss integration point of the element \( e \). The average nodal stress can be seen as a weighted average of stresses of elements sharing \( N_k \), the weighting factor being their respective mass contributions. Traction vectors for each inactive cohesive facet \( f \) attached to \( N_k \) are derived by contracting \( \sigma^k_{avg} \) with \( n_f \), and then evaluated using the half-spheroid criterion. Since the activation criterion is investigated for each individual node, the cohesive facet is marked as failed with respect to node \( N_k \). In this regard, partial activation of cohesive zones is feasible.

### 4.4.3.3 Failure path method

The failure path method, as detailed in [59], seeks all admissible geometrical paths that virtually subdivide an elemental partition adjacent to \( N_k \) into two sub-partitions. As the number of sought paths can become extremely high in 3D, this methodology must be carefully employed. Since granular structures with only inter-granular failure are involved in the scope of this work, the number of admissible failure paths is affordable. A node \( N_k \) located at the intersection of \( p \) grains exhibits \( \frac{p(p+1)}{2} \) admissible failure paths. Each admissible failure path consists of internal facets for which the traction vector, provided by Equations (4.23), is submitted to the half-spheroid criterion which acts as the mechanical failure criterion. If the latter is fulfilled, the cohesive facet is marked as failed with respect to node \( N_k \). The cohesive facet is then activated under the condition that the geometric activation criterion, explained in the next paragraph, is fulfilled for the failure path considered. If, even in the presence of failed cohesive facets, none of the admissible failure paths fulfills the geometrical activation criterion, then no node splitting occurs.

The failure path method has the great advantage to evaluate a traction vector that directly correlates with the theoretical cohesive traction vector at failure initiation. In this respect, time continuity of the acceleration vector upon failure is automatically fulfilled. It must be underlined that satisfying the half-spheroid criterion for a facet does not necessarily mean that the common traction vector \( T^k_{init} \) exactly lies on the facet-specific spheroidal surface. This originates not only from the temporal discretization, but also from the mathematical requirement to fulfill Inequation (4.3) for all facets involved in the failure path simultaneously. Therefore,
some cohesive zones may exert an initial cohesive traction beyond the prescribed spheroidal bounds, see Figure 4.9. This deviation converges to zero when the absolute value of the difference between $180^\circ$ and the angles between the cohesive facets goes to zero, i.e. when the failure path tends to flatness.

In the simulations conducted in this work, a balance between computation-time efficiency and precision must be achieved. Since the number of discrete breakable facets in the computed RVEs is significant, a rigorous analysis of all candidate failure paths for each interfacial node proves to increase the computational effort noticeably. A judicious solution consists in adopting a hybrid cohesive zone criterion, making use of the top-bottom stress criterion and of the failure path method. In the first step, breakable facets are marked as effectively failed if they fulfill the top-bottom stress criterion. If a failure path can be drawn around a given node, cohesive zone elements are inserted in a second step and exert cohesive tractions on that node according to Equations (4.23). The achieved cohesive traction values may, though, diverge from those located on the facet-specific half-spheroids. As a replacement solution, the half-spheroid of each failed facet is scaled to match the initial cohesive traction vector that has been evaluated with the failure path method.

4.4.3.4 Geometrically-based activation
For the sake of simplicity, a two-dimensional case is outlined here. Figure 4.10-a illustrates a planar assembly of triangles sharing the
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Evidently, the edges of the triangles represent internal facets. Thin solid lines correspond to non-breakable internal facets. Dotted lines represent breakable but inactive cohesive facets, where the mechanical failure criterion has not been fulfilled at the node $N_k$ yet, whereas bold solid lines depict mechanically-activated cohesive facets.

Figure 4.10: Step decomposition of a multiple node split. a) Activation of one cohesive facet. b) Activation of a second cohesive facet that builds up a failure path. c) Primary node split and activation of a new cohesive facet that builds up a new failure path. d) Secondary node split.

The duplication of node $N_k$ is prohibited if and only if a chain of elements adjacent to $N_k$ and connected over intact facets can be found between the upper and lower sides of at least one mechanically-activated cohesive facet. Otherwise, node splitting is enabled. According to this principle, no node splitting can occur in the a) case as the chain of elements forms a group that is interconnected by either unbreakable (solid) or breakable, but not yet activated (dotted) facets, although one activated face (bold) is already present. On the contrary, the b) case depicted in Figure 4.10-b
shows that a so-called failure path divides the elemental assembly into two sub-partitions, thus enabling splitting of $N_k$ into $N_{k1}$ and $N_{k2}$. The subsequent activation of a new cohesive facet after primary node split immediately results in a secondary node split, see Figure 4.10-c and Figure 4.10-d. This is explained by the impossibility to draw a connecting path across an existing failure path.

When addressing three-dimensional configurations, the same condition for a failure path as in the two-dimensional case can be used. However, the required number of mechanically-activated cohesive facets to induce node splitting is higher. As in 2D, secondary node splitting is enhanced by existing failure paths, but generally requires more than one active cohesive facet to take place.

4.5 New improvements of Cohesive-Zone-Elements

In the light of the previous sections addressed in this chapter, still open questions concern the treatment of multiple node split on the one hand, and the treatment of negative normal displacements at small openings on the other hand. In particular, time continuity of nodal accelerations in the context of successive node splits must be permanently fulfilled. These issues are addressed in the following subsections, and remedies are concomitantly developed and portrayed.

4.5.1 A novel methodology for dealing with multiple node split

As outlined in the previous section, the failure path method is the most convenient way to ensure time continuity of nodal accelerations. This subsection tackles the question of further secondary node splitting following a primary node split.

4.5.1.1 Issue

The argumentation is developed in 2D for a node $N_k$ undergoing a primary node duplication, followed by a secondary node duplication for one of its two sub-nodes. Such a scenario has already been sketched out in Figure 4.10 and is reframed more purposively in Figure 4.11.
During the primary node split, $N_k$ is split into $N_{k1}$ and $N_{k23}$, concomitantly with the emergence of two cohesive zones $C^I$ and $C^{II}$. The cohesive forces are, during the decohesion process, given by:

$$f^{coh}_{k1\leftarrow k23} = f^{I}_{k1\leftarrow k23} + f^{II}_{k1\leftarrow k23} = -f^{coh}_{k23\leftarrow k1} \quad (4.25)$$

In the secondary duplication phase, $N_{k23}$ is further split into $N_{k2}$ and $N_{k3}$ and a third cohesive zone $C^{III}$ emerges. The new cohesive force between $N_{k2}$ and $N_{k3}$ is thus given by:

$$f^{coh}_{k2\leftarrow k3} = f^{III}_{k2\leftarrow k3} = -f^{coh}_{k3\leftarrow k2} \quad (4.26)$$

The cohesive interaction between $N_{k1}$ and the newly split nodes $N_{k2}$ and $N_{k3}$ is inherited from the primary cohesive interaction and needs to be properly evaluated. In standard FE code implementations, the total cohesive force on a given node is generally derived from the cohesive tractions of its adjacent cohesive zone elements. Applying this principle to the present case means that $N_{k2}$ would be subjected to the cohesive tractions of $C^I$ and $C^{III}$ and $N_{k3}$ to the cohesive tractions of $C^{II}$ and $C^{III}$. Unavoidably, time discontinuities in nodal accelerations are to be expected for each individual sub-node. Issues conveyed by this pure geometrical formulation can be circumvented by enforcing time continuity on nodal accelerations at any secondary node split initiation time.
4.5.1.2 Remedy
Analogously to the time continuity condition given by Equations (4.22), the initial cohesive force induced by the primary node split is given by:

\[ f_{coh\,init}^{k_{1}\leftarrow k_{23}} = \frac{m_{k_{23}} f_{int}^{k_{1}} - m_{k_{1}} f_{int}^{k_{23}}}{m_{k_{1}} + m_{k_{23}}} = -f_{coh\,init}^{k_{23}\leftarrow k_{1}} \]  

(4.27)

It is assumed for the secondary node split, regardless of the primary cohesive interactions between \( \mathcal{N}_{k_{1}} \) and \( \mathcal{N}_{k_{23}} \), that the cohesive force between the new sub-nodes \( \mathcal{N}_{k_{2}} \) and \( \mathcal{N}_{k_{3}} \) can be set up as if they had undergone a primary split:

\[ f_{coh\,init}^{k_{2}\leftarrow k_{3}} = \frac{m_{k_{3}} f_{int}^{k_{2}} - m_{k_{2}} f_{int}^{k_{3}}}{m_{k_{2}} + m_{k_{3}}} = -f_{coh\,init}^{k_{3}\leftarrow k_{2}} \]  

(4.28)

Cohesive interactions between secondary split nodes \( \mathcal{N}_{k_{2}} \) and \( \mathcal{N}_{k_{3}} \), respectively, and the primary split node \( \mathcal{N}_{k_{1}} \) still need to be determined. For this purpose, the discrete equation of linear momentum conservation upon the secondary node split is set up for node \( \mathcal{N}_{k_{23}} \) before splitting and its sub-nodes \( \mathcal{N}_{k_{2}} \) and \( \mathcal{N}_{k_{3}} \) after splitting. Reciprocity of cohesive forces, i.e. \( f_{i\leftarrow j} = -f_{j\leftarrow i} \) according to Newton’s Third Law, has also been accounted for:

\[ \ddot{u}_{k_{23}} = \frac{f_{coh}^{k_{23}\leftarrow k_{1}} - f_{int}^{k_{2}} - f_{int}^{k_{3}}}{m_{k_{2}} + m_{k_{3}}} \]  

(4.29a)

\[ \ddot{u}_{k_{2}} = \frac{f_{coh}^{k_{2}\leftarrow k_{1}} + f_{coh\,init}^{k_{2}\leftarrow k_{3}} - f_{int}^{k_{2}}}{m_{k_{2}}} \]  

(4.29b)

\[ \ddot{u}_{k_{3}} = \frac{f_{coh}^{k_{3}\leftarrow k_{1}} - f_{coh\,init}^{k_{3}\leftarrow k_{2}} - f_{int}^{k_{3}}}{m_{k_{3}}} \]  

(4.29c)

The equality of nodal accelerations owing to the time continuity condition, i.e. \( \ddot{u}_{k_{23}} = \ddot{u}_{k_{2}} = \ddot{u}_{k_{3}} \), reduces this third-row system of equations to a second-row one. As the only unknowns are \( f_{coh}^{k_{2}\leftarrow k_{1}} \) and \( f_{coh}^{k_{3}\leftarrow k_{1}} \), the system can be fully resolved. After a few simplifications, their expressions are given by:
The cohesive force $f_{k2\rightarrow k1}^{coh}$ node $N_{k1}$ exerts on $N_{k23}$ after the primary node split is, from the secondary node split, distributed over nodes $N_{k2}$ and $N_{k3}$:

$$f_{k2\rightarrow k1}^{coh} = \frac{m_{k2}}{m_{k2} + m_{k3}} \cdot f_{k23\rightarrow k1}^{coh} \quad (4.30a)$$

$$f_{k3\rightarrow k1}^{coh} = \frac{m_{k3}}{m_{k2} + m_{k3}} \cdot f_{k23\rightarrow k1}^{coh} \quad (4.30b)$$

Moreover, it is worth noticing that the distribution of cohesive forces after the secondary node split is performed according to a mass weighting of $N_{k2}$ and $N_{k3}$ with respect to $N_{k23}$.

$$f_{k23\rightarrow k1}^{coh} = f_{k2\rightarrow k1}^{coh} + f_{k3\rightarrow k1}^{coh} \quad (4.31)$$

4.5.1.3 Example of application
To better illustrate the benefits of the presented methodology, a simple pseudo-2D problem is considered. A triangle, subdivided into three irregularly-sized triangular finite elements $e_\alpha$, $e_\beta$ and $e_\gamma$ is considered, see Figure 4.12. Since the hydrocode SOPHIA only addresses 3D geometries, the triangular finite elements are artificially connected to an additional non-planar node in order to build up tetrahedrons. In the following, the argumentation is led in the triangular plane only.
Figure 4.12: Schematic sequence of a multi-node split on a 2D assembly of three triangular finite elements sharing a common inner node. At $t_1$, a primary node split occurs at $N_k$ and separates $e_\alpha$ from the $(e_\beta, e_\gamma)$ cluster. At $t_2$, a secondary node split separates $e_\beta$ from $e_\gamma$. Instants of time $t_3$ and $t_4$ depict more advanced decohesion steps for which cohesive tractions gradually soften.

All three finite elements are connected by breakable surfaces, i.e. which are susceptible to failure upon the achievement of a critical traction. The applied boundary conditions are described by tensile velocities acting at the three outer nodes. Accordingly, cohesive zone elements can only be partially activated at the inner node $N_k$. At time $t_1$, a primary node split between $e_\alpha$ and the $(e_\beta, e_\gamma)$ cluster occurs, concomitantly with the emergence of two cohesive zone elements. From time $t_2$, a secondary node split occurs between $e_\beta$ and $e_\gamma$ and a third cohesive zone element arises accordingly. Time continuity of node accelerations is surveyed here for the sub-node $N_{k3}$ attached to $e_\gamma$. In order to better capture potential time discontinuity effects from cohesive zone elements on $N_{k3}$, the internal force contribution by element $e_\gamma$ is subtracted from the node acceleration of $N_{k3}$, such that a pseudo-cohesive node acceleration can be defined:
\[ \ddot{u}_{k3}^{ps-coh} = \ddot{u}_{k3} - \frac{f_{int}^y}{m_{k3}} = \ddot{u}_{k3} + \frac{f_{int}^y}{m_{k3}} \]  

(4.32)

From the secondary node split initiation time, \( \ddot{u}_{k3}^{ps-coh} \) directly mirrors the accelerations imparted by the cohesive zone elements and acting on \( N_{k3} \). Prior to the secondary node split, \( \ddot{u}_{k3}^{ps-coh} \) is only regarded as a pseudo-cohesive acceleration since it accounts not only for already activated cohesive zone elements, but also for non-activated ones for which a virtual cohesive force, in the spirit of Equation (4.22b), can be computed. Figure 4.13 shows a temporal diagram of \( \ddot{u}_{k3}^{ps-coh} \) for the pure geometrical and time-continuous formulations.

![Figure 4.13: Pseudo-cohesive acceleration of node \( N_{k3} \) over time for the pure geometrical (red) and time-continuous (green) formulations. The four sketched instants of time are correlated to those indicated in Figure 4.12.](image)

As both acceleration profiles show, an acceleration jump at the secondary node split time \( t_2 \) occurs such that the norm of \( \ddot{u}_{k3}^{ps-coh} \) overestimates its time-continuous counterpart. This acceleration discrepancy extends over the whole subsequent decohesion process and demonstrates how far time-discontinuity effects may induce misjudgment of the failure response of materials subjected to multi-branched fracturing.
4.5.2 A novel methodology addressing small or negative normal separations

4.5.2.1 Issue
A common issue with the extrinsic cohesive approach, as opposed to the intrinsic approach, is encountered when cohesive unloading sets in promptly after cohesive activation. In such a case, the slope of the reversible unloading branch is significantly steep and even reaches infinity if no separation has occurred yet. To illustrate this with a concrete example, a simple model, consisting of two tetrahedrons connected by a breakable surface, is considered, see Figure 4.14-left. A tensile boundary condition, in the form of two temporal velocity profiles, is applied on the two end nodes, i.e. on those not belonging to the breakable surface. Both velocity vectors are oriented orthogonally to the breakable surface and are of opposite signs. For testing purposes, the velocity temporal evolution is described by a sawtooth-shaped ramp over the time interval \([t_0, t_2]\) with achievement of a maximum velocity at \(t_1\), see Figure 4.14-right. From \(t_2\), the boundary condition is completely removed and the geometry is solely submitted to its internal forces. The purpose therewith is to analyze the spring-like behavior of an initiated cohesive zone element at small separations upon removal of boundary conditions.
Figure 4.14: Simulation results of a tensile test on a two-tetrahedral setup without any corrective algorithm. Six instants of time are highlighted. Boundary conditions are fully removed from $t_2$. Left: graphical representation of the geometrical setup with blue-colored tetrahedrons and red-colored cohesive zone element. Right: temporal evolution of the effective traction $T^{eff}$ (blue), normal separation $\delta_n$ (red) and velocity boundary condition $U_{bc}$ (green). No quantitative values have been given for the sake of simplicity.

From the observations that can be made in Figure 4.14, a cohesive zone element emerges shortly after $t_0$ and expands until $t_2$. This decohesion phase is corroborated by the traction curve decrease discernable in the time interval $[t_0, t_2]$. From $t_2$, all velocity boundary conditions are removed and the cohesive traction elastically releases. Due to the still high stiffness exhibited by the unloading path, the normal separation strongly oscillates between positive and negative values, as witnessed by the traction behavior in the time interval $[t_2, t_5]$. Accordingly, the effective traction $T^{eff}$ is affected by the oscillating behavior of $\delta_n$. The instants of time $t_3$ and $t_4$, picked out from the diagram during the oscillating regime, graphically highlight the alternation of inverted and upright states of the cohesive zone element. At $t_5$, the oscillations are evanescent and the cohesive zone element tends back to flatness. The element interpenetration issue, as is strikingly evidenced by the present example, can be prevented by a corrective algorithm that is developed in the following paragraph.
4.5.2.2 Remedy
To counteract negative separations as have been portrayed by the previous example, a corrective acceleration is applied on pairs of nodes which tend to draw nearer or interpenetrate. In practice, the separation vector \( \delta \) is enforced to constancy upon achievement of the so-called backward-separation criterion, i.e. if its norm \( \| \delta \| \) drops or if its normal component \( \delta_n \) gets negative.

For illustration purposes, let \( \mathcal{N}_k \) be two nodes separating from each other with respective vector positions \( \mathbf{u}_{k1}^{(n)} \) and \( \mathbf{u}_{k2}^{(n)} \) at time \( t^{(n)} \). Owing to the leapfrog integration scheme, see Equations (3.14), the following system of equations with regards to the separation vector \( \delta = \mathbf{u}_{k2} - \mathbf{u}_{k1} \) can be derived:

\[
\begin{align*}
\delta^{(n+\frac{1}{2})} &= \delta^{(n-\frac{1}{2})} + \Delta t^{(n)} \dot{\delta}^{(n)} \\
\delta^{(n+1)} &= \delta^{(n)} + \Delta t^{(n+\frac{1}{2})} \delta^{(n+\frac{1}{2})}
\end{align*}
\] (4.33)

As Equation (4.33) shows, the achievement of the backward separation criterion is dictated by the separation velocity \( \delta^{n+\frac{1}{2}} \) which, if oriented backwards, results in \( \| \delta^{(n+1)} \| < \| \delta^{(n)} \| \), see Figure 4.15 for illustration.

Figure 4.15: Schematic representation of a primary node split at \( t^{(n-1)} \) followed by decohesion at \( t^{(n)} \) and release at \( t^{(n+1)} \) of the associated cohesive zone element. The separation vector \( \delta \) and the separation rate vector \( \dot{\delta} \) are also represented. A traction-separation curve, on which the three instants of time are highlighted, is provided on the right-hand side of the figure.
Upon achievement of the backward-separation criterion, corrective acceleration increments \( \Delta \tilde{u}_k^{(n)} \) are applied on \( N_1 \) and \( N_2 \) such that their resulting corrected accelerations are expressed by \( \tilde{u}_k^{(n)} = \hat{u}_k^{(n)} + \Delta \tilde{u}_k^{(n)} \). By enforcing equality between the corrected accelerations for \( N_1 \) and \( N_2 \), the corrected separation acceleration \( \tilde{\delta}^{(n)} \) drops to zero. As a result, the corrected separation velocity \( \tilde{\delta}^{(n+\frac{1}{2})} \) equals the previous separation velocity \( \delta^{(n-\frac{1}{2})} \). Since the latter is forward-oriented or at least zero, the corrected separation \( \tilde{\delta}^{(n+1)} \) outreaches or at least equals the previous separation \( \delta^{(n)} \) in norm as requested. The backward-separation criterion is then surveyed again for the next time step.

The choice of the node acceleration correction is not arbitrary but is based upon a virtual merging of both separating nodes and, concomitantly, upon a concatenation of their respective elemental partitions as if no cohesive zone element had arisen. Indeed, if the backward-separation criterion is assumed to be instantaneously met after the emergence of the cohesive zone element, the corrected node accelerations intuitively have to correspond to those prevailing right before cohesive zone activation in order to fulfill the time continuity condition. Following this principle, the corrective acceleration increments and the resulting corrected accelerations are given by following equations:

\[
\Delta \tilde{u}_{k1} = \frac{1}{m_{k1}} \left( m_{k2} f_{k1}^{\text{int}} - m_{k1} f_{k2}^{\text{int}} \right) \left( -f_{k1-k2}^{\text{coh}} \right) \quad (4.34a) \\
\Delta \tilde{u}_{k2} = \frac{1}{m_{k2}} \left( m_{k1} f_{k2}^{\text{int}} - m_{k2} f_{k1}^{\text{int}} \right) \left( -f_{k2-k1}^{\text{coh}} \right) \quad (4.34b) \\
\tilde{u}_{k1} = \tilde{u}_{k2} = \frac{-f_{k1}^{\text{int}} - f_{k2}^{\text{int}}}{m_{k1} + m_{k2}} \quad (4.34c)
\]

In the light of Equation (4.22b), the corrective acceleration increments are close to zero for any backward-oriented separation succeeding the cohesive zone element activation. For more advanced separation states, a noticeable discrepancy between the cohesive force and the weighted internal forces may arise. The resulting time discontinuity in the node acceleration though remains acceptable provided the corrective algorithm only acts at
small separations, where backward-oriented separations are the most critical. Generally, a user-defined threshold value $\delta_{\text{stab}}$ stands for the critical separation vector norm beyond which the corrective algorithm is disabled. A non-growing separation vector $\delta$ and a non-negative separation rate $\dot{\delta}$ are thus guaranteed with this corrective procedure, and instability issues related to excessive stiff unloading are circumvented.

4.5.2.3 Example of application
The previous two-tetrahedral geometry is considered again. The tensile loading case is simulated using the corrective algorithm and is graphically sketched in Figure 4.16-left. From $t_2$, the cohesive zone element opening remains constant in spite of traction removal. Figure 4.16-right corroborates this static behavior as the normal traction and separations remain at a constant level from $t_2$. Accordingly, the corrective algorithm is proved to prevent backward-oriented separations from arising. Thence, it imparts an enhanced stability to the cohesive zone formulation, especially at small separations where the elastic unloading issue is crucial.

![Figure 4.16: Simulation results of a tensile test on a two-tetrahedral setup using the corrective algorithm. Six instants of time are highlighted. Boundary conditions are fully removed from $t_2$. Left: graphical representation of the geometrical setup with blue-colored tetrahedrons and red-colored cohesive zone element. Right: temporal evolution of the effective traction $T^{\text{eff}}$ (blue), normal separation $\delta_n$ (red) and velocity boundary condition $U_{bc}$ (green). No quantitative values have been given for the sake of simplicity.](image)
5 Development of a novel mesoscale simulation model for Split-Hopkinson-Bar-Tests in spallation configuration

The purpose of this chapter is to ascertain the inter-granular dynamic failure strength of quartzite and sandstone on the mesoscale. While the elastic behavior of quartz grains can be explicitly determined, the achievement of reliable data on inter-granular interfaces remains particularly challenging. As the formation of sandstone is driven by geological processes over extremely long time scales, e.g. sedimentation and cementation, the strength of quartz grain boundaries is, by nature, hard to predict. To gain qualitative and quantitative insight into the inter-granular behavior of geologic materials, a specific numerical model for quartzite and sandstone is devised on the basis of experimental Split-Hopkinson-Bar-Tests. The latter are generally employed to investigate dynamic properties of materials. A large dynamic range of strain rates can be covered, although they lie well below shock conditions. Using a specific setup, namely the spallation configuration, the dependency of dynamic tensile strength on strain rate can be investigated. For instance, a bilinear tensile strength-strain rate function has been assessed for concrete in [88][82]. In the following sections, the evaluation of dynamic tensile strength and dynamic fracture energy will be explained in some detail as the calibration of mesoscale parameters will be done by evaluating mesoscale simulations in the same way as the experiments such that direct comparisons can be made. A preliminary study where pseudo-realistic quartzite and sandstone mesostructures were submitted to tensile loading cases can be found in [30].

5.1 Reference experiments and data

5.1.1 Experimental setup

The reference experiments used for assessing the mechanical behavior of quartzite and sandstone are modified Split-Hopkinson-Bar-Tests in spallation configuration [58][69][80][88][103]. They involve thin cylindrical rods; the corresponding geometrical assembly is depicted in Figure 5.1.
The employed materials are, from left to right, an impactor, an aluminum rod called an incident bar and the investigated specimen of study. The latter is, depending on the experimental purpose envisaged, glued or weakly attached to the free end of the incident bar.

Figure 5.1: Schematic setup of a Split-Hopkinson-Bar-Test in spallation configuration. The experimental arrangement is from left to right: an impactor, an incident bar and the investigated specimen. Stress wave profiles at different instants of time are schematically represented. $\sigma_i$, $\sigma_r$ and $\sigma_t$ respectively stand for the incident, reflected and transmitted stresses with respect to the incident bar-specimen interface and $T_{crit}$ denotes the dynamic critical traction or dynamic tensile strength. The geometrical setup has not been drawn to scale in order to provide a more comprehensible representation of the pulses.

Figure 5.1 gives a schematic overview of what happens in a Split-Hopkinson-Bar spallation experiment. As the impactor hits the incident bar, a bidirectional compressive pulse is generated. While the right-traveling pulse propagates through the incident bar, the left-traveling
pulse is reflected at the impactor free end and an unloading wave runs back into the impactor and the incident bar. As a result, one single right-traveling compressive pulse, the wave length of which is dictated by the impactor length, propagates in the incident bar. It is called incident wave. As it reaches the incident bar-specimen interface, a part of the incident wave is reflected back into the incident bar, while the other part is transmitted into the specimen. Due to the small diameter-to-length ratio of the rods, a one-dimensional longitudinal stress state can be assumed in all bars and the specimen, i.e. no transverse stresses are supposed to act on the lateral surfaces. As can be mathematically supported by stress and velocity equilibrium equations (see again section 2.3), the impedance contrast between the incident bar and the specimen determines the transmitted wave amplitude in the specimen. As the compressive wave reaches the specimen free end, it is reflected into a left-traveling tensile wave. Since the applied stress loading is purely elastic, both symmetric compressive and tensile waves superimpose each other and can be summed up. Due to the well-defined shape of the waves, the points in the specimen see a compression, then unloading and tensile loading. When a critical traction, called dynamic tensile strength $T_{exp}^{crit}$, is reached, the specimen fails. The strains in the incident bar and in the specimen are measured with strain gauges (SG) and the free-end velocity of the specimen is measured by an accelerometer (AC), see Figure 5.2. In the rest of this chapter, the transmitted wave that propagates in the specimen will be labeled as incident wave since the specimen is regarded as the reference material of study.
Figure 5.2: Experimental setup for a Split-Hopkinson-Bar-Test in spallation configuration. Strain gauges are glued on the incident bar and the specimen, and an accelerometer is placed at the specimen free end. Dimensions are given in mm. The notch depicted in the specimen is drilled only when the fracture energy is investigated.

The signals delivered by the experiments allow, after some analysis, for the assessment of two key material properties in the specimen, namely the dynamic tensile strength and the dynamic fracture energy. The employed methodology will be described in the following subsection; it is described in more detail in [88]. When the dynamic tensile strength is investigated, the specimen is glued onto the incident bar to ensure a proper wave transmission. In the case of fracture energy investigation, a notched specimen is prepared and appended onto the incident bar. This way, the location of the main fracture plane is pre-determined and the probability of generating multiple simultaneous cracks, which complicates evaluations, is reduced. The smooth and planar nature of the incident wave is slightly altered by the notch, but this effect is usually small compared to the measured variations in typical geomaterials. The notch is filled with some cement in order to minimize its effects on the wave transmission.
5.1.2 Determination of dynamic material properties

5.1.2.1 Longitudinal wave speed and dynamic Young’s modulus

The longitudinal wave speed or sound speed in the specimen can be determined by measuring the time $\Delta t$ the wave needs to travel over a longitudinal distance $d$. Hereby, it is assumed that the wave is not altered when propagating in the specimen and thus, keeps a constant speed. For an accurate determination of the wave speed, two remote measurement points are selected. This way, structural inhomogeneities, which could affect the wave speed locally, are averaged. In practice, the wave arrival times observed at the accelerometer and at one of the three strain gauges attached to the specimen (SG 5-6-7) are compared. To ensure a proper analysis, the free-end velocity signal is scaled such that its amplitude conforms to that of the strain signal. It is then temporally shifted to the strain signal interval until a good signal superimposition is achieved, see Figure 5.3.

By calling $\Delta t$ the temporal shifting and $d$ the distance separating the strain gauge from the specimen free end, the longitudinal sound speed $C_{spe}$ in the specimen can be calculated:

$$C_{spe} = \frac{d}{\Delta t}$$  \hspace{1cm} (5.1)
With the assumption of a one-dimensional stress state, the Young’s modulus $E_{spe}$ of the specimen is directly given by:

$$E_{spe} = \rho_{spe} C_{spe}^2$$  \hspace{1cm} (5.2)

where $\rho_{spe}$ is the density of the specimen.

5.1.2.2 Dynamic tensile strength
As outlined in the previous subsection, the dynamic tensile strength $T_{crit}^{exp}$ can be determined by the use of unnotched specimens. With the notch, some wave diffraction would occur. When failure occurs, a crack emerges which can be regarded as an interface from the point of view of wave mechanics. Owing to the subsequent disruption process, waves are reflected at the crack interface as though they would encounter a material of lower impedance $\rho C$. Consequently, the left-traveling tensile wave partly reflects at the crack location into a right-traveling compressive wave. As it reaches the free end of the specimen, the new release wave counteracts the declining trend of the free-end velocity and produces a kink-up as sketched by Figure 5.3. The resulting free-end velocity difference, called pull-back velocity and depicted by $\Delta U_{pb}$ in Figure 5.3, allows for the calculation of the dynamic tensile strength $T_{crit}^{exp}$ [88]:

$$T_{crit}^{exp} = \frac{1}{2} \rho_{spe} C_{spe} \Delta U_{pb}$$  \hspace{1cm} (5.3)

The range of validity of this formula will be addressed in paragraph 5.2.5.1.

5.1.2.3 Dynamic fracture energy
As mentioned above, the dynamic fracture energy is often determined by means of notched specimens in order to enforce the crack location and to avoid secondary cracks. For this purpose, an energy balance is conducted between two instants of time $t_1$ and $t_2$. The former one corresponds to the failure initiation time $t_{fail}$, at which a crack starts to develop. The latter one relates to the full separation of the two resulting fragments. In [88], it is suggested to estimate the dynamic fracture energy by calcu-
lating the product of the impulse transfer $\Delta I$ between the two fragments and the crack opening velocity $\delta_{\text{crack}}$, expressed by:

$$G_{\text{exp}}^{\text{crit}} = \Delta I \delta_{\text{crack}}$$  (5.4)

By convention, the impulse transfer over the time span $[t_1, t_2]$ is considered to flow from the left fragment with mass $m_1$ and average velocity $U_1$ to the right fragment with mass $m_2$ and average velocity $U_2$:

$$\Delta I = \Delta I_{1 \rightarrow 2} = (U_2(t_1) - U_2(t_2)) m_2$$  (5.5)

Accordingly, the crack opening velocity is the relative velocity of the right fragment with respect to the velocity of the left fragment:

$$\delta_{\text{crack}} = \frac{(U_2(t_1) + U_2(t_2))}{2} - \frac{(U_1(t_1) + U_1(t_2))}{2}$$  (5.6)

In order to better apprehend the frame of hypotheses adopted in the calculation of the dynamic fracture energy, an identical expression can be established by recourse to momentum and energy conservation equations. Energy conservation bases on the assumption that the dynamic fracture energy $G_{\text{exp}}^{\text{crit}}$ stands for the exact loss in kinetic energy between $t_1$ and $t_2$. In this respect, the following system of equations can be set up:

$$\begin{cases} 
    m_1 U_1(t_1) + m_2 U_2(t_1) = m_1 U_1(t_2) + m_2 U_2(t_2) \\
    m_1 U_1^2(t_1) + m_2 U_2^2(t_1) = m_1 U_1^2(t_2) + m_2 U_2^2(t_2) + G_{\text{exp}}^{\text{crit}}
\end{cases}$$  (5.7)

Using Equations (5.5), (5.6) and (5.7), and solving for $G_{\text{exp}}^{\text{crit}}$, it turns out that the same expression for the dynamic fracture energy $G_{\text{exp}}^{\text{crit}}$ as in Equation (5.4) is obtained.

The failure initiation time $t_1$ is indirectly determined by measuring the pull-back time $t_{pb}$ at the specimen free end, i.e. the arrival time of the release wave as a consequence of cracking. By defining $L$ the specimen length, and knowing the notch position $x_c$ and the wave speed $C_{\text{spe}}$ in the specimen, the following relationship can be intuitively set up:
\[ t_1 = t_{\text{fail}} = t_{pb} - \frac{L - x_c}{C_{spe}} \] (5.8)

The concomitant velocities \( U_1(t_1) \) and \( U_2(t_1) \) can be determined by using wave theory since pure elastic conditions are met prior to \( t_1 \). Calculation details can be found in paragraph 5.2.5.1. The full failure time \( t_2 \) is, however, conditioned by the experimental observation of a full crack pattern. Accordingly, the velocities \( U_1(t_2) \) and \( U_2(t_2) \) are determined from high-speed camera pictures. The exact failure time is actually not required, it just has to be late enough, i.e. after the full separation of the fragments. As for the dynamic tensile strength, it will be shown in paragraph 5.2.5.2 how far the validity of hypotheses used for the calculation of the dynamic fracture energy is met or not.

5.1.3 Results for quartzite and sandstone

5.1.3.1 Photographs of specimens
Results from Split-Hopkinson-Bar experiments for Wasa quartzite and Seeberger sandstone, which will be used as a basis for the mesoscale simulations, can be found in [84] and [70]. In both quartzite and sandstone, up to two spallation cracks developed using the unnotched preparation. Due to the fine striation in the sandstone specimens, the cracks in unnotched sandstone are not planar but may extend over a length of about 15 mm. In notched quartzite and notched sandstone, however, only one localized and planar crack developed. Figure 5.4 shows exemplary photographs of failed sandstone specimens for both unnotched and notched preparations.
5.1.3.2 Measured signals
In the following, experimental results for one quartzite and one sandstone experiment are explained in more detail. The experiments were performed and evaluated in [84]. Experimental signals are plotted on one diagram for each rock type, see Figure 5.5.
Figure 5.5: Experimental signals for a quartzite specimen (top) and a sandstone specimen (bottom) published in [84]. The left vertical axis belongs to two strain gauge measurements in the incident bar (SG 2, blue and SG 3, red) and one in the specimen (SG 5, green). The right vertical axis belongs to the accelerometer signal in terms of velocity (AC, black). The pull-back time is denoted by $t_{pb}$ and the pull-back velocity by $\Delta U_{pb}$.

The strain gauges SG 2 and SG 3 attached to the incident bar deliver, aside from the temporal shifting due to wave propagation, quasi-identical compressive strain signals. The strain gauge SG 5, which is glued on the specimen, exhibits a compressive strain of the same shape, but with a higher amplitude. The difference in impedance between the incident bar and the specimen is the reason for this compressive enhancement, as has been demonstrated using theory in section 2.3. The velocity signal at the
free end of the specimen is calculated using time integration of the acceleration measured in AC and refers to the right axis in the diagram. The geometrical shape of the free-end velocity signal is in good agreement with the geometrical shapes of the strain profiles. This accordance is valid until the release wave, which originates at the crack location, has reached the free end of the specimen. The arrival of the release wave results in a local kink-up of the free-end velocity profile while it releases from the incident compressive wave. As introduced in the previous subsection, this feature allows for the evaluation of the pull-back velocity $\Delta U_{pb}$.

5.1.3.3 Macroscopic experimental data
As only a preliminary evaluation of the experiments was available when the analysis in this work started, values given in Table 5.1 differ slightly from the published values in [84] and [70]. However, the differences are small, particularly for the average values, which are the basis for further numerical analyses presented below.

Table 5.1: Measured fracture properties of quartzite and sandstone determined in Split-Hopkinson-Bar experiments in spallation configuration. The values are given in terms of average and standard deviation, see [84] and [70].

<table>
<thead>
<tr>
<th>Material</th>
<th>Tensile strength [MPa]</th>
<th>Fracture energy [N/m]</th>
<th>Young’s modulus [GPa]</th>
<th>Strain rate [s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartzite</td>
<td>16.7 ± 2.3</td>
<td>180 ± 120</td>
<td>52.79 ± 2.8</td>
<td>28</td>
</tr>
<tr>
<td>Sandstone</td>
<td>5.5 ± 1.0</td>
<td>160 ± 40</td>
<td>13.55 ± 0.5</td>
<td>23</td>
</tr>
</tbody>
</table>

For each material variant, three specimens have been investigated to check for reproducibility. For each value of Table 5.1, the first number represents the average value of the three experiments and the second one the standard deviation thereof. Two important findings shall be explained in more detail. First, the Young’s moduli for both materials, which are determined from the dynamic experiments, are significantly lower than the values determined in quasi-static and ultrasound measurements. For quartzite, the value from the dynamic experiment is 52.79 GPa, while around 80 GPa are typically measured in the quasi-static regime. A possible explanation for this discrepancy is the type of quartz
involved in the experiments, i.e. Wasa quartzite. This quartzite variant possesses some impurities and thus may exhibit a lower stiffness compared to pure quartzite. Similarly, the Young’s modulus of sandstone in the quasi-static regime is 23 GPa, which was measured by an acoustic test, while 13.55 GPa were determined in the dynamic case. Sandstone, as it possesses a high granularity and a significant porosity, tends to disturb the compressive wave transmitted by the incident bar. Nonlinear material behavior and damage occurring on the microscale at the applied stress amplitude could also be reasons for the observed stiffness reductions which cannot be explained quantitatively yet. However, it remains essential to use the measured Young’s moduli of quartzite and sandstone in simulations to make a direct comparison between numerical and experimental results possible.

Second, the variability of the dynamic fracture energy, especially in quartzite, is relatively high compared to extensively investigated materials such as concrete. The low number of experiments available for notched quartzite and sandstone specimens partly explains the low informative value of the fracture energy measurements. Moreover, the simplifications made in the evaluation of the dynamic fracture energy compared to a purely theoretical evaluation also contribute to this variability, see paragraph 5.2.5.2. In the final publication of [84], however, a smaller variability value is given. As mentioned above, only the average value is relevant for the mesoscale material model parameters, therefore this difference is not relevant for the analysis conducted in this work.

5.2 Mesoscale model setup

In the following, new numerical mesoscale models for sandstone and quartzite, aimed at replicating Split-Hopkinson-Bar-Tests in spallation configuration, are presented. To ensure a proper modeling, a discretized geometrical model, representative of the experimental geometrical setup, is first built up. Initial and boundary conditions achieved in the experimental setup are transposed to the numerical model and adapted to conform to the geometrical simplifications necessitated by the modeling. Material models for quartzite and sandstone are fed by known parameters either available in the literature or directly obtained from experimental results. Unknown inter-granular parameters are varied in the frame of a para-
meter study and indirectly compared to experimental data via the setup of an appropriate numerical instrumentation.

5.2.1 Geometrical setup

A principal difficulty in mesoscale modeling of Split-Hopkinson-Bar experiments is the geometric scales involved. In order to sufficiently resolve the details of the mesoscale structure and keep the computational cost reasonable, the RVE is about half a millimeter edge-sized, whereas the experimental specimen is a cylindrical rod with a length of 250 mm and a diameter of 75 mm. At the same time, the computational effort of the entire model should not be orders of magnitude higher than the effort for simulating the RVE alone. This limits the number of tetrahedral elements. As introduced in section 5.1, the low diameter-to-length ratio of the rods involved in the Hopkinson configuration leads to a more or less, one-dimensional stress state. The specimen thickness in the computational model can therefore be the same as the RVE thickness, provided that the outer lateral surfaces are kept stress-free.

Considering the longitudinal dimension, a grain-scale modeling of the whole specimen is obviously not necessary as, outside the crack area, the specimen is only subjected to moderate dynamic compressive and tensile stresses within the elastic regime. The use of an equivalent isotropic model without representing material failure outside the RVE is thus appropriate in this region. Within the crack area, however, the location of which is either pre-determined by notches or can be determined by wave propagation analysis, tensile failure is modeled in detail using the RVE. The proposed geometrical setup is represented in Figure 5.6 in the case of quartzite.
Figure 5.6: Model of the 250-mm long quartzite specimen used in Split-Hopkinson-Bar simulations. Homogeneous material is represented in pale yellow and the fine-meshed quartzite RVE with grain contours. The location of the RVE is determined by the location of the crack, which here corresponds to the location of a notch drilled at a distance of 100 mm from the free end of the specimen.

In order to keep the total number of tetrahedrons as small as possible, a very coarse mesh can be used for the non-failing region which represents more than 99% of the whole specimen. A smooth transition from the homogenized region to the RVE and vice versa is realized with a specifically developed mesh generation algorithm that uses consecutive coarsening steps. At each coarsening step, two cross-sectional surfaces, facing each other and segmented into triangular meshes with different resolutions, are joined by a pure tetrahedral meshing. The ultimate coarsening step ends with two triangles covering the cross-sectional surface. If the dimensional specifications require further mesh prolongation, the coarse pattern can be perpetuated by repeating cubes composed of five tetrahedrons. Figure 5.7 sketches the different coarsening steps, departing from the RVE outer surface up to the final five-tetrahedral cube.
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Figure 5.7: Representation of three gradual coarsening steps. The fine mesh on the left represents the outer RVE surface, the cube on the right is the final mesh composed of five tetrahedrons.

Figure 5.8 gives an overview of the mesh geometry that respectively represents a quartzite specimen and a sandstone specimen in a Split-Hopkinson-Bar configuration. Color coding is attributed to individual grains within the RVE while pale yellow indicates homogeneous material.
Figure 5.8: Mesh geometry representing the transition from RVE to homogeneous material. Top: quartzite. Bottom: sandstone. Three gradual mesh coarsening steps have been used. For the sake of clarity, the very fine tetrahedral mesh of the RVE is not displayed.

For sandstone, a specific porous RVE, the generation of which is described in the appendix chapter 11, is employed. As the wavelength of the pulse that represents the stress loading is much larger than the largest element and the pulse itself is smooth, no reflections occur at the mesh transitions.

5.2.2 Boundary conditions

In order to save computational effort, neither the striker nor the incident bar is considered explicitly in the mesoscale model. Instead, the transmitted part of the compressive wave from the incident bar into the specimen is prescribed at the left boundary of the specimen using a time-dependent velocity boundary condition $U_{bc}(t)$. The determination of relationships between strain and velocity waves involved in materials of different impedances can be achieved by elastic wave theory, see again section 2.3.
5.2.2.1 Derivation of boundary conditions from experimental signals

In order to get a satisfying estimate of the velocity function $U_{bc}(t)$ that shall be prescribed at the left end of the rock specimen, the instrumentation attached to both aluminum incident bar and specimen is used. Note that, in the following, wave functions which are equal, except for a temporal shift, will be categorized as congruent.

The amplitude of $U_{bc}(t)$ can be indirectly determined with the help of the accelerometer that measures the velocity $U_{AC}(t)$ at the free end of the specimen. According to Equation (2.52), the velocity of the transmitted wave, here the velocity at the free end, amounts to twice the velocity of the incident velocity. This property leads to the congruence relation: $U_{AC} \equiv 2U_{bc}$. The shape of $U_{bc}(t)$ is provided by a strain gauge attached to the aluminum incident bar, here SG3. The shape of the accelerometer signal is not recommended, since it is influenced by the release wave originating at the crack initiation, also called pull-back signal.

The consistency of experimental wave signals with each other can be checked by recourse to elastic wave theory. Since, from the incident bar point of view, the strain pulse $\varepsilon_{SG3}(t)$ is associated to the incident wave and the boundary condition $U_{bc}(t)$ to the transmitted wave, it follows from Equations (2.38) and (2.51) that:

$$\frac{U_{AC}}{\varepsilon_{SG3}} \equiv \frac{2 \rho_{alu} C_{alu}^2}{\rho_{spe} C_{spe} + \rho_{alu} C_{alu}} \quad (5.9)$$

The theoretical ratio of Equation (5.9) has been compared to its experimental counterpart and showed for both quartzite and sandstone that the error does not exceed 8 %, which is acceptable.

A further important aspect to consider is the ratio of wave length to specimen length. As far as failure processes are concerned, the decohesion process following failure initiation often needs a relatively long time. In quartzite, for example, longitudinal elastic waves propagate at 4464 m/s. Thus, a wave takes 112 µs to propagate through the 250 mm-long specimen and back. Yet, as the incident compressive stress pulse temporally extends to about 250 µs, its tail superimposes the head of its reflected counterpart at the incident bar-specimen interface. As a result, a secondary reflected wave, induced by the aluminum-rock material
impedance contrast, arises and propagates into the specimen, thus superimposing the incident wave initially conveyed by the incident bar. Similarly, longitudinal waves propagate in sandstone at 2570 km/s and accordingly take 195 µs for a back-and-forth travel. As the incident compressive wave is prescribed within a time slot of 250 µs, a secondary wave reflection, although somewhat delayed when compared to quartzite, occurs at the incident bar-specimen interface as well. In this regard, the incident stress signal prescribed at the latter interface needs to be modified after a delay time given by $t_{\text{delay}} = \frac{2L}{c_{\text{spe}}}$, where $L$ is the specimen length and $c_{\text{spe}} = \sqrt{\frac{E_{\text{spe}}}{\rho_{\text{spe}}}}$ is the longitudinal wave speed. This delay time corresponds to the duration of a back-and-forth wave propagation in the specimen. In practice, the modification of the velocity boundary condition from $t_{\text{delay}}$ consists in superimposing both incident compressive and secondary reflected waves via the use of elastic wave theory. The raw velocity boundary conditions, which are transmitted by the incident bar, and the modified ones due to secondary wave reflection at the incident bar-specimen interface, which will be used in the following, are sketched for quartzite and sandstone in Figure 5.9. For illustration, the corresponding stresses are also given.
Using the velocity boundary condition over time and the assumption of purely elastic waves, stress distributions in the specimen can be analytically determined at any instant of time. A sample wave snapshot sequence for quartzite is depicted in Figure 5.10. The total stress wave $\sigma_{\text{tot}}$ (red), or resulting stress wave, and its decomposition into the incident stress wave $\sigma_{i}$ (green) and the reflected stress wave $\sigma_{r}$ (blue) arising at the free end of the specimen are shown. All three stresses are related by the wave superimposition rule $\sigma_{\text{tot}} = \sigma_{i} + \sigma_{r}$. The secondary reflected stress wave, which arises at $t = 112 \mu s$ at the incident bar-specimen interface, is not represented here since its contribution to the resulting stress amplitude is negligible in the time sequence considered.
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Figure 5.10: Analytically calculated elastic wave profiles in a 250 mm-long quartzite rod in terms of longitudinal stress at different instants of time. The incident wave (green) and reflected wave (blue), when summed up, provide the resulting wave (red).

Figure 5.11 represents a wave snapshot sequence in sandstone. Again, the secondary reflected stress wave is not represented owing to its negligible amplitude in this time sequence.
Figure 5.11: Analytically calculated elastic wave profiles in a 250 mm-long sandstone rod in terms of longitudinal stress at different instants of time. The incident wave (green) and reflected wave (blue), when summed up, provide the resulting wave (red).

For each material, the last frames show that the resulting stress wave is of tensile nature and progressively gains in amplitude. Depending on the tensile strength prevailing in the specimen, one or several cracks may be initiated within the represented time slot.
5.2.3 Numerical modeling of notched specimen vs. unnotched specimen

As outlined in subsection 5.1.2, the determination of macroscale failure properties when conducting Split-Hopkinson-Bar experiments in spallation configuration requires two distinct specimen preparations: notched and unnotched. In this subsection, it will be shown that only a geometrical setup, allowing for the simultaneous determination of both dynamic tensile strength and dynamic fracture energy, is required in the simulation model.

5.2.3.1 Notched specimen
Split-Hopkinson-Bar-Tests on notched specimens are intended to enforce a localized planar failure pattern at the notch location. The emergence and evolution of fracture surfaces are consequently prescribed by the specimen preparation and the dynamic fracture energy $G_{\text{exp}}^{\text{cr}}$ can be fairly well measured. The notch, drilled at a distance of 100 mm from the specimen right free end, is described in the modeling by centering the RVE on the notch location. It must be strongly emphasized that, in the modeling, the RVE itself does not need to be notched since it is the only part of the model where failure is allowed.

As depicted in the previous subsection, wave superimposition needs to be taken into account in order to correctly represent the boundary condition for the specimen. Since the incident bar and the specimen are weakly appended to each other, any interfacial tension immediately calls the separation of both rods forth. In practice, both compressive tail and tensile head contributions compete with each other until tension preponderates. From this instant of time, both rods dissociate. In the model, this is realized by interrupting the boundary condition.

5.2.3.2 Unnotched specimen
Split-Hopkinson-Bar-Tests on unnotched specimens are aimed at measuring the dynamic tensile strength as precisely as possible. Due to the absence of a notch, the propagating wave is planar and the crack location is not enforced. The unpredictability of the crack location though requires that the RVE be put in the right place to match the experimental crack location.
In quartzite, cracks observable in experiments are very localized and are orthogonal to the longitudinal direction. In sandstone, cracks do not emerge orthogonally to the wave propagation direction, but with an inclination angle, and sprawl over a longitudinal band of about 15-20 mm in length. The low density of contact areas between quartz grains, and thus the relatively small dissipation-prone fracture energy, may explain this pattern. For each rock type, a high variability in the crack locations can be observed among the different specimens investigated. This effect is particularly pronounced in sandstone owing to its weak structural cohesion. Apart from the natural scattering pertaining to geological rocks, this variability is also attributed to the flattening of the resulting stress wave signal over a given spatial length. The plateau of the resulting stress curve spatially ranges over a few tens of millimeters, see again the last snapshots of Figure 5.10 and Figure 5.11 for illustration.

Among the plurality of cracks that may emerge in the specimen, the very right one, i.e. the closest one with respect to the free end of the specimen, obviously engenders the pull-back signal. In order to get an estimate of the presumable location of this crack from a theoretical point of view, the evolution of the resulting stress wave over time as e.g. illustrated in Figure 5.10 and Figure 5.11 can be used. It can be mathematically proven that, at the failure initiation time, the locus of the very right crack always matches the locus of the peak tensile stress of the reflected wave. An additional condition to fulfill this mathematical property is that the incident wave profile monotonically increases up to a maximum value and then monotonically decreases, which is met here. Thence, the resulting stress prevailing at the variable position reached by the peak reflected stress can be tracked over time. Depending on the tensile strength of the specimen, the locus and time at which the very right crack emerges can thus be determined analytically.

Figure 5.12 portrays the amount of resulting tensile stress registered at the locus of the peak reflected stress, respectively over time (left) and over this locus (right). The latter curve starts at 250 mm, i.e. at the free end of the specimen, and then moves to the left along with the left-traveling reflected tensile wave.
Figure 5.12: Plot of the analytically calculated resulting tensile stress at the locus of the peak reflected stress over time (left) and over this locus (right) for purely elastic quartzite and sandstone. The curves in the right diagram start at 250 mm, i.e. the free end of the specimen, which keeps a value of 0 while the rest of the specimen is compressed. When the incident wave is reflected at the free end of the specimen, the locus of the peak reflected tensile stress moves to the left.

In the simulation model, only one crack can be captured since, owing to the need for saving computational effort, only one RVE is modeled. The latter should be preferentially placed at the location of the very right crack in order to reproduce the emergence of the pull-back signal as in the experiment. In order to estimate the most suitable position of the RVE that matches the very right crack in the experiment, the average dynamic tensile strength $\overline{T}_{\text{exp}}$ measured in the experiment is taken as reference. From Table 5.1, it amounts to 16.7 MPa for quartzite and to 5.5 MPa for sandstone. On this basis, the locus of the reflected peak tensile stress for which the resulting stress amounts to $\overline{T}_{\text{exp}}$ is read off from Figure 5.12-right for both rock types. Values for quartzite and sandstone are 182.8 mm and 216.6 mm, respectively.

In spite of the previous information, the RVE will be placed, as in the notched specimens, at the position 150 mm for both quartzite and sandstone. Three main reasons can be stated. First, numerical testing showed that the identification of the pull-back time $t_{pb}$ becomes inaccurate when the RVE is too close to the free end of the specimen, especially in sandstone. Second, the scattering in the position of the very right crack does not give any clue about the ideal crack position to define in the model. This scattering is corroborated by the standard deviation of the dynamic tensile strength in quartzite and sandstone. Third, a numerical method that permits the determination of the tensile strength
of the specimen can be reliably employed, even though the crack position is prescribed, see paragraph 5.2.5.1 for more details.

Using this approach, a considerable advantage is that only one geometrical setup is required to investigate the dynamic tensile strength and dynamic fracture energy of each rock type. However, two distinct simulations must be conducted to determine both macroscale failure quantities since, depending on whether the specimen is glued or appended on the incident bar, dissimilar reflected wave signals have to be dealt with once the incident wave has traveled back and forth through the specimen.

5.2.4 Material model

5.2.4.1 Model for quartz grains and homogeneous material
The strain rates involved in Split-Hopkinson-Bar-Tests correspond to the moderate dynamic regime, thence no shock wave occurs. Furthermore, the stress levels achieved in quartzite and sandstone do not exceed 100 MPa. Since the onset of plasticity in quartz is at stresses in the magnitude of Gigapascals, see [94] and [42], a linear isotropic elastic behavior can be assumed for quartz. Hence, only two independent parameters, e.g. the Young’s modulus $E$ and the bulk modulus $K$, are needed. The bulk modulus $K$ can be derived from the shock-suited Analytical Equation of State or ANEOS for quartz, for which a linear behavior can be assumed in the low compressive regime. The ANEOS model will be addressed in more detail in Chapter 6. The Young’s modulus $E$ is directly taken from Table 5.1. Parameters for quartz grains in the RVE, as well as for homogeneous quartzite and sandstone outside the crack area, are summarized in Table 5.2.
Table 5.2: Material parameters for quartz grains, homogeneous quartzite and homogeneous sandstone adopted in the Split-Hopkinson-Bar simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density ([\text{mg/mm}^3])</th>
<th>Young’s modulus (E) [GPa]</th>
<th>Bulk modulus (K) [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartz grains</td>
<td>2.65</td>
<td>52.79</td>
<td>37.76</td>
</tr>
<tr>
<td>Homogeneous quartzite</td>
<td>2.65</td>
<td>52.79</td>
<td>37.76</td>
</tr>
<tr>
<td>Homogeneous sandstone</td>
<td>1.992</td>
<td>13.35</td>
<td>8.04</td>
</tr>
</tbody>
</table>

Note that the quartz properties are set equal to those of quartzite since neither porosity nor grain anisotropy is modeled here. For sandstone, a Poisson’s ratio of 0.223 has been determined in quasi-static tensile simulations using a porous RVE. Using this Poisson’s ratio value and the measured Young’s modulus in acoustic tests, i.e. 23 GPa, the bulk modulus amounts to 14.03 GPa. In order to make the homogeneous sandstone model conform to the measured dynamic Young’s modulus in Split-Hopkinson-Bar experiments, both stiffness coefficients \(E\) and \(K\) are downscaled by the same factor. The stiffness contrast between homogeneous sandstone (13.35 GPa) and the RVE (23 GPa) has a negligible influence on the longitudinal wave speed since the RVE represents less than one percent of the whole specimen in length. This methodology, although open for improvements, presents the advantage that the wave signal simulated in the specimen mirrors experimental waves spatially and temporally.

5.2.4.2 Inter-granular failure model
Inter-granular failure is modeled with the Cohesive-Zone-Element formulation, as has been extensively addressed in Chapter 4. The purpose therewith is to model inter-granular failure adequately on the basis of a dissipating energy. This way, the dependency of the simulation results on the mesh size can be limited. For each type of material, a specific set of failure parameters \((T_{\text{meso}}^{\text{crit}}, C_{\text{meso}}^{\text{crit}})\) will be investigated within the frame of the parameter study. For practical reasons, when conducting the parameter study, the normal component \(T_{n,\text{meso}}^{\text{crit}}\) and the tangential
component $T_{t,meso}^{crit}$ of the mesoscopic cohesive law will be set equal to one single value, namely $T_{meso}^{crit}$.

Besides, the question of whether it is necessary to model contact of initially not contacted grain surfaces could be raised. In sandstone, as it contains pores, such contacts could occur under the incident compressive wave that precedes the reflected tensile wave. Nevertheless, the compressive strain levels achieved in sandstone do not exceed 0.1%. Moreover, tensile stresses are locally prevailing during the cracking process. Therefore, contact can reasonably be disregarded.

5.2.5 Numerical instrumentation

The numerical instrumentation covers two major aspects. On the one hand, it has to mimic the laboratory instrumentation, namely strain gauges and acceleration sensor, by delivering strain and velocity signals at identical locations in the specimen as in experiments. On the other hand, it employs further physically-based numerical methods that outperform the capability of the laboratory instrumentation. This way, the numerical instrumentation is able to deliver more accurate estimates of the physical parameters of interest. The variability in the results can subsequently be tested among the different methods used.

5.2.5.1 Measuring the macroscale dynamic tensile strength

Three different evaluation techniques for the macroscale dynamic tensile strength $T_{macro}^{crit}$ in the simulation model will be presented in the following. All three methods require the knowledge of the failure initiation time $t_{fail}$. This instant of time can be determined by Equation (5.8) knowing the RVE position, i.e. the crack position $x_c$, the wave length $C_{spe}$ in the specimen and, via the analysis of velocity profiles at the free end of the specimen, the pull-back time $t_{pb}$.

The first method (Method T1-theory) bases on elastic wave theory and makes use of the prescribed velocity wave and subsequent reflections in the specimen, to provide a theoretical stress value at the spatiotemporal locus $(x_c,t_{fail})$. To determine the number of reflections the elastic wave has experienced in the specimen at crack initiation, let the integer $n$ be
defined as the integer part of $\frac{t_{fail}}{C_{spe}}$. Then, the following inequation can be set up: $\frac{nL}{C_{spe}} \leq t_{fail} < \frac{(n+1)L}{C_{spe}}$ where $n$ corresponds to the number of wave reflections in the specimen. The theoretical velocity and stress acting at the crack location are then derived from Equations (2.54):

\[
U(x_c, t_{fail}) = \sum_{2k=0}^{n} \left( \alpha^k U_{bc} \left( t_{fail} - \frac{2kL + x_c}{C_{spe}} \right) \right) + \sum_{2k=0}^{n} \left( \alpha^k U_{bc} \left( t_{fail} - \frac{2(k + 1)L + x_c}{C_{spe}} \right) \right)
\]

(5.10a)

\[
\sigma(x_c, t_{fail}) = -\rho_{spe}C_{spe} \sum_{2k=0}^{n} \left( \alpha^k U_{bc} \left( t_{fail} - \frac{2kL + x_c}{C_{spe}} \right) \right) + \rho_{spe}C_{spe} \sum_{2k=0}^{n} \left( \alpha^k U_{bc} \left( t_{fail} - \frac{2(k + 1)L + x_c}{C_{spe}} \right) \right)
\]

(5.10b)

where: $\alpha = \frac{\rho_{spe}c_{spe} - \rho_{alu}c_{alu}}{\rho_{spe}c_{spe} + \rho_{alu}c_{alu}}$

Here, the impedance ratio relative to the right interface vanishes since the latter is a free surface.

The second method (Method T2-rve) solely catches the numerically averaged RVE stress $\sigma_{RVE}$ in the simulation at $t_{fail}$.

The third method (Method T3-exp) applies elastic wave theory on the free-end velocity profile $U_{AC}(t)$ that is recorded in the simulation. To evaluate $U_{AC}(t)$ over time in the simulation, history points are placed at the right free end of the specimen and their values are averaged. Again, an expression for the velocity at the free end at any time $t$ can be derived from Equation (2.54a):

\[
U_{AC}(t) = U(L, t) = 2 \sum_{2k=0}^{n} \left( \alpha^k U_{bc} \left( t - \frac{(2k + 1)L}{C_{spe}} \right) \right)
\]

(5.11)
Noteworthy is that the left-traveling and right-traveling waves induce the same velocity at the specimen free surface. In order to find a relationship between the free-end velocity and the velocity at the spatiotemporal locus \((x_c, t_{fail})\), the free-end velocity is evaluated at \(t_{fail} - \frac{L - x_c}{c_{spe}}\) and \(t_{fail} + \frac{L - x_c}{c_{spe}}\), respectively. From Equations (5.10) and (5.11), it turns out that:

\[
\sigma(x_c, t_{fail}) = \frac{\rho_{spe} c_{spe}}{2} \left( U_{AC} \left( t_{fail} - \frac{L - x_c}{c_{spe}} \right) - U_{AC} \left( t_{fail} + \frac{L - x_c}{c_{spe}} \right) \right) \tag{5.12}
\]

This formula, since it points out the difference of two free-end velocities at two instants of time, is reminiscent of Equation (5.3) which is used in the experiment. In Equation (5.12), both times in the right member are symmetric to each other with respect to \(t_{fail}\). The first term stands for the recorded signal at the free surface such that, after acoustic propagation in the specimen, its arrival time at the crack location is \(t_{fail}\). Symmetrically, the second term designates the pull-back signal originating from the crack at \(t_{fail}\) and arriving after acoustic propagation. Compared to Equation (5.3), Equation (5.12) presents the advantage that the tensile strength evaluated in the RVE is always correct, even though the crack location is enforced and does not necessarily match the expectable location of the very right crack in the experiment. In the quantitative analysis that will be conducted in subsection 5.3.2, Method T3-exp will be the reference method for calibrating the mesoscale critical traction \(T_{crit}^{meso}\).

The reason why Method T1-theory and Method T2-rve are employed is to check how far they match the reference method (Method T3-exp) and thus, whether they are legitimate.

5.2.5.2 Measuring the macroscale fracture energy
The macroscale fracture energy \(G_{crit}^{macro}\) is measured by four different techniques. The close-to-experiment method (Method G1-exp) tracks the spatial average velocities of the two separating fragments at two instants of time. The first time \(t_1\) corresponds to the failure initiation time \(t_{fail}\) while the second time \(t_2\) is associated to a full visual crack opening, or more practically, to the annihilation of the average RVE stress \(\sigma_{RVE}\). The spatial average velocity of each fragment is numerically determined by
performing a discrete averaging of node velocities. For this purpose, evaluation voxels, distributed all over the fragment length, are exploited. Their underlying principle will be explained in more detail in Chapter 6. The fracture energy \( G_{\text{exp}}^{\text{crit}} \) is then determined by applying Equation (5.4) to the numerically determined averaged velocities. This method will be taken as a reference for calibrating the mesoscale fracture energy \( G_{\text{meso}}^{\text{crit}} \).

The second method (Method G2-theory) compares the energy prevailing in the specimen at \( t_2 \), after full cracking, to the theoretical energy at \( t_2 \) if failure is inactive. The difference of both energies shall provide the energy dissipated by the failure process. To this, a complete energy balance, discarding the simplifications made in the Method G1-exp, is set up. The total energy can be decomposed into a kinetic energy and an internal energy contribution. The volumetric total energy \( e_{\text{tot}} \) at any spatio-temporal locus \((x,t)\) in the specimen is, assuming a pure elastic behavior and small strains, given by:

\[
e_{\text{tot}}(x,t) = e_{\text{kin}} + e_{\text{int}} = \frac{1}{2} \rho_{\text{spe}} U(x,t)^2 + \frac{1}{2} \sigma(x,t) \varepsilon(x,t)
\]  

where \( \sigma(x,t) \varepsilon(x,t) = \frac{\sigma(x,t)^2}{\rho_{\text{spe}} c_{\text{spe}}^2} \).

Integration over the specimen length provides a surface-specific total energy:

\[
E_{\text{tot}}(t) = \frac{1}{2} \rho_{\text{spe}} \int_0^L U(x,t)^2 \, dx + \frac{1}{2} \rho_{\text{spe}} c_{\text{spe}}^2 \int_0^L \sigma(x,t)^2 \, dx 
\]  

In numerical simulations in which failure occurs, both velocity \( U(x,t) \) and stress \( \sigma(x,t) \) profiles are provided by history variables. In theoretical analysis, in which failure is disregarded, velocity and stress profiles are provided by the mathematical expressions (2.54a) and (2.54b). The dynamic fracture energy \( G_{\text{theory}}^{\text{crit}} \) is then computed as the difference between the virtual total energy of an intact specimen at \( t_2 \) and the actual total energy of the failed specimen at \( t_2 \):

\[
G_{\text{theory}}^{\text{crit}} = E_{\text{tot}}^{\text{intact}}(t_2) - E_{\text{tot}}^{\text{failed}}(t_2)
\]
By comparing the expression of the theoretical fracture energy via Equations (5.14) and (5.15) and that of the experimental one described by Equation (5.4), the simplifications made in the experimental analysis can be pointed out. First, $G_{\text{crit}}^\text{exp}$ disregards internal energy and only considers kinetic energy as though the two fragments were rigid bodies. Second, $G_{\text{crit}}^\text{exp}$ calculates the kinetic energy on the basis of a spatially-averaged velocity, thus assuming that the velocity of each fragment is spatially homogenous. Lastly, the energetic variations induced by the still contacting incident bar at the incident bar-specimen interface between $t_1$ and $t_2$ should be subtracted from the experimental energy balance. The evaluation of the experimental energy at the failure initiation time ($t_1 = t_{\text{fail}}$) rather than at the full failure time ($t_2$) would be appropriate if the two fragments would constitute an isolated system, in which no more external energy were supplied to the specimen in the time slot $[t_1, t_2]$.

The third method (Method G3-rve) focuses on the crack location and consists in integrating the average RVE stress $\sigma_{\text{RVE}}$ over the RVE elongation $\delta_{\text{RVE}}$ between $t_1$ and $t_2$. Since the initial RVE length $L_{\text{RVE}}$ is negligible with respect to the involved wave lengths, the RVE elongation $\delta_{\text{RVE}}$ can be assimilated to the actual crack opening $\delta_{\text{crack}}$. This method presents the advantage that stress and displacement are evaluated in the direct vicinity of the crack and thus does not need to consider the velocity distribution throughout the specimen.

The last method (Method G4-cohesive) uses the intrinsic variable in the hydrocode SOPHIA that cumulates local dissipated energies relatively to the expansion and the extinction of cohesive zone elements. This method also accounts for localized interrupted cracks that do not contribute to the macroscopic transverse crack, see Figure 5.13.
Figure 5.13: Schematic view of a sandstone RVE (middle) with a visible macroscopic crack and partially opened cracks. The macroscopic crack is associated to a series of full damaged cohesive zone elements (left), while partially opened cracks are associated to partially damaged cohesive zone elements (right).

In order to harmonize all fracture energy definitions, the fracture energy computed with Method G4-cohesive is normalized by the planar cross-section of the RVE, even though the real fracture pattern is highly non-planar and irregular, especially in sandstone. Mathematically, this is expressed by:

$$
G_{\text{cohesive}}^{\text{crit}} = \sum_k D_k G_{\text{meso}}^{\text{crit}} \frac{S_k}{S_{\text{section}}} \tag{5.16}
$$

where $k$ is an index running over all activated and extinguished cohesive zone elements, $D_k$ and $S_k$ are respectively, the damage and mid-surface area of the $k$-th cohesive zone element, and $S_{\text{section}}$ is the cross-sectional area of the RVE.

Although Method G1-exp mirrors the experimental analysis, its physical validity is called into question, as has been pointed out by Method G2-theory. The latter method, as well as the numerically-based methods, G3-rve and G4-cohesive, shall thus provide macroscale fracture energy values that are closer to physics. Accordingly, discrepancies between the experimentally-based evaluation and the latter three ones will be brought forward in the quantitative analysis in subsection 5.3.2.
5.2.6 Parameter study setup

The parameter study presented in the following is aimed at showing the dependence and sensitivity of the macroscopic response with respect to mesoscale parameters. A set of mesoscale parameters, for which the equivalent macroscopic response replicates the experimental measurement satisfactorily, is selected. The mesoscale parameters that are varied are related to the cohesive zone formulation, namely the mesoscale critical traction $T_{\text{meso}}^{\text{crit}}$ and the mesoscale fracture energy $G_{\text{meso}}^{\text{crit}}$.

In order to start the parameter calibration with relevant mesoscale values, some intuitive analysis is carried out. For this purpose, separate hypotheses are adopted for quartzite and sandstone due to their differences in nature. For quartzite, the interval of variation $T_{\text{meso}}^{\text{crit}}$ is set below the experimental tensile strength. The reason is that inertial effects delay the actual failure initiation and consequently raise the macroscale tensile strength. The macroscale fracture energy, as it might involve secondary cracks aside from the main macroscopic crack, tends to overestimate its mesoscale counterpart. Therefore, it is relevant to investigate quartzite $G_{\text{meso}}^{\text{crit}}$ values that are smaller than the experimental values. In sandstone, however, the porosity weakens the tensile strength of the material and considerably reduces the available internal surfaces across a cross-section. In this regard, the investigation of $T_{\text{meso}}^{\text{crit}}$ and $G_{\text{meso}}^{\text{crit}}$ values that overrate the experimental values is of relevance. The set of mesoscale parameters varied in the parameter study are summarized for each rock type in Table 5.3.

Table 5.3: Set of parameters varied for the mesoscale critical traction $T_{\text{meso}}^{\text{crit}}$ and the mesoscale fracture energy $G_{\text{meso}}^{\text{crit}}$, for both quartzite and sandstone.

<table>
<thead>
<tr>
<th>Rock type</th>
<th>Critical traction $T_{\text{meso}}^{\text{crit}}$ [MPa]</th>
<th>Fracture energy $G_{\text{meso}}^{\text{crit}}$ [N/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quartzite</td>
<td>6 – 10 by steps of 1</td>
<td>10 – 100 by steps of 10</td>
</tr>
<tr>
<td>Sandstone</td>
<td>6 – 12 by steps of 1</td>
<td>160 – 440 by steps of 40</td>
</tr>
</tbody>
</table>
5.3 Numerical results and interpretation

A qualitative analysis of failure mechanisms occurring at the RVE level will be conducted before the quantitative evaluation of results. Stress concentrations within quartz grains and the rate of damage progress at grain interfaces will be highlighted. The following detailed quantitative analysis of stress waves and dissipative fracture energy shall provide equivalent macroscale properties. Due to their different geological nature, quartzite and sandstone are modeled with different mesoscale parameter sets and are analyzed separately.

5.3.1 Qualitative analysis

For the sake of clarity, the qualitative analysis is, for each material, focused on one fixed set of mesoscale parameters. This condensed analysis is aimed at reporting on general features pertaining to the Split-Hopkinson-Bar-Tests in a straightforward manner.

5.3.1.1 Quartzite specimen

For quartzite, the selected set of mesoscale parameters is given by: $T_{\text{meso}}^{\text{crit}}$ = 7 MPa and $G_{\text{meso}}^{\text{crit}}$ = 30 N/m. Figure 5.14 shows a series of six snapshots focused on the RVE and its immediate vicinity at six different instants of time. The upper part of the picture represents a color coding of the longitudinal stress in the specimen. The lower part highlights damage footprints relatively to emerging and developing cohesive zone elements. In order to convey a better perception of the current state within the continuous failure process, a temporal RVE stress diagram, in which the current instant of time is emphasized, is embedded in each snapshot.
Figure 5.14: Snapshots of quartzite focused on the crack area at six different failure stages. Top: longitudinal stress contours. Bottom: only cohesive zone elements are displayed with damage contours. In the left-lower part of each snapshot, a temporal RVE stress diagram is plotted, in which the current time is highlighted by a red dot.
The first snapshot highlights stress inhomogeneities just before macroscopic failure sets in. These are attributed to localized activation of cohesive zones, thus inducing local wave reflections within quartz grains. The longitudinal stress is limited by the prescribed mesoscale critical traction in the vicinity of grain boundaries but may exceed 15 MPa in the core of grains. In the second snapshot, tensile stresses get degraded concomitantly with advancing damage. A pale stripe in the middle of the RVE indicates a stress release induced by an emerging but not yet visible crack. The third snapshot stands for a highly advanced decohesion phase, in which a full cross-sectional footprint of highly damaged cohesive zone elements can be observed. In the fourth and fifth snapshots, a large amount of cohesive zones is deleted after they reached complete damage and a macroscopic crack emerges. The last snapshot depicts an ultimate stage beyond the fracturing time range, in which the macroscopic crack pattern is consolidated. Few cohesive zones still exist, however, the damage is so high that they do not carry considerable further inter-granular forces.

5.3.1.2 Sandstone specimen
For sandstone, the selected set of mesoscale parameters is given by: $T_{\text{meso}}^{\text{crit}} = 7$ MPa and $G_{\text{meso}}^{\text{crit}} = 280$ N/m. Again, six snapshots are represented in Figure 5.15.
Figure 5.15: Snapshots of sandstone focused on the crack area at six different failure stages. Top: longitudinal stress contours. Bottom: only cohesive zone elements are displayed with damage contours. In the left-lower part of each snapshot, a temporal RVE stress diagram is plotted in which the current time is highlighted by a red dot.
The first snapshot is taken well before the onset of failure. The visible stress variations are caused by the porous nature of sandstone. In the second snapshot, macroscopic failure has just begun and is accompanied by high tensile stress concentrations in the core of quartz grains. The third and fourth snapshots illustrate stages of low and advanced damage, respectively. There, tensile stresses degrade and compressive areas develop locally as a result of wave reflections at free grain boundaries. No distinct crack pattern can be distinguished since the macroscopic release wave is diluted in the network of these free surface reflections. The fifth snapshot corresponds to a highly advanced decohesion phase in which stresses are mostly annihilated. The last snapshot displays the consolidated macroscopic crack pattern at a late instant of time, it also indicates a few remaining cohesive zone elements, the stiffness of which is vanishing.

5.3.2 Quantitative analysis

Owing to the homogenization methodology introduced in subsection 5.2.5, each set of mesoscale parameters delivers, for each evaluation method, a macroscale tensile strength and a macroscopic fracture energy. By compiling all macroscale parameters together, inter-scale relationships can be explicitly set up. As an example, the influence of the mesoscale critical traction on its macroscopic counterpart at fixed mesoscale fracture energy will be assessed. The strengths and weaknesses of the different homogenization techniques will also be discussed in the quantitative analysis.

5.3.2.1 Quartzite specimen

In order to gain insight into the evolving stress acting at the crack location prior to, during and after the cracking process, longitudinal RVE stress profiles are plotted over time for a variety of mesoscale parameters. The reference parameter set is $T_{\text{meso}}^{\text{crit}} = 8 \text{ MPa}$ and $G_{\text{meso}}^{\text{crit}} = 50 \text{ N/m}$. In Figure 5.16-left, the mesoscale critical traction $T_{\text{meso}}^{\text{crit}}$ is varied at fixed mesoscale fracture energy $G_{\text{meso}}^{\text{crit}}$, while in Figure 5.16-right, this is the other way round. A non-failing case is adjoined to the diagram for comparison.
Figure 5.16: Longitudinal RVE stress profiles in quartzite over time. Left: fixed \( G_{\text{meso}}^{\text{crit}} = 50 \text{ N/m} \) and varying \( T_{\text{meso}}^{\text{crit}} \) from 6 MPa to 10 MPa. Right: fixed \( T_{\text{meso}}^{\text{crit}} = 8 \text{ MPa} \) and varying \( G_{\text{meso}}^{\text{crit}} \) from 10 N/m to 90 N/m.

Noticeably, the achieved tensile stresses increase with increasing \( T_{\text{meso}}^{\text{crit}} \) values. This finding is intuitive since higher \( T_{\text{meso}}^{\text{crit}} \) values delay the activation of cohesive zone elements and, subsequently, the onset of fracturing on the macroscale. At a fixed \( T_{\text{meso}}^{\text{crit}} \) value, the macroscopic stress peak remains constant but is followed by a gentler softening, the higher \( G_{\text{meso}}^{\text{crit}} \) is. Indeed, high fracture energies are associated with long dissipation processes to achieve full cracking. Incidentally, it must be emphasized that the observable macroscopic peak stress does not strictly mirror the macroscale tensile strength \( T_{\text{macro}}^{\text{crit}} \). As a plausible explanation for this, inertial effects related to wave mechanics tend to further raise the RVE stress in the few instants of time following failure initiation. A proper determination of \( T_{\text{macro}}^{\text{crit}} \) is, as outlined in paragraph 5.2.5.1, supported by the evaluation of the actual failure initiation time \( t_{\text{fail}} \) via the analysis of the pull-back velocity profile.

Figure 5.17 gives a representation of the free-end velocity signals for the same variations of parameter sets as previously. Note the kink-up during the velocity release phase, which is due to cracking and indicates the arrival time \( t_{\text{pb}} \) of the release wave at the specimen free end, also called pull-back time, see again Figure 5.5.
Figure 5.17-left shows that the pull-back time increases with growing $T_{\text{meso}}^{\text{crit}}$ values. Since failure initiation is delayed at higher $T_{\text{meso}}^{\text{crit}}$ values, so is the emergence of the release wave at the crack location. Figure 5.17-right shows a good agreement of all $t_{pb}$ values if $T_{\text{meso}}^{\text{crit}}$ is fixed. Obviously, the macroscale tensile strength $T_{\text{macro}}^{\text{crit}}$ according to Method T3-exp, see again Equations (5.12) and (5.8), is not sensitive to variations of $G_{\text{meso}}^{\text{crit}}$.

In the following, the influence of the mesoscale parameter set $(T_{\text{meso}}^{\text{crit}}, G_{\text{meso}}^{\text{crit}})$ on the macroscale tensile strength $T_{\text{macro}}^{\text{crit}}$ is evaluated. The reference mesoscale set $T_{\text{meso}}^{\text{crit}} = 8 \text{ MPa}$ and $G_{\text{meso}}^{\text{crit}} = 50 \text{ N/m}$ is used again. Figure 5.18-left represents, for each of the three methods presented in paragraph 5.2.5.1, $T_{\text{macro}}^{\text{crit}}$ values as a function of $G_{\text{meso}}^{\text{crit}}$ at different $T_{\text{meso}}^{\text{crit}}$ values. Reversely, Figure 5.18-right represents $T_{\text{macro}}^{\text{crit}}$ values as a function of $T_{\text{meso}}^{\text{crit}}$ at different $G_{\text{meso}}^{\text{crit}}$ values.
The three evaluation methods T1-T2-T3 show a very good accordance with each other, since they all refer to a more or less direct evaluation of the RVE stress at \( t_{\text{fail}} \). The Method T1-theory, which calculates a pure theoretical stress without resorting to the simulation model, slightly overestimates the two other ones. This slight discrepancy can be attributed to the emergence of small defects in the specimen prior to \( t_{\text{fail}} \) which, although not noticeably affecting wave mechanics, tends to attenuate the macroscopic tensile stress in the simulation when compared to a non-failing specimen.

The increasing trend of \( T_{\text{crit,macro}} \) with growing \( T_{\text{crit,meso}} \) values, see Figure 5.18-left, confirms the intuitive finding relative to the RVE stress profile analysis from Figure 5.16-left. Besides, the analysis of Figure 5.18-right corroborates the aforementioned observation in Figure 5.16-right for which \( T_{\text{macro}} \) remains approximately constant when \( G_{\text{meso}} \) varies. Energy dissipation mechanisms pertaining to local decohesion processes play a very limited role here since only failure initiation is considered.

In order to impart a better overview of the combined effects of both mesoscale \( T_{\text{crit,meso}} \) and \( G_{\text{meso}} \) parameters on the macroscale tensile strength, the function \( T_{\text{crit,macro}}(G_{\text{meso}}) \) is represented in Figure 5.19 for...
different $T_{\text{crit}}^{\text{meso}}$ values. To this, only the reference Method T3-exp is considered.

The tendencies observed in the diagrams in Figure 5.18 are confirmed in Figure 5.19. Since the mesoscale fracture energy hardly affects the macroscale tensile strength, the calibration of the correct $T_{\text{crit}}^{\text{meso}}$ value can be made independently of $G_{\text{crit}}^{\text{meso}}$. The case $T_{\text{crit}}^{\text{meso}} = 10$ MPa delivers a macroscale tensile strength $T_{\text{crit}}^{\text{macro}}$ which roughly equals the experimental average $T_{\text{exp}}^{\text{crit}} = 16.7$ MPa. This value will be considered the calibrated value of the mesoscale critical traction $T_{\text{meso}}^{\text{crit}}$. Note that the macroscale tensile strength is always higher than its mesoscopic counterpart. This finding is in accordance with the prediction made in the parameter study setup, see again subsection 5.2.6.

The second important aspect to investigate is the influence of the mesoscale parameter set $(T_{\text{crit}}^{\text{meso}}, G_{\text{crit}}^{\text{meso}})$ on the macroscale fracture energy $G_{\text{macro}}$. Figure 5.20 represents, for each of the four methods presented in paragraph 5.2.5.2, the functions $G_{\text{macro}}(T_{\text{crit}}^{\text{meso}})$ and $G_{\text{macro}}(G_{\text{meso}}^{\text{crit}})$, respectively. The mesoscale set $T_{\text{meso}}^{\text{crit}} = 8$ MPa and $G_{\text{meso}}^{\text{crit}} = 50$ N/m is further taken as reference.
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Figure 5.20: Macroscale fracture energy $G_{macro}^{crit}$ in quartzite according to four determination methods. Left: fixed $G_{meso}^{crit} = 50 \text{ N/m}$ and varying $T_{meso}^{crit}$ from 6 MPa to 10 MPa. Right: fixed $T_{meso}^{crit} = 8 \text{ MPa}$ and varying $G_{meso}^{crit}$ from 10 N/m to 100 N/m. The average and standard deviation of the experimentally determined fracture energy are also depicted.

Figure 5.20-left shows that $G_{macro}^{crit}$ is more or less independent of $T_{meso}^{crit}$ up to about 9 MPa. For higher $T_{meso}^{crit}$ values, however, the $G_{macro}^{crit}$ function, according to Method G1-exp, exhibits a declining trend. This is due to the reduction of critical separation values $\delta_{meso}^{crit}$ in cohesive zone elements when $T_{meso}^{crit}$ increases and $G_{meso}^{crit}$ is kept constant. As a consequence, the material behaves more and more brittle and fewer secondary cracks arise, meaning that less energy is dissipated by the cracking process. Methods G2-G3-G4 show a somewhat more constant behavior in $G_{macro}^{crit}$ with varying $T_{meso}^{crit}$ values since $G_{meso}^{crit}$ variations do not outreach $\pm 25 \text{ N/m}$. Furthermore, they all remain close to and do not diverge from each other by more than 60 N/m. Figure 5.20-right shows the dependence of $G_{macro}^{crit}$ on $G_{meso}^{crit}$ at a fixed $T_{meso}^{crit}$ value. For all four methods, a monotonic increasing behavior is expectedly observed since an increase in local fracture energy naturally raises the macroscale fracture energy.

An overview of the combined influence of $T_{meso}^{crit}$ and $G_{meso}^{crit}$ on $G_{macro}^{crit}$ is sketched in Figure 5.21. The Method G1-exp and Method G4-cohesive are respectively depicted on the Figure 5.21-left and Figure 5.21-right. As already mentioned in paragraph 5.2.5.2, the former method is the reference method used for calibrating $G_{meso}^{crit}$ while the latter method is
relatively close to physics. Method G4-cohesive accounts for the total energy dissipated by cohesive zone elements, including partially damaged cohesive zone elements.

The diagrams show for both evaluation methods that \( G_{\text{macro}}^\text{crit} \) declines when \( T_{\text{meso}}^\text{crit} \) and \( G_{\text{meso}}^\text{crit} \) are conjointly high. As already evidenced above, the material adopts a brittle behavior when \( T_{\text{meso}}^\text{crit} \) increases at fixed \( G_{\text{meso}}^\text{crit} \) values. At lower \( G_{\text{meso}}^\text{crit} \) values, this declining trend is less prominent. Indeed, the brittleness imparted by growing \( T_{\text{meso}}^\text{crit} \) values becomes imperceptible compared to the brittleness already present in a material with a low mesoscale fracture energy. Besides, the ascending behavior of \( G_{\text{macro}}^\text{crit} \) with growing \( G_{\text{meso}}^\text{crit} \) values at fixed \( T_{\text{meso}}^\text{crit} \) values is confirmed in Figure 5.21 for both evaluation methods. However, this tendency is not valid any more at higher \( T_{\text{meso}}^\text{crit} \) values in Method G1-exp and may be attributed to deficiencies pertaining to Method G1-exp, see the excursus in the next paragraph. Another finding is that the amount of dissipative energy according to Method G4-cohesive permanently exceeds the mesoscale fracture energy. This finding corroborates the hypothesis that the macroscopic failure surface extends over more than a smooth planar cross-section. In the investigated mesoscale parameter range, the macroscale fracture energy varies between 30 and 240 N/m. Departing from the already calibrated traction value \( T_{\text{meso}}^\text{crit} = 10 \) MPa, the mesoscale fracture energy
energy $G_{meso}^{crit}$ must be selected such that its macroscopic counterpart approximates the experimental average $G_{exp}^{crit} = 180$ N/m. Because of the decline of $G_{macro}^{crit}$ in the range of 10 MPa, the maximum macroscale fracture energy is achieved for $G_{meso}^{crit} = 50$ N/m and amounts to 145 N/m according to Method G1-exp. In this respect, the value of 50 N/m will be considered the calibrated value of the mesoscale fracture energy $G_{meso}^{crit}$. The associated $G_{macro}^{crit}$ value according to Method G4-cohesive is 111 N/m.

5.3.2.2 Excursus: about the accuracy of evaluating the macroscale fracture energy in the simulation

In order to gain more insight into the non-stable nature of the macroscale fracture energy according to Method G1-exp, the bounds of the time window $(t_1, t_2)$, which have been defined at the beginning of paragraph 5.2.5.2 and within which stress integration is conducted, are set as variables. Accordingly, two mono-variable functions $G_{macro}^{crit}(t_1)$ at fixed $t_2$ and $G_{macro}^{crit}(t_2)$ at fixed $t_1$ are set up. Figure 5.22 shows both function plots for an exemplary set $T_{meso}^{crit} = 8$ MPa and $G_{meso}^{crit} = 60$ N/m.

![Figure 5.22: Fictive macroscale fracture energy $G_{macro}^{crit}$ as a function of $t_1$ at fixed $t_2=200$ µs (left) and fracture energy as a function of $t_2$ at fixed $t_1 = t_{fail}$ (right). On the left diagram, energy evaluations according to Methods G1-exp and G3-rve are represented. Negative, unphysical energy values according to Method G1-exp have been removed from the diagram. On the right diagram, all four energy methods are represented from $t_2 = t_{fail}$. The RVE stress profile is additionally plotted with the right vertical axis for reference.](image-url)
When the time $t_2$ of supposed full cracking is fixed, the macroscale fracture energy according to Method G1-exp shows a high sensitivity to $t_1$ values in the vicinity of $t_{fail}$. For the mesoscale parameter set considered here, $G_{macro}^{crit}$ according to Method G1-exp takes the value 200 N/m at $t_1 = t_{fail}$, see Figure 5.22-left, but deviates by $\pm$ 25 N/m for $t_1$ values varying by $\pm$ 1 $\mu$s. In this time slot, however, the $G_{macro}^{crit}$ values computed using Method G3-rve keep a quite constant level of 138 N/m $\pm$ 1 N/m. These observations confirm the robustness of Method G3-rve when compared to Method G1-exp. When the full cracking time is set as a variable, see Figure 5.22-right, all four methods exhibit constant $G_{macro}^{crit}$ values from the $t_2$ value which corresponds to the RVE stress annihilation. This finding demonstrates that the energy integration up to late instants of time, i.e. beyond the effective fragment separation, does not affect the assessment of the macroscale fracture energy. Indeed, no more energy is dissipated during the post-failure process.

5.3.2.3 Sandstone specimen
As for quartzite, temporal RVE stress profiles are plotted for sandstone by varying the set of mesoscale parameters, see Figure 5.23. Here, the reference parameter set is $T_{meso}^{crit} = 8$ MPa and $G_{meso}^{crit} = 320$ N/m.

![Figure 5.23](image-url)

Figure 5.23: Longitudinal RVE stress profiles in sandstone over time. Left: fixed $G_{meso}^{crit} = 320$ N/m and varying $T_{meso}^{crit}$ from 6 MPa to 10 MPa. Right: fixed $T_{meso}^{crit} = 8$ MPa and varying $G_{meso}^{crit}$ from 240 N/m to 400 N/m.
Previously analyzed features for quartzite are also noticeable for sandstone, such as the increase of the maximum tensile stress with growing $T_{meso}^{crit}$ values and its constancy if $T_{meso}^{crit}$ is fixed and $G_{meso}^{crit}$ varies. The dependency of the softening behavior on $G_{meso}^{crit}$ is, although less pronounced than in quartzite, perceptible. In Figure 5.24, free-end velocity profiles are shown using the same set of mesoscale parameters.

![Figure 5.24: Free-end velocity profiles in sandstone over time. Left: fixed $G_{meso}^{crit} = 320 \text{ N/m}$ and varying $T_{meso}^{crit}$ from 6 MPa to 10 MPa. Right: fixed $T_{meso}^{crit} = 8 \text{ MPa}$ and varying $G_{meso}^{crit}$ from 240 N/m to 400 N/m.](image)

Again, the velocity kink-up, which is characteristic of the arrival of the release wave, occurs later, the higher $T_{meso}^{crit}$ is.

The behavior of the macroscale tensile strength with respect to the mesoscale parameter set ($T_{meso}^{crit}, G_{meso}^{crit}$) is sketched in Figure 5.25 at fixed $G_{meso}^{crit}$ (left) and fixed $T_{meso}^{crit}$ (right), respectively. The reference parameter set is kept unchanged.
Figure 5.25: Macroscale tensile strength $T_{macro}^{crit}$ in sandstone according to three determination methods. Left: fixed $G_{meso}^{crit} = 320 \text{ N/m}$ and varying $T_{meso}^{crit}$ from 6 MPa to 12 MPa. Right: fixed $T_{meso}^{crit} = 8 \text{ MPa}$ and varying $G_{meso}^{crit}$ from 160 N/m to 440 N/m. The average and standard deviation of the experimentally determined tensile strength are also depicted.

As for quartzite, the macroscale tensile strength $T_{macro}^{crit}$ is a growing function of its mesoscopic counterpart. The three methods T1-T2-T3 show very similar $T_{macro}^{crit}$ values and do not deviate from each other by more than 0.3 MPa. Figure 5.25-right confirms once again the quasi-independence of $T_{macro}^{crit}$ on $G_{meso}^{crit}$.

Figure 5.26 gives for Method T3-exp a more complete representation of the function $T_{macro}^{crit}(G_{meso}^{crit})$ for different $T_{meso}^{crit}$ values.
Figure 5.26: Macroscale tensile strength $T_{\text{macro}}^{\text{crit}}$ in sandstone as a function of $G_{\text{meso}}^{\text{crit}}$ for different $T_{\text{meso}}^{\text{crit}}$ values using Method T3-exp. The average and standard deviation of the experimentally determined tensile strength are also depicted.

The negligible variations of $T_{\text{macro}}^{\text{crit}}$ with respect to $G_{\text{meso}}^{\text{crit}}$ are validated in Figure 5.26. To conform to the experimental average traction $T_{\text{exp}}^{\text{crit}} = 5.5$ MPa, a mesoscale value $T_{\text{meso}}^{\text{crit}} = 10$ MPa has to be opted for. Remarkably, the macroscale tensile strength always lies underneath its mesoscopic counterpart, which is opposite to the findings for quartzite. As prognosticated in subsection 5.2.6, brittle inter-granular interfaces due to the porous nature of sandstone are responsible for a global lowering of the macroscale tensile strength.

The dependency of the macroscale fracture energy $G_{\text{macro}}^{\text{crit}}$ on the mesoscale parameter set $(T_{\text{meso}}^{\text{crit}}, G_{\text{meso}}^{\text{crit}})$ is investigated in the following. Figure 5.27 represents the functions $G_{\text{macro}}^{\text{crit}}(T_{\text{meso}}^{\text{crit}})$ and $G_{\text{macro}}^{\text{crit}}(G_{\text{meso}}^{\text{crit}})$ by keeping the aforementioned reference mesoscale set.
Figure 5.27: Macroscale fracture energy $G^{\text{macro}}_{\text{crit}}$ in sandstone according to four determination methods. Left: fixed $G^{\text{meso}}_{\text{crit}} = 320 \text{ N/m}$ and varying $T^{\text{meso}}_{\text{crit}}$ from 6 MPa to 12 MPa. Right: fixed $T^{\text{meso}}_{\text{crit}} = 8 \text{ MPa}$ and varying $G^{\text{meso}}_{\text{crit}}$ from 160 N/m to 440 N/m. The average and standard deviation of the experimentally determined fracture energy are also depicted.

In contrast to quartzite, the macroscale fracture energy according to Method G1-exp shows a global ascending behavior, apart from some local variations. Again, the role played by porosity can be put forward. At low $T^{\text{meso}}_{\text{crit}}$ values, the low amount of available internal crack surfaces leads to stress concentrations which call a rapid macroscopic crack forth. At higher $T^{\text{meso}}_{\text{crit}}$ values, the macroscopic failure is postponed and is in favor of the emergence of additional irregular, non-planar crack surfaces, thus raising the macroscale fracture energy. The increase of $G^{\text{macro}}_{\text{crit}}$ according to Methods G2-G3-G4 is also noticeable but less pronounced than in Method G1-exp. The three methods G2-G3-G4 show mutual deviations not exceeding 20 N/m and own variations limited to 30 N/m. At fixed $T^{\text{meso}}_{\text{crit}}$, the macroscale fracture energy monotonically increases with $G^{\text{meso}}_{\text{crit}}$ for all four methods and thus comes along with the physical intuition. An extensive representation of $G^{\text{macro}}_{\text{crit}}$ as a function of $(T^{\text{meso}}_{\text{crit}}, G^{\text{meso}}_{\text{crit}})$ is provided in Figure 5.28 for Method G1-exp and Method G4-cohesive.
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Figure 5.28: Macroscale fracture energy $G_{\text{macro}}^{\text{crit}}$ in sandstone as a function of $T_{\text{meso}}^{\text{crit}}$ for different $G_{\text{meso}}^{\text{crit}}$ values. Left: Method G1-exp. Right: Method G4-cohesive. The average and standard deviation of the experimentally determined fracture energy are also depicted.

The growing trend of $G_{\text{macro}}^{\text{crit}}$ with increasing $G_{\text{meso}}^{\text{crit}}$ values is confirmed in Figure 5.28 at any fixed $T_{\text{meso}}^{\text{crit}}$ value for both methods. Note that $G_{\text{meso}}^{\text{crit}}$ values in sandstone considerably underrate their mesoscopic counterparts in contrast to quartzite, as has been prognosticated in the parameter study setup. Again, the porosity and structure topology in sandstone offer a reduced amount of internal surfaces and thus are in favor of this drastic energy reduction. Within the investigated mesoscale parameter range, the macroscale fracture energy according to Method G4-cohesive fall within an amplitude interval of 70 N/m. The calibration of the mesoscale fracture energy $G_{\text{meso}}^{\text{crit}}$ is now carried out on the basis of the already calibrated critical traction $T_{\text{meso}}^{\text{crit}} = 10$ MPa. From the analysis of iso-$G_{\text{meso}}^{\text{crit}}$ profiles, see Figure 5.28-left, it turns out that a reasonable calibration to the experimental average $\bar{G}_{\text{exp}}^{\text{crit}} = 160$ N/m is achieved by defining $G_{\text{meso}}^{\text{crit}} = 240$ N/m. The associated $G_{\text{macro}}^{\text{crit}}$ value according to Method G4-cohesive is 78 N/m.

More generally, it can be noticed that the changes of macroscale fracture energy, due to variations of the mesoscale set $(T_{\text{meso}}^{\text{crit}}, G_{\text{meso}}^{\text{crit}})$, are smaller in sandstone than they are in quartzite, indistinctively of the evaluation method employed. This trend qualitatively corroborates the standard deviations of $G_{\text{exp}}^{\text{crit}}$ measured in experiments, which are 120 N/m and 40 N/m for quartzite and sandstone, respectively.
5.4 Summary: main findings

In this chapter, a new mesoscale model has been developed that adequately represents geometry and boundary conditions for Split-Hopkinson-Bar-Tests in spallation configuration. The purpose therewith has been to determine a set of failure-related parameters on the mesoscale that correctly describes inter-granular failure, i.e. the decohesion process between quartz grains in quartzite and sandstone, under dynamic tensile loading. The two mesoscale unknown parameters, which are related to the cohesive zone formulation, are the critical traction \( T^\text{crit}_{\text{meso}} \) and the fracture energy \( G^\text{crit}_{\text{meso}} \). Since only macroscale failure quantities, i.e. the dynamic tensile strength \( T^\text{crit}_{\text{macro}} \) and the dynamic fracture energy \( G^\text{crit}_{\text{macro}} \), can be measured in the experiment, macroscale equivalent properties have been evaluated using an equivalent numerical instrumentation in order to enable a direct comparison with experimental data. By varying the mesoscale failure parameters over a user-defined interval, a parameter study has been conducted to achieve the best satisfying fit between the numerical and experimental macroscopic quantities. To ensure a proper calibration, the macroscale quantities have been evaluated not only on the same basis as the experimental instrumentation, but also via the use of additional evaluation methods closer to physics. The latter methods have been intended to test the validity of the experimental evaluation methods.

It has been shown that the three evaluation methods for determining the macroscopic tensile strength deliver \( T^\text{crit}_{\text{macro}} \) values that are in good accordance with each other. This finding confirms the validity of the experimental analysis of the dynamic tensile strength, which is represented in the simulation model by Method T3-exp. As regards the macroscopic fracture energy, the three physically-based methods show that \( T^\text{crit}_{\text{macro}} \) values are in quite good agreement with each other, but also all considerably diverge from those computed by the experimentally-based method. Limitations related to the latter method have been pointed out in this chapter. While the experimentally-based evaluation needs to be taken as reference for calibration purposes, the \( G^\text{crit}_{\text{macro}} \) values that physically describe the dissipating failure energy in quartzite and sandstone are those computed by Method G4-cohesive.
Table 5.4 summarizes the $T_{\text{meso}}^{\text{crit}}$ and $G_{\text{meso}}^{\text{crit}}$ parameters that have been calibrated on the basis of the averaged values of experimental data $T_{\text{exp}}^{\text{crit}}$ and $G_{\text{exp}}^{\text{crit}}$, as well as the macroscopic values $T_{\text{macro}}^{\text{crit}}$ and $G_{\text{macro}}^{\text{crit}}$ that have been evaluated by Methods T3-exp and G4-cohesive.

Table 5.4: Summary of mesoscale parameters $T_{\text{meso}}^{\text{crit}}$ and $G_{\text{meso}}^{\text{crit}}$ calibrated for quartzite and sandstone on the basis of the averaged values of experimental data $T_{\text{exp}}^{\text{crit}}$ and $G_{\text{exp}}^{\text{crit}}$, and derivation of the physically-based macroscopic failure quantities according to Methods T3-exp ($T_{\text{macro}}^{\text{crit}}$) and G4-cohesive ($G_{\text{macro}}^{\text{crit}}$).

<table>
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<th>Parameter</th>
<th>Quartzite</th>
<th>Sandstone</th>
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<tbody>
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<td>10</td>
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<tr>
<td>Mesoscale fracture energy $G_{\text{meso}}^{\text{crit}}$ [N/m]</td>
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<td>240</td>
</tr>
<tr>
<td>Critical separation $\delta_{\text{meso}}^{\text{crit}}$ [mm]</td>
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<td>0.048</td>
</tr>
<tr>
<td>Experimental average tensile strength $T_{\text{exp}}^{\text{crit}}$ [MPa]</td>
<td>16.7</td>
<td>5.5</td>
</tr>
<tr>
<td>Experimental average fracture energy $G_{\text{exp}}^{\text{crit}}$ [N/m]</td>
<td>180</td>
<td>160</td>
</tr>
<tr>
<td>Macroscopic tensile strength $T_{\text{macro}}^{\text{crit}}$ using Method T3-exp [MPa]</td>
<td>16.7</td>
<td>5.5</td>
</tr>
<tr>
<td>Macroscopic fracture energy $G_{\text{macro}}^{\text{crit}}$ using Method G4-cohesive [N/m]</td>
<td>111</td>
<td>78</td>
</tr>
</tbody>
</table>
In this chapter, the focus is set on compressive shock loading in quartzite and sandstone on the mesoscale. First, a literature review focusing on standard shock data of quartzite and sandstone is given in section 6.1. A mesoscale model setup inspired by Planar-Plate-Impact tests is then developed in section 6.2. The experimental setup consists of a cylindrical plate striking a second one with the same geometry, thus initiating a planar shock wave. Deeper details on the experimental setup of Planar-Plate-Impact tests can be found in [83] in an application for the characterization of mortar and granite. In these tests, the high-rate loading conditions are produced by generating a planar shock wave that propagates in the axial direction of the cylindrical plate. Due to the high radius-to-thickness ratio of the specimen, no transverse displacements occur at the center of the plate and a one-dimensional strain state can be assumed. Two discretization methods are used for modeling. On the one hand, the SPH method is applied to idealized material geometries since grain boundaries cannot be captured. Parameters such as quartz strength, porosity and water saturation are varied to assess their influence on the macroscopic material response. The SPH model builds up on previous work in [29]. On the other hand, a FE model is employed for realistic microstructures, as has been the case in the Split-Hopkinson-Bar model setup developed in Chapter 5. Owing to the explicit geometrical modeling of grains in the FE model, quartz anisotropy effects can be investigated. Due to the use of two discretization methods, a detailed parameter study can be conducted in order to gain insight into pore collapse mechanics and to derive macroscopic shock Hugoniots from mesoscale quantities. Since quartzite and sandstone both consist of quartz grains with identical properties in the modeling, the differences to be expected in their macroscopic behavior are essentially attributed to their different microstructural nature. The description of the different models and all attendant findings addressed in this chapter can also be found in [32].
6.1 Literature review of shock data

Shock conditions on geological materials are only sparsely addressed in the literature. Two main reasons can be put forward. First, the application of shock conditions on the laboratory scale demands highly specialized and expensive equipment such as for example Planar-Plate-Impact facilities. Such equipment is only available in a few laboratories worldwide. Secondly, most applications in shock physics concern military research, where metals and alloys are more widely investigated than geological materials or rocks. Trunin et al. [98] present a large collection of shock data that has been gathered from the late 1940’s to the end of 2000 by the All-Russian Research Institute of Experimental Physics. As far as quartzite and sandstone are concerned, shock Hugoniot relations such as shock velocity-particle velocity \((U_s - U_p)\) relationships or pressure-density relationships can be found for silica \(\text{SiO}_2\). The covered particle velocities range from 250 m/s to more than 20 000 m/s. Limited data for sandstone with different porosities is also available. Shipman et al. [90] present shock data inferred from shock wave loading on Coconino sandstone from the Meteor crater in Arizona. The particle velocities and pressures achieved by their light gas gun facility range up to 6500 m/s and 14 GPa, respectively. Ahrens and Gregson [1] conducted shock experiments on a variety of crustal rocks by recourse to explosives. Shock data on Sioux quartz, Eureka quartz, Coconino sandstone and Massilon sandstone was obtained in a low shock regime, for which the particle velocity \(U_p\) does not exceed 2000 m/s.

Figure 6.1 presents a collection of \(U_s - U_p\) data extracted from the aforementioned literature references for quartzite and sandstone. The lower shock regime, i.e. \(U_p < 2000\) m/s, is separately focused on in Figure 6.1-left in order to highlight the elastic-shock transition more properly. The complete data set is represented in Figure 6.1-right. A bi-logarithmic axis scale for the complete data set is employed in order to condense shock data for the lower and the higher shock velocity regimes into one interpretable diagram.
For Sioux quartz, depicted by crossed symbols, a velocity pseudo-plateau can be observed for the lowest particle velocities, followed by a drastic drop at about \( U_p = 300 \text{ m/s} \) and a subsequent slight increase until \( U_p = 800 \text{ m/s} \). The somewhat more remote crossed symbol at \( U_p = 1400 \text{ m/s} \) was obtained by an alternative experimental arrangement and shall not be interpreted here. Shock data of Eureka quartz, which is only available up to \( U_p = 300 \text{ m/s} \) and depicted by upside triangles, also exhibits a plateau-like behavior and fits satisfactorily to data of Sioux quartz. As has been addressed in subsection 2.4.4 and particularly portrayed by Figure 2.12, this initial plateau-like behavior is not attributed to shock but to elastic conditions at which the involved stresses are below the Hugoniot Elastic Limit. Quartz data from Trunin et al. [98], as it only departs from \( U_p = 250 \text{ m/s} \), does not show evidence of such an elastic regime. Nevertheless, the data remarkably stretches out over a very large particle velocity range up to \( U_p = 22 \, 500 \text{ m/s} \). Noteworthy is a curvature breakpoint around \( U_p = 2500 \text{ m/s} \) beyond which the slope of the shock velocity steepens. The origin of this feature will be debated in section 6.3.

The shock velocities observed in dry sandstone lie underneath those achieved in quartz. This finding is intuitive since the presence of porous cells hinders wave propagation, as will be pointed out in more details in subsection 6.3.1. Coconino sandstone was investigated in the frame of
two distinct works. While Ahrens and Gregson [1] focused on the lower shock regime below $U_p < 2000 \text{ m/s}$, see circle symbols, Shipman et al. [90] swept particle velocities from 750 m/s to 6500 m/s, see upside-down triangles. No initial elastic plateau is observed for sandstone. Rather than the sudden drop observed in quartz from the Hugoniot Elastic Limit, a declining trend of the velocity is observed in sandstone for $U_p < 300 \text{ m/s}$, followed by a monotonic increase at higher particle velocities. Only the very first circle symbol does not fit in this interpretation, it needs to remain unclear why this is the case. It is worth noticing that shock data from both sources is in very good accordance within the overlapping $U_p$ range [750 m/s, 2000 m/s]. By merging both Coconino databases, shock data for Coconino sandstone is available for particle velocities ranging from 70 m/s to 6500 m/s. Furthermore, an elastic behavior in sandstone is observable in the limited shock data for Massilon sandstone at $U_p < 500 \text{ m/s}$, represented by rhombic symbols.

To gain insight into the shock stresses, the $U_s - U_p$ data extracted from literature can be converted into $\sigma_L - U_p$ relationships using the equation $\sigma_L = \rho_0 U_s U_p$, namely the second Rankine-Hugoniot Equation (2.63b) for which pressures $P$ are generalized to longitudinal compressive stresses $\sigma_L$. The compressive longitudinal stress $\sigma_L$ is sometimes set equal to the pressure $P$. This assumption is not valid if the material has shear strength, but can be reasonably met if volumetric pressures override shear stresses by far, especially in the high compressive regime. Figure 6.2 bases upon the shock data of Figure 6.1 to derive $\sigma_L - U_p$ data. Again, the data is partitioned into two sub-plots and a bi-logarithmic axis scale is applied for the full range of shock data.
Figure 6.2: Compressive longitudinal stress $\sigma_L$ vs. particle velocity $U_p$ calculated from $U_S-U_p$ literature data. Left: lower shock regime for $U_p < 2000$ m/s. Right: complete data set plotted on bi-logarithmic scale.

For these material variants in which an elastic behavior could be ascertained from the $U_S-U_p$ data, a short linear branch is exhibited in the $\sigma_L-U_p$ curve, followed by a flattening slope, thus indicating the wave velocity drop from the elastic to the shock regime. At particle velocities above 300-500 m/s, the combined ascending trends of shock velocity and particle velocity lead to a high-order increase of the compressive longitudinal stress.

6.2 Mesoscale model setup

An idealized model is first developed using the SPH discretization method. The SPH method, as a Lagrangian method and in contrast to the Eulerian Finite-Volume method used in [42], naturally tracks material points over time. Due to the meshfree nature of the SPH method, grain boundaries are not necessarily conserved during a loading process, and might even get undefined. In a second approach, a refined mesoscale model of quartzite and sandstone is proposed by using a Lagrangian Finite Element discretization with explicit time integration. There, the intent is to explicitly resolve quartz grain shapes, orientations and mutual positions via the use of a structure generator and a tetrahedral meshing tool. The geometrical refinement is of particular relevance when local mechanisms
shall be investigated, since this cannot be done in idealized geometries. The refined model is able to represent grain anisotropy according to the crystallographic nature of quartz \cite{38,78} and grain-to-grain contact. These key mesoscale features, generally not captured by the available mesoscale models in the literature, may have an important influence on the macroscopic material behavior. In particular, the influence of quartz shear strength on macroscopic constitutive laws will be assessed over a wide range of prescribed particle velocities for quartzite and sandstone. Preliminary work addressing shock wave dynamics in pseudo-realistic sandstone structures can be found in \cite{31}. Both discretization methods have assets and drawbacks. The SPH method, owing to its meshfree nature, is particularly convenient for the modeling of Hyper-Velocity processes but lacks an explicit description of material interfaces. The FE method, on the contrary, is able to capture grain-to-grain interactions to a degree not achievable by the SPH method but is more prone to instability issues, such as severe mesh distortions or failing contact algorithms characterized by element interpenetration.

6.2.1 Geometrical setup

6.2.1.1 SPH model

Realistic RVE geometries, which have already been employed in Chapter 5 for Split-Hopkinson-Bar simulations, are reused in this chapter. In the SPH model, however, these geometries need to be reshaped into more simplistic geometries. As grain interfaces can hardly be adequately represented in SPH simulations on the scale considered here, idealized RVEs are defined for that case. A two-dimensional geometry with planar symmetry is employed to reduce the computation time. The symmetry is justified since the wave propagates under macroscopic, one-dimensional strain conditions. The quartzite RVE is a compact quartz matrix and is depicted in Figure 6.3-left. By removing a volume fraction from the quartz matrix, an idealized sandstone RVE is derived. In a first approximation, regularly distributed closed, square pores will be assumed in sandstone, see Figure 6.3-middle. Porosity amounts to 25 % of the total material volume. A second RVE represents water-saturated sandstone, in which the pores are filled with water, see Figure 6.3-right.
Figure 6.3: Idealized two-dimensional RVE geometries of quartzite (left), dry sandstone (middle) and water-saturated sandstone (right) using the SPH formulation. The latter two geometries are peppered with regularly distributed square pores.

Although no corresponding shock data is available, water-filled sandstone offers the opportunity to enrich the comprehension of pore collapse dynamics with respect to dry sandstone. Moreover, in the prospect of homogenization, the water-filling degree may be integrated into a macroscale model via the definition of an appropriate macroscopic variable. The effect of water on the material response will be demonstrated at both mesoscale and macroscale in the results analysis in section 6.3. Partially water-filled sandstone is not investigated here as it would require the setup of a large porous geometric domain to ensure a random distribution of water-filled and dry pores.

6.2.1.2 FE model
The FE geometries used for quartzite and sandstone are identical to the RVEs employed in Chapter 5 for dynamic fracture analysis, i.e. have been engendered by the Voronoi-based and GEOSTAT structure generators, respectively. In order to ensure that wave propagation and pore crushing be captured over an appreciable spatial interval, RVEs are duplicated and appended on each other in the longitudinal direction. A two-millimeter long rod, comprised of four concatenated half-millimeter-sized RVEs, proves to be a good compromise in regard to the informative value of results and a reasonable computational effort, see Figure 6.4.
Development of a novel mesoscale simulation model for compressive shock loading

6.2.2 Boundary conditions

The SPH numerical model is built up as follows: a first rod, consisting of a compact quartz matrix, strikes a second block, in which the specimen to be investigated is sandwiched between two quartz matrices. A zero displacement condition is imposed on the lateral upper and lower boundaries. This way, the macroscopic one-dimensional longitudinal strain state relative to the Planar-Plate-Impact configuration can be mimicked in the simulation model. A schematic representation of the simulation setup for investigating sandstone is provided in Figure 6.5.
The quartz matrix in front of the specimen is intended to ensure the arrival of a smooth wave signal in the specimen by avoiding non-plane wave perturbations in the impact area. As both impactor and target consist of the same compact material near the impact point, two symmetrical shock waves are initiated and propagate in opposite directions. The quartz matrix behind the specimen facilitates the wave analysis by preventing the shock wave from reflecting and interfering with the incident wave. In practice, only one row of pores is set up throughout the longitudinal direction. Due to the imposed lateral confinement, this geometrical configuration is, from a mechanical point of view, equivalent to an infinitely wide rod in which the elementary porous pattern would be repeated indefinitely. When quartzite is investigated, the target simplifies to a homogeneous quartz block with no material contrast.

Since it does not have to consider remote interaction between mass points, the FE model can be reduced to the sandwiched specimen denoted as sandstone in Figure 6.5, the left end of which is prescribed a constant velocity boundary condition. Noteworthy is that the FE model allows for the direct setting of the boundary particle velocity, while in the SPH model, the particle velocity is indirectly controlled by the prescription of the impact velocity $U_{impact}$. 

Figure 6.5: Schematic representation of the simulated Planar-Plate-Impact test for investigating sandstone in the SPH model: a compact quartz block impacts a sandstone specimen sandwiched between two compact quartz matrices with a velocity $U_{impact}$. A zero displacement condition is imposed on the lateral upper and lower boundaries.
6.2.3 Material model for quartz

6.2.3.1 Equation of State
A phase diagram of quartz, bringing to light the microstructural variety the mineral can adopt as a function of the prevailing thermodynamic conditions, has been sketched and described in subsection 1.2.3. The intent of the present mesoscale modeling is not to delve into microstructural transformations of shock-loaded quartz in detail, but rather, to construct a predictive model that takes advantage of equivalent properties manageable on the mesoscale. This presupposes a preliminary homogenization from microscale to mesoscale. To address this issue, the Analytical Equation of State (ANEOS), a physics-based code developed at Sandia National Laboratories [64][67][97], is employed. The ANEOS code necessitates a large set of parameters as input, which covers amongst others atomism, chemistry and thermodynamics, including phase transitions. It computes the Helmholtz free energy $\mathcal{F}$, a two-variable function of density $\rho$ and temperature $T$, by interpolating in a table of predefined values. According to the principles of thermodynamics, partial derivatives of $\mathcal{F}$ with respect to $\rho$ and $T$, respectively, deliver the pressure $P$ and the mass-specific entropy $S$:

$$d\mathcal{F} = -SdT + \frac{P}{\rho^2} d\rho = \left. \frac{\partial \mathcal{F}}{\partial T} \right|_{\rho} dT + \left. \frac{\partial \mathcal{F}}{\partial \rho} \right|_{T} \frac{1}{\rho^2} d\rho$$ (6.1)

For a deepened comprehension of the physical background of the ANEOS code, the theory manual in [97] can be looked up. In practice, no direct analytical functions are returned by the ANEOS code, but a set of discretized values are. These are written out in the form of a tabulated tuple of thermodynamic variables $(P, \rho, T, S, e, ...)$). In most hydrocodes, such as SOPHIA, the Equation of State is ruled by the function $P = P(\rho, e)$ for each computational cycle. Due to the discrete nature of the ANEOS, expressed by $P_{l,j} = P_{l,j}(\rho_l, e_j)$, the actual pressure $P$ is approximated by a bi-linear interpolation of $P_{l,j}$ with respect to $(\rho_l, e_j)$. Let $l$ and $J$ be two indices such that $\rho_l \leq \rho < \rho_{l+1}$ and $e_j \leq e < e_{j+1}$. The actual pressure $P = P(\rho, e)$ is thus approximated by:
Development of a novel mesoscale simulation model for compressive shock loading

\[ P = \rho_{i,j}^P + \frac{e - e_j}{e_{j+1} - e_j}(\rho_{i,j+1}^P - \rho_{i,j}^P) \]  \hspace{1cm} (6.2)

where:

\[ p_{k,l}^p = p_{k,l} + \frac{\rho - \rho_k}{\rho_{k+1} - \rho_k}(p_{k+1,l} - p_{k,l}) \]  \hspace{1cm} (6.3)

ANEOS input data for quartzite can be found in [67]. The initial density of quartz is \( \rho_0 = 2.65 \text{ g/cm}^3 \). In addition to the tuple \((P, \rho, T, S, e, \ldots)\), by-product data can be returned by the ANEOS code, such as isotherms \( P_T(\rho) \) and isobars \( T_p(\rho) \), see Figure 6.6. These isolines enable a better identification of material-specific features, e.g. phase transitions that are recognizable by graphical plateaus. In each diagram, a shock Hugoniot curve, standing for ideal shock conditions, is represented. Upon phase transition, the Hugoniot curve crosses pressure and temperature ranges of respectively 20-25 GPa and 600-800 K. From the micromechanical point of view, these thermodynamic loci \((P, T)\) are correlated to crystal amorphization in the vicinity of the PDF-diaplectic glass transition, see again Figure 1.4.

![Figure 6.6: Plot of isotherms (left) and isobars (right) basing upon the ANEOS code. The phase transitions appear as plateaus and are also visible in the shock Hugoniot curve.](image)

In the current SOPHIA implementation, the ANEOS model can only be used in combination with a SPH formulation. As it is not yet implemented for the FE solver, a Mie-Grüneisen Equation of State as given by Equa-
tion (2.68) and associated to a linear $U_s(U_p)$ relationship, see Equation (2.65), is used as an alternative solution. Parameter values for the model are $\rho_0 = 2.65 \text{ g/cm}^3$, $C_B = 3775 \text{ m/s}$, $\Gamma = 0.9$ and $s = 1.695$. The initial density $\rho_0$ and the bulk sound speed $C_B$ of quartz have been derived from the initial ANEOS state while the Mie-Grüneisen coefficients $\Gamma$ and $s$ have been taken out from the quartz material library in the commercial program AUTODYN [5]. Due to the absence of phase transition, the equivalent bulk modulus, defined as the first derivative of the Hugoniot pressure with respect to the compressive volumetric strain $\zeta$, monotonically grows with pressure. In other words, quartz volumetrically stiffens the more it gets compressed.

6.2.3.2 Shear strength model
When applying a far-field volumetric load on purely homogeneous quartzite, pure volumetric stresses are expected to act within the matrix. If the same external loading is applied on porous sandstone, the presence of pores disturbs the volumetric stress homogeneity and induces local shear stresses at pore walls, see [95]. This observation is particularly crucial when compressive shock waves are involved, since pore crushing dynamics are preponderantly governed by the matrix shear strength. The stronger the framework of grains is, the more it resists crushing. This effect will be investigated for both SPH and FE models in section 6.3.

Quartz grains possess by nature a crystallographic structure, i.e. they exhibit preferential crystallographic orientations. Owing to this property, and assuming that quartz grains are single crystals, each quartz grain can be modeled with a locally-oriented anisotropic elastic stiffness tensor. For each quartz grain, a local anisotropic reference frame is defined, the axes of which are defined via three randomly generated angles. Ab initio calculations of loadings in single lattice directions of quartz crystals were performed in [38][78] to determine the local stiffness tensor of quartz. The linear elastic equation is expressed by Equation (6.4) in a local anisotropic reference frame using Voigt notation.
The stiffness coefficients $C_{ij}$ are not constant but depend on the instantaneous pressure prevailing in the material. Table 6.1 summarizes the values of stiffness coefficients for different pressure values.

Table 6.1: Pressure-dependent stiffness coefficients of quartz in GPa [38][78].

<table>
<thead>
<tr>
<th>Pressure (GPa)</th>
<th>$C_{11}$</th>
<th>$C_{33}$</th>
<th>$C_{44}$</th>
<th>$C_{12}$</th>
<th>$C_{13}$</th>
<th>$C_{14}$</th>
<th>$C_{66}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>86.74</td>
<td>107.2</td>
<td>57.94</td>
<td>6.99</td>
<td>11.91</td>
<td>-17.9</td>
<td>39.88</td>
</tr>
<tr>
<td>1</td>
<td>86.4</td>
<td>103.3</td>
<td>43.6</td>
<td>13.5</td>
<td>14.8</td>
<td>-17</td>
<td>36.2</td>
</tr>
<tr>
<td>2</td>
<td>84.2</td>
<td>105</td>
<td>40.8</td>
<td>18.2</td>
<td>16.7</td>
<td>-15.4</td>
<td>32.2</td>
</tr>
<tr>
<td>5</td>
<td>80.8</td>
<td>111.2</td>
<td>31.6</td>
<td>32.1</td>
<td>23.1</td>
<td>-9.9</td>
<td>24.6</td>
</tr>
<tr>
<td>8</td>
<td>81.2</td>
<td>119.2</td>
<td>22.2</td>
<td>44.5</td>
<td>30.2</td>
<td>-3.0</td>
<td>18.3</td>
</tr>
<tr>
<td>10</td>
<td>84.2</td>
<td>124.6</td>
<td>18</td>
<td>52.2</td>
<td>35.5</td>
<td>12.1</td>
<td>15.8</td>
</tr>
<tr>
<td>10.5</td>
<td>84.6</td>
<td>125</td>
<td>17.7</td>
<td>53.3</td>
<td>36</td>
<td>16.7</td>
<td>15.7</td>
</tr>
<tr>
<td>11</td>
<td>85.1</td>
<td>125.8</td>
<td>17.5</td>
<td>54</td>
<td>36</td>
<td>22.5</td>
<td>15.6</td>
</tr>
<tr>
<td>12.5</td>
<td>86.2</td>
<td>128.3</td>
<td>16.4</td>
<td>56.6</td>
<td>38.2</td>
<td>38.2</td>
<td>15.2</td>
</tr>
</tbody>
</table>

Noteworthy is that at increasing pressures, the diagonal terms $C_{44}$ and $C_{66}$, which relate to shear stiffness coefficients, exhibit a decaying behavior.

In an isotropic linear elastic model, the deviatoric stress-strain relations and the volumetric stress-strain relations can be set up independently of each other, as already pointed out in subsection 2.2.2. In an anisotropic elastic model, however, deviatoric stresses, respectively strains, are additionally coupled to volumetric strains, respectively stresses. By using the decomposition of the stress tensor and of the strain tensor into their deviator and volumetric parts, it follows:
\[ \sigma = S - P \mathbf{1}, \quad \varepsilon = \varepsilon_{\text{dev}} - \frac{1}{3} \zeta \mathbf{1} \]  

(6.5)

The stress-strain relationship for anisotropic materials is given by:

\[ S = C_{\text{dev}} : \varepsilon_{\text{dev}} + A \zeta, \quad P = B : \varepsilon_{\text{dev}} + K_{\text{aniso}} \zeta \]  

(6.6)

where \( C_{\text{dev}} \) is the anisotropic deviatoric stiffness tensor and \( K_{\text{aniso}} \) is the anisotropic bulk modulus, similarly to those defined in isotropic materials. \( A \) and \( B \) are anisotropy-related stiffness tensors of second order and couple deviatoric stresses, respectively pressure, and compressive volumetric strains, respectively deviatoric strains, together. All these four stiffness parameters can be analytically determined by inserting the tensor decompositions from Equations (6.5) into the global stress-strain relationship \( \sigma = C : \varepsilon \).

A major issue when dealing with nonlinear Equations of State for anisotropic materials is the discrepancy between the volumetric pressure term \( K_{\text{aniso}} \zeta \), derived from the anisotropic stiffness tensor \( C \), and the pressure term \( P_{\text{EOS}} \) prescribed by the Equation of State. In order to overcome this shortcoming, [2] suggest to enforce the replacement of \( K_{\text{aniso}} \zeta \) by \( P_{\text{EOS}} \). This way, the high-pressure thermodynamics pertaining to the Equation of State can be incorporated into an anisotropic material model. This methodology, when applied to quartz, works satisfactorily, especially at low confining pressures where a good accordance of both pressure terms is met. Moreover, the incorporation of an external Equation of State into the anisotropic model permits to extrapolate the material description well beyond the pressure range indicated in Table 6.1.

Since the anisotropic model presupposes that quartz grain boundaries be explicitly resolved, it is only applicable in the FE model. An alternative solution is thus proposed for the SPH model. Quartzite, as a high-concentrated conglomerate of randomly arranged and oriented quartz grains, is assumed to exhibit in average an isotropic behavior. This assessment is generally valid for any poly-granular structure in which grain mechanical orientations are uniformly distributed all over the tridimensional space. For this purpose, equivalent isotropic stiffness coefficients can be established for the quartz matrix. Owing to the classical Hooke's
law, two independent stiffness coefficients need to be determined. Departing from an anisotropic material law, [46] demonstrated that equivalent bulk and shear moduli can be estimated between a lower Reuss bound and a higher Voigt bound. A detailed calculation of these bounds is also provided in [46]. An estimate of the equivalent isotropic stiffness coefficients is proposed by taking the arithmetic average of the Voigt and Reuss bounds:

\[
K_{\text{iso}} = \frac{K_{\text{Voigt}} + K_{\text{Reuss}}}{2}, \quad G_{\text{iso}} = \frac{G_{\text{Voigt}} + G_{\text{Reuss}}}{2}
\]  

(6.7)

At zero confining pressure, the equivalent bulk and shear moduli for quartzite are: \(K_{\text{iso}}^0 = 37.76\) GPa and \(G_{\text{iso}}^0 = 42.62\) GPa. At increasing pressures, the equivalent shear modulus \(G_{\text{iso}}(P)\) has a decreasing behavior as it strongly depends on the decaying diagonal terms \(C_{44}\) and \(C_{66}\). This aspect will be further debated in section 6.3 for the pressure-dependent stiffness model.

Depending on the discretization scheme, it turns out that a pressure-dependent anisotropic model and a pressure-dependent isotropic model are the reference shear strength models for quartz. In the parameter study presented in the next subsection, an isotropic case with constant shear stiffness, i.e. \(G_{\text{iso}}^0\), and an isotropic case without shear stiffness will be additionally considered.

A last and important aspect that must be considered in order to enrich the shear strength model for quartz is plasticity. In the upcoming parameter study, quartz will be alternatively modeled with pure elasticity, as has been assumed until now in the aforementioned anisotropic and isotropic models, and then with elasticity, perfect plasticity. In the latter case, a constant yield stress \(Y = 1.73\) GPa is adopted for quartz, see [94][42]. Elasticity, perfect plasticity is associated to plastic flowing without build-up of any additional stress. As a result, in shock-related deformation states, the shear resistance of the quartz matrix is negligible compared to its volumetric resistance.
6.2.4 Parameter study setup

In order to better apprehend individual effects of quartz material parameters on the shock response of quartzite and sandstone, a parameter study is proposed in the following. Table 6.2 gives an overview of the parameters investigated within this study. In the SPH numerical study, all simulations are conducted using the ANEOS model. Quartz is alternately deprived of shear stiffness or outfitted with linear isotropic elasticity, perfect plasticity using the above-mentioned parameters $G_{iso}^0$ and $Y$. Anisotropic and pressure-dependent elasticity effects are discarded in the SPH model. Instead, water-saturated sandstone is investigated in addition to quartzite and dry sandstone. For this purpose, water-filled pores are attributed a water-specific ANEOS model. In summary, the influence of quartz shear strength, porosity and pore content on pore crushing dynamics, macroscopic stresses and shock velocities are investigated in the SPH model.

In the FE configuration, the Mie-Grüneisen Equation of State is employed. Here, the focus is set on different variants of quartz shear strength models. In particular, the effects of quartz anisotropy, shear stiffness and plastic yielding on the macroscopic material shock response are qualitatively and quantitatively assessed for quartzite and dry sandstone.

| Table 6.2: Set of material model and parameters variations for SPH and FE models. |
|---------------------------------------------|---------------------------------------------|
| SPH model | FE model |
| Quartz EOS | ANEOS | Mie-Grüneisen |
| Quartz shear strength model | No shear stiffness | Linear isotropic elasticity $G_{iso}^0$, perfect plasticity $Y$ |
| | No shear stiffness | Linear isotropic elasticity $G_{iso}^0$, perfect plasticity $Y$ |
| | Linear anisotropic elasticity $C_{ij}$ |
| | Pressure-dependent isotropic elasticity $G_{iso}(P)$ |
| Rock type | Quartzite | Quartzite |
| | Dry sandstone | Dry sandstone |
| | Water-saturated sandstone | |
| Porosity in sandstone | 25 % | 23 % |
| | 36 % | |
| | 56 % | |
6.3 Numerical results

6.3.1 Qualitative analysis

6.3.1.1 SPH simulations with idealized geometries

In this paragraph, it is investigated how far pore collapse mechanisms, taking place under shock wave loading in sandstone, are affected by quartz material properties. To impart a good comprehension of these mechanisms, first the SPH simulations are analyzed qualitatively. The choice of large and isolated pores in idealized geometries prevents the collapse of each individual pore from interfering with reflecting waves that originate at neighboring pore walls. In this idealized setting, pore collapse mechanisms can be properly observed and analyzed. Two essential influence factors are quartz shear strength and pore content. In Figure 6.7, pore collapse and the surrounding pressure field are depicted for three sandstone variants: dry sandstone without quartz shear stiffness, dry sandstone with elastic, perfect plastic quartz and water-saturated sandstone without quartz shear stiffness.

![Pressure contours in shock-loaded sandstone using an idealized geometry in SPH simulations. Impact velocity: 1000 m/s. Porosity: 25 %. Pore edge length: 120 µm. Snapshots were taken from left to right every 10 ns. From top to bottom: dry sandstone without quartz shear stiffness, dry sandstone with elastic, perfect plastic quartz and water-saturated sandstone without quartz shear stiffness.](image-url)
The following conclusions can be drawn. In dry sandstone, the way pores are crushed is correlated to the shear strength of the quartz matrix. Quartz, when lacking shear stiffness, offers no shear resistance to local stress concentrations in the vicinity of pore walls. Upon arrival of the shock wave, the quartz matrix consequently jets into the pore towards the opposite pore wall. This phenomenon is depicted as jetting. Alternatively, when quartz is outfitted with shear strength, here elasticity, perfect plasticity, the quartz matrix exhibits a shear resistance against pore crushing. Pore compaction is thus delayed and not localized to the upper pore wall only. The resulting uniformly-distributed compaction process is called shrinking. Both jetting and shrinking phenomena are extensively addressed in [56] and are supported by experimental data. In water-saturated sandstone, water-filled pores hardly get compressed as the shock wave passes by. This originates from the very low compressibility of water which strongly acts against external pressures.

An increase in the impact velocity, say beyond 2000 m/s, results in higher local deformations in dry sandstone. Owing to the elastoplastic quartz model, the shear resistance is constrained by the limiting yield envelope. As the pressures further increase, the shock loading is characterized by a volumetric-dominated regime, in which shear stresses become negligible. To corroborate this velocity-dependent effect, shock simulations are conducted on sandstone with elastoplastic quartz at velocities of 500 m/s, 1000 m/s and 2000 m/s, respectively. Pore crushing dynamics are depicted in Figure 6.8.
The tendency observed in Figure 6.8 confirms the attenuation of the quartz shear stiffness with increasing impact velocities. This phenomenon is in agreement with the basic finding of [56]. According to that reference, pore shrinking occurs in weakly shocked rocks and jetting is a consequence of moderate and high shocks.

The effect of using different pore sizes has been investigated for dry sandstone modeled with quartz without shear stiffness. While the overall porosity was kept constant, the pore size has been reduced by subdividing the large pores into smaller ones across the specimen width. Figure 6.9 illustrates the compaction process in dry sandstone with different pore sizes, respectively amounting to one, two and four pores across the specimen width.
Figure 6.9: Pressure contours in shock-loaded dry sandstone with quartz without shear stiffness. Impact velocity: 1000 m/s. Porosity: 25 %. Pore edge length from left to right: 120 µm, 60 µm and 30 µm.

For any of the three material variants, no noticeable differences in the position of the shock wave front can be assessed, as corroborated in [11]. From a local point of view, small and compacted pores tend to concentrate higher pressure peaks compared to large and sparsely distributed pores. From a macroscopic point of view, however, calculations show that the average shock pressure is not affected by the pore size or pore distribution, but solely by the overall porosity. The methodology for calculating the average shock pressure or homogenized shock pressure will be presented in paragraph 6.3.2.1.

6.3.1.2 FE simulations with realistic geometries
The influence of quartz shear strength on pore crushing and shock velocity is corroborated by FE simulations, in which realistic dry sandstone geometries are used. For robustness purposes, the ANEOS is replaced by the Mie-Grüneisen Equation of State to model the volumetric behavior of quartz in the FE solver. Figure 6.10 shows three exemplary snapshots of the sandstone geometry with pressure contours at three different instants of time. The upper frames show results for dry sandstone with linear isotropic elastic quartz, the lower ones represent dry sandstone with elastic, perfect plastic quartz. The prescribed particle velocity is $U_p = 1500$ m/s.
Figure 6.10: Pressure contours in a longitudinal cross-sectional view of dry sandstone at different instants of time. The prescribed velocity is $U_p = 1500 \text{ m/s}$. Upper row: linear isotropic elastic quartz model. Lower row: elastic, perfect plastic quartz model.

In the purely elastic model, pores are moderately deformed and pressure peaks are somewhat scattered in the form of isolated spots. These are mostly located in contact areas. In the elastoplastic model, pores located behind the shock wave get entirely crushed and pressure concentrations spread out over most of the specimen volume. Furthermore, the shock wave propagation is much faster in the purely elastic model than in the elastoplastic model. In the latter model, the shock velocity is attenuated along with the vanishing shear resistance as the material plastically flows. The quantitative influence of porosity and pore content on macroscopic pressures will be demonstrated by recourse to homogenization techniques, as developed in the next subsection.

6.3.2 Quantitative analysis

6.3.2.1 Homogenization technique
The intent of homogenization is to summarize local mesoscopic results and derive meaningful macroscopic relationships, see [13] for further details. Among the latter, the macroscopic $U_s - U_p$ and $\sigma_t - U_p$ relationships are commonly employed in shock analysis. To set them up, a mathematical average of local variables needs to be calculated over an adequate reference volume $V_{ref}$. Whether a mass- or volumetric-averaging is conducted depends on the nature of the variable of interest. It must be done
consistently with the basic physical conservations for mass, momentum and energy. This way, it can be shown that velocities are mass-related, whereas stresses are volume-related quantities. The averaging is accordingly provided by the following integrals:

\[
\bar{\sigma}_L = \frac{1}{V_{\text{ref}}} \int_{V_{\text{ref}}} \sigma_L \, dV 
\]

(6.8)

\[
\bar{U}_p = \frac{1}{m_{\text{ref}}} \int_{m_{\text{ref}}} U_p \, dm = \frac{1}{m_{\text{ref}}} \int_{V_{\text{ref}}} U_p \rho \, dV 
\]

(6.9)

where \(V_{\text{ref}}\) and \(m_{\text{ref}}\) are respectively the reference volume and reference mass over which the homogenization is performed.

Two types of homogenization are proposed. In the first case, the specimen geometry is subdivided into a finite set of thin sub-volumes oriented orthogonally to the wave propagation direction and denoted by \(V_{\text{voxel}}\). By conducting for every sub-volume a local variable averaging and by appending their results to each other, one-dimensional variable profiles can be elaborated across the target length. In this respect, intermediate-scale aspects not covered by global averaging, such as stress concentrations induced by a collapsing pore, can be investigated. An artistic view of sandstone, overlaid with history voxels, is schematized in Figure 6.11 to impart a better comprehension of this methodology.

![Figure 6.11: Schematic representation of an artistic sandstone specimen partitioned into history voxels. The material volume of a history voxel considers solid matter only, whereas the voxel volume additionally accounts for pore space.](image)

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In practice, the variable integration is, due to the numerical discretization scheme, reduced to a discrete variable summation over a finite number of so-called history points. Depending on the analysis strategy that is pursued, history points can be defined in a twofold manner. On the one hand, Eulerian history points are fixed in space and track material points that successively flow therethrough. On the other hand, Lagrangian history points follow the motion of individual material points from the initial configuration. In the Eulerian case, the reference volume $V_{ref}$ is fixed in space and equals the voxel volume $V_{voxel}$. The associated reference mass $m_{ref}$ is not fixed in time but is steadily updated along with mass inflow and outflow across the voxel boundaries. In the Lagrangian case, $V_{ref}$ merely captures the solid phase, initially located in $V_{voxel}$ and posteriorly transported across the neighboring voxels. Accordingly, the reference mass remains unchanged over time. While the Lagrangian averaging scheme invariably bases upon the initial compact volume, the Eulerian averaging scheme captures the real-time material filling degree in each voxel volume and, as a result, the evolving crushing porosity as the shock wave passes by. In the light of the latter features, the Eulerian method will be relevantly adopted in the following. In this regard, the voxel-specific homogenization is described by the following equations:

$$\overline{\sigma}_{L_{\text{voxel}}} = \frac{1}{V_{\text{voxel}}} \int_{V_{\text{voxel}}} \sigma_L \, dV \approx \frac{1}{V_{\text{voxel}}} \sum_{hist} \sigma_{L_{hist}} \, V_{hist}$$

$$\overline{U}_{p_{\text{voxel}}} = \frac{1}{m_{\text{voxel}}} \int_{V_{\text{voxel}}} U_p \, \rho \, dV \approx \frac{1}{m_{\text{voxel}}} \sum_{hist} U_{p_{hist}} \, \rho_{hist} \, V_{hist}$$

where the subscript $hist$ denotes all history points used in the discrete summation inside a specific history voxel volume $V_{voxel}$. By concatenating all voxel-averaged quantities together, one-dimensional variable profiles can be elaborated across the specimen length. The effects the compact-porous material interface has on the shock material response can thus be evidenced, such as pressure oscillations or shock front propagation hampering, see the next paragraph as regards the SPH results.

In the second case, a global homogenization is performed. The purpose therewith is to deliver one homogenized variable value that is representative of each loading configuration, namely an impact velocity, a porosity
degree and a pore material. To achieve this, a homogenization volume, embracing all material points of the specimen that are momentarily submitted to shock, is defined. The forefront of the homogenization volume is unequivocally associated to the shock wave front and its rear side is defined as the moving quartz-sandstone interface, see Figure 6.12. To ensure a proper homogenization analysis, rarefaction waves, which may originate from the reflection of the rearward-traveling shock wave at the free end of the impactor, must be prevented from entering the homogenization volume. This can be achieved by the setup of a sufficiently long impactor with respect to the targeted time frame in which the shock analysis is conducted. Figure 6.12 schematically illustrates the shock wave propagation in a sandstone specimen sandwiched between two quartz matrices at three different instants of time. The impactor has been blended out for the sake of clarity.

The blue area corresponds to shocked quartz as a result of impact at the uppermost target boundary. Once the incident shock wave reaches the quartz-sandstone interface, it decomposes into a reflected part and a transmitted part, as sketched by the ongoing stretching orange area. The hatched region, bounded by the downward moving quartz-sandstone
interface and the shock wave front in sandstone, stands for the homogenization volume. In practice, the subdivision of the homogenization volume into computation voxels proves to be a relevant and practical way to conduct global homogenization properly. To identify the shocked volume hatched in Figure 6.12, a contiguous row of so-called shocked voxels is sought. A voxel is marked as shocked if its average particle velocity has overridden a critical value that depends on the applied impact velocity. Since a numerical shock wave is not ideally steep but exhibits smeared ascending and descending phases, this critical value is defined as the halfway value of the particle velocity value to be attained at full shocked state. Using this approach, the shock velocity in the specimen can be determined by tracking the position of the shock front over time.

6.3.2.2 Homogenized results for idealized geometries in SPH simulations
In order to better apprehend local pore effects on shock wave mechanics, such as shock pressure or particle velocity, one-dimensional profiles are plotted over the specimen depth, see Figure 6.13. In the SPH results presented below, quartz has no shear stiffness, therefore the compressive longitudinal stress $\sigma_L$ and the pressure $P$ are identical and can be interchanged.
Figure 6.13: Pressure profile (black) over depth at 1 µs after impact. Impact velocity: 2000 m/s. Left: dry sandstone. Right: water-saturated sandstone. In both cases, quartz has no shear stiffness. The pressure profiles correspond to sandstone geometries in Figure 6.7-top (dry sandstone) and Figure 6.7-bottom (water-saturated sandstone). The initial (resp. second) interface corresponds to the interface between the first (resp. second) quartz matrix and the sandwiched specimen in the configuration at rest, where the first (resp. last) pore is encountered. The current interface points to the position of the initial interface at the current time, which is here 1 µs after impact. The pure quartz pressure line corresponds to the macroscopic (identical to mesoscopic here) pressure level achieved in quartz or compact quartzite.

The oscillations observable in Figure 6.13 are caused by the occurrence of porous cells in the sandstone specimen. The deeper the shock wave propagates in the target, the larger is the amount of porosity the wave has run over. As a result, pressure oscillations keep growing in amplitude along with the shock wave front progression. However, this amplitude enlargement is counteracted by the pore crushing process taking place behind the shock front. Under shock compression, pores absorb a part of the shock energy available and thus attenuate the oscillating amplitude. Despite their non-constant amplitude throughout the target depth, pressure oscillations tend to be centered on a constant pressure value, as highlighted by the dash-dotted vertical lines in Figure 6.13. This graphical estimate is actually correlated to the macroscopic pressure that is derived from summation of local pressure over the whole shocked area schematized in Figure 6.12.

To better capture the influence of impact velocity and porosity on macroscopic variables, Figure 6.14 depicts macroscopic $U_s - U_p$ and
\( \sigma_L - U_p \) (or \( P - U_p \)) curves for quartzite and dry and water-saturated sandstones with different porosities, respectively. The underlying quartz models have here no shear stiffness. It must be emphasized that shock data of quartzite has been replaced by the theoretical shock Hugoniot for the sake of exactness. The latter has been directly provided by the ANEOS code and is reproduced in the SPH model very accurately.

![Figure 6.14: Macroscopic \( U_L - U_p \) (left) and \( \sigma_L - U_p \) (right) curves for quartzite, dry sandstone and water-saturated sandstone. Porosities in sandstone are 25 %, 36 % and 56 %. In all cases, quartz has no shear stiffness.](image)

In the diagram, the changes of curvature located at particle velocities between 1500 and 2500 m/s, which reflects the phase transition in quartz, can easily be noticed. In dry and water-saturated sandstone, shock velocity and pressure levels decrease if the porosity degree increases. This is in accordance with physics, since porosity causes local wave reflections and slows down the shock velocity. Moreover, pore crushing irreversibly consumes energy, thereby attenuating the macroscopic pressure. Water-saturated sandstone, in comparison to dry sandstone, exhibits higher macroscopic shock velocities and pressures. Water-filled pores possess high wave impedances and thus, efficiently resist crushing. Quartzite, depicted with solid lines, surmounts all porous cases in terms of shock velocities and pressures since it exhibits a high wave impedance.

Subsidiary analyses show, in the frame of idealized pore geometries, that macroscopic variables are not affected by pore size or shape, as long as the overall porosity is kept unchanged. For instance, half-sized pores, due
to the reduced impedance barrier they represent, smooth the oscillations and locally reduce pressure. Nevertheless, their twice as high population globally enhances pore reflections and thus counteracts the size-related smoothing effects.

6.3.2.3 Homogenized results for realistic geometries in FE simulations
As opposed to SPH results in Figure 6.13, the analysis of one-dimensional profiles in FE simulations does not evidence stress oscillations across the longitudinal direction of the sandstone specimen, but rather a more or less constant stress level. This observation can be explained by the well-balanced distribution of porosity in the realistic three-dimensional sandstone geometry, where homogenization smooths out potential stress concentrations. Accordingly, the observable stress plateau directly stands for the macroscopic compressive longitudinal stress.

In the FE simulations, five different quartz shear strength models have been investigated, see again Table 6.2. The first two strength models consider, as in the SPH simulations, shear-unresisting quartz and elastic, perfect plastic quartz, respectively. The third one assumes linear isotropic elasticity without plasticity and the fourth one represents its anisotropic counterpart. To this end, the stiffness coefficients $C_{ij}^0$ of the anisotropic model are taken out of Table 6.1 at zero confining pressure. The last quartz variant, closer to the physical one determined in [78], employs pressure-dependent equivalent isotropic coefficients $G_{iso}(P)$ and discards plasticity.

For each of these model variants, macroscopic $U_s - U_p$ and $\sigma_L - U_p$ relationships are plotted and compared with each other. The investigated particle velocities in this parameter study range from 50 to 4000 m/s. The pure isotropic and anisotropic elastic models are plotted in Figure 6.15 for both quartzite and sandstone.
Regardless of the anisotropy degree attached to the quartz model, the shock velocity $U_s$ and the compressive longitudinal stress $\sigma_L$ show to monotonically increase, with respect to the particle velocity $U_p$. Moreover, the macroscopic quantities $U_s$ and $\sigma_L$ in quartzite prevail over those in sandstone. These properties are in accordance with the SPH simulation results and are corroborated by Equations (2.74) and (2.63b) which can be rewritten into the condensed form:

$$U_s = \sqrt{\frac{\bar{K}_{EOS} + \frac{4}{3} \bar{G}}{\rho_0}}$$  \hspace{1cm} (6.12)$$

$$\sigma_L = \rho_0 U_p U_s = \rho_0 U_p \sqrt{\frac{\bar{K}_{EOS} + \frac{4}{3} \bar{G}}{\rho_0}}$$  \hspace{1cm} (6.13)$$

where $\bar{K}_{EOS} = \Delta P \left(\frac{\Delta \rho}{\rho_0}\right)^{-1}$ is the non-constant, apparent bulk modulus prescribed by the Equation of State, defined as the ratio of pressure to compressive volumetric strain, and $\bar{G} = -\Delta s_{11} \left(\frac{\Delta \rho}{\rho_0}\right)^{-1}$ is the apparent shear modulus, defined as the ratio of shear stress to shear strain, see Equation (2.74). In sandstone, pore crushing attenuates the material resistance to compression and thus lowers the bulk modulus. Thus, at a
fixed particle velocity, shock velocities and compressive longitudinal stresses in sandstone undervalue those in quartzite.

When comparing the anisotropic and isotropic cases together, no significant differences in shock velocities and stresses can be noticed. In quartzite, the relative difference lies below 0.5 % and is thus negligible, and demonstrates that the equivalent isotropy hypothesis, as proposed in [46] for polygranular aggregates with randomly oriented grains, is fulfilled. In sandstone, a slightly more meaningful relative difference, up to 5 %, can be observed. The presence of pore spaces may induce some sensitivity to anisotropy since the crystallographic orientation of pore-neighboring grains might influence pore crushing locally. Figure 6.16 sketches macroscopic relationships in quartzite for linear isotropic elastic, pressure-dependent isotropic elastic, elastoplastic and shear-unresisting quartz.

![Graph](image)

**Figure 6.16:** Macroscopic $U_s - U_p$ (left) and $\sigma_L - U_p$ (right) curves for quartzite with linear isotropic elastic quartz (solid lines, dotted symbols), pressure-dependent isotropic elastic quartz (dash-dotted lines, upside triangles), elastic, perfect plastic quartz (dotted lines, upside-down triangles) and shear-unresisting quartz (dashed lines, pentagon symbols).

For the elastoplastic quartz model, the ascending slope of the shock velocity is conspicuously preceded by a drop localized in the very low particle velocity range, i.e. below $U_p = 250$ m/s. This feature is commonly observed in real materials and in elastoplastic models, since elastic precursors propagate faster than elastic-plastic waves. In mathematical
terms, the apparent shear modulus $\tilde{G}$ becomes, upon plastic yielding, constrained by the yielding envelope and asymptotically drops towards zero. In parallel, the volumetric contribution $K_{\text{EOS}}$ increases since it represents the dominating stiffness term from $U_p = 250 \text{ m/s}$. Accordingly, the shock velocity goes through a local minimum preliminary to the ascending phase. In the case of pressure-dependent elastic quartz, a similar but much less pronounced drop can also be noticed. This phenomenon can be explained by the decay of the anisotropic coefficients $C_{44}$ and $C_{66}$ with increasing pressure, see Table 6.1, since these essentially monitor the equivalent shear modulus $G_{\text{iso}}(P)$. The latter, as it asymptotically drops to 17 GPa at pressures beyond 10 GPa, weakens the decay of the apparent shear modulus $\tilde{G}$ compared to the elastoplastic case. In this regard, the pressure-dependent elastic quartz model represents, in terms of shear stiffness, an intermediate case between pure linear elastic and elastoplastic quartz. In the shear-unresisting case, no elastic precursor is expected to propagate as only the volumetric behavior is modeled. Accordingly, the $U_s - U_p$ curve diverges from those relative to the shear-resisting variants at low particle velocities and converges to the bulk sound speed $C_B = \sqrt{K_{\text{iso}}/\rho_0}$ as $U_p$ tends to zero. Nevertheless, it rapidly catches up the elastoplastic curve at $U_p = 250 \text{ m/s}$ since the shear stresses in the elastoplastic model quickly get negligible with respect to volumetric pressures.

Regarding longitudinal stresses, no drop can be evidenced for the low shear-resisting models, but rather a lower ascending slope in the lower particle velocity range. A closer look at Equation (6.13) justifies this behavior in that the decreasing behavior of the shock velocity $U_s$ is counteracted by the slopes of the more rapid increasing behavior of the particle velocity $U_p$. In the very high particle velocity range, the relative differences for both longitudinal stress and shock velocity decrease since shear resistance gets more and more negligible in favor of volumetric resistance.

Analogously, Figure 6.17 depicts shock data for sandstone with the same parameter variations as for quartzite.
Development of a novel mesoscale simulation model for compressive shock loading

In sandstone, similar trends can be observed depending on the quartz material model considered. Noteworthy is that the shock velocity tends to zero if the particle velocity converges to zero and if shear stiffness is discarded. This feature can be attributed to the pore crushing mechanism. Since inertial forces are low and shear resistance does not exist in quartz, most of the available shock energy is consumed for pore closure and the shock front gets rapidly extinguished. In the elastoplastic case, a much more pronounced shock velocity drop can be observed in sandstone when compared to quartzite. The conjunction of plastic yielding and pore crushing mechanics at low velocities is responsible for this phenomenon.

6.3.2.4 Main findings and comparison of simulation results with literature data

The purpose of this paragraph is to emphasize the essential findings gained in the previous quantitative analysis and to compare them to literature data. In a preliminary step, shock simulation results are compared with each other. The purpose therewith is to evaluate to which extent the Mie-Grüneisen and ANEOS models correlate with each other. Furthermore, the legitimacy of using simplistic geometries in the SPH setup rather than realistic geometries in the FE setup needs to be verified. Figure 6.18 represents shock data of quartzite and sandstone for a
restricted set of quartz models, all without shear stiffness. Here, shock data of the ANEOS-based quartzite model has been replaced by the theoretical shock Hugoniot curve issued by the ANEOS code.

The first finding that can be derived from the diagrams is the good accordance of shock data between both FE and SPH setups. The SPH-related curve does not deviate from the FE-related curve by more than 5%. This validates the legitimacy of the use of idealized geometries as far as shock loading conditions, disregarding quartz shear stiffness, are concerned. The second finding is related to the type of Equation of State attached to quartz and its influence on the macroscopic shock behavior. At low particle velocities, the $U_s - U_p$ curves of ANEOS and Mie-Grüneisen models are in good accordance. From $U_p = 1300$ m/s, the curve of the ANEOS model flattens due to the phase transition. This flattening is quite smooth in sandstone but particularly pronounced in quartzite. Consequently, the shock velocities achieved in the Mie-Grüneisen model overestimate those achieved in the ANEOS model at higher particle velocities. The excess of shock velocity amounts to a roughly constant value of 2000 m/s for quartzite, and moderately grows for sandstone from 0 m/s to 1000 m/s when $U_p$ varies from 1300 m/s to 2300 m/s.
Now, the numerical results are compared to literature data. In Figure 6.19, experimental literature data and selected numerical results are plotted together for quartzite.

The theoretical shock Hugoniot curves from the ANEOS model, for which quartz shear stiffness is disregarded, are plotted in the diagrams. For the FE setup, and for the sake of conciseness, only the elastoplastic and the pressure-dependent stiffness quartz models are represented. In the lower shock regime, i.e. below 1300 m/s, a number of data points for Sioux quartz and Eureka quartz are available [1]. They show, after a short elastic plateau, a significant drop of the shock velocity at about $U_p = 300$ m/s. This drop can be interpreted as loss of shear stiffness due to plastic yielding. The initial elastic plateau can be represented well by the model with pressure-dependent elasticity. The elastoplastic quartz model combined with the Mie-Grüneisen Equation of State is capable of capturing the drop and the subsequent increase of the shock velocity up to a particle velocity of about 1300 m/s. Beyond this threshold, the Trunin experimental data [98] shows a plateau that represents the aforementioned phase transition. This feature is only included in and well represented by the model with the ANEOS. However, that model fails to represent the first elastic plateau and the drop in the region of lower
particle velocities since it omits quartz shear stiffness. In a similar way, Figure 6.20 summarizes shock Hugoniot curves for sandstone.

![Figure 6.20: Macroscopic $U_s - U_p$ (left) and $\sigma_L - U_p$ (right) curves for sandstone. Solid lines stand for the ANEOS quartz model in the SPH setup, dotted lines stand for the pressure-dependent stiffness quartz model and dashed lines for the elastic, perfect plastic quartz model in the FE setup.](image_url)

In the lower particle velocity regime, data on Coconino sandstone and Massillon sandstone from Ahrens and Gregson [1] shows a rapid decline of the shock velocity. This decrease is more pronounced than in quartzite since local plastic deformations and damage lead to crushing of pores and thus to drastically reduced shock velocities. The pressure-dependent elastic model fails to represent this process and therefore exhibits overestimated shock velocities. The elastoplastic quartz model combined with the Mie-Grüneisen Equation of State captures the shock velocity drop well as well as the subsequent increase of shock velocities up to $U_p = 1200$ m/s. At higher particle velocities, the role played by the phase change in quartz is evidenced by the divergence of shock Hugoniot curves between the Mie-Grüneisen and ANEOS models. In the higher pressure region, only the ANEOS model satisfactorily mirrors experimental data on Coconino sandstone from Shipman et al. [90] and demonstrates how primordial phase transition effects need to be accounted for in the modeling.
6.3.3 Suggestions for further improved mesoscale modeling

From this detailed analysis, improvement suggestions for future mesoscale modeling can be formulated. A combination of the ANEOS Equation of State, pressure-dependent stiffness and plasticity in one single material model for quartz is of high relevance. The purpose therewith is to achieve a macroscopic behavior in quartzite and sandstone as close to reality as possible over the entire particle velocity range for which experimental data is available, i.e. from zero to several thousand meters per second. The modeling results shall primarily provide input for improved macro-scale shock-related Equations of State for meteorite impact modeling, but they may also be used for in-depth investigations on grain-to-grain interactions and pore crushing processes. Therefore, correlations between mesoscale simulation results with small scale shock features observed in materials that were loaded by experimentally simulated or real-scale meteorite impacts may be found. A further research topic is the combination of the mesoscale models with material models which cover inelastic processes inside the crystals in more detail.
7    Multiaxial mesoscale simulations

In this chapter, the quartzite and sandstone RVEs are successively subjected to a variety of multiaxial loads at different strain rates. The stress states, at which yielding or failure occur, are then mapped to the principal stress space. The concatenation of the different yield and failure points registered for each loading state result in a realistic homogenized three-dimensional failure surface or yield surface. Material properties of quartz are defined in the light of the numerical studies conducted in the previous Chapters 5 and 6.

7.1    Model setup

7.1.1    Material model

Since the applied loading conditions do not involve short wave pulses but employ linear strain distributions, the Equation of State does not require an accurate modeling of shock-related compressive states. Accordingly, the ANEOS will be discarded in favor of the Mie-Grüneisen Equation of State. The latter has been conveniently employed in the FE shock wave simulations in Chapter 6. Besides, as the applied loading is circumscribed to small deformations, stress levels are not expected to outreach the yield initiation point, the order of magnitude of which is the Gigapascal. Accordingly, and since anisotropic effects are limited in quartzite and sandstone, the shear strength model is restricted to isotropic quartz elasticity with constant shear stiffness. The shear modulus is taken out from the equivalent isotropic model of quartz, see Equation (6.7), i.e. $G = 42.62$ GPa. Inter-granular strength is modeled for each material variant by the use of the mesoscopic set of parameters ascertained from the simulated Split-Hopkinson-Bar-Tests in Chapter 5. In this respect, a mesoscopic material model capable of modeling tensile failure and compressive states shall constitute the baseline of the upcoming analysis. The material model setup is summarized in Table 7.1:
Table 7.1: Summary of the quartz material model and inter-granular model used in the multiaxial mesoscale simulations.

<table>
<thead>
<tr>
<th>Equation of State</th>
<th>Mie-Grüneisen ( \rho_0 = 2.65 \text{ mg/mm}^3 ), ( \Gamma = 0.9 ), ( C_B = 3775 \text{ m/s} ), ( \sigma = 1.695 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shear strength</td>
<td>Linear isotropic elasticity, ( G = 42.62 \text{ GPa} )</td>
</tr>
<tr>
<td>Inter-granular failure</td>
<td>( T_{\text{meso}}^{\text{crit}} = 10 \text{ MPa}, \ G_{\text{meso}}^{\text{crit}} = 50 \text{ N/m} )</td>
</tr>
<tr>
<td>in quartzite</td>
<td></td>
</tr>
<tr>
<td>Inter-granular failure</td>
<td>( T_{\text{meso}}^{\text{crit}} = 10 \text{ MPa}, \ G_{\text{meso}}^{\text{crit}} = 240 \text{ N/m} )</td>
</tr>
<tr>
<td>in sandstone</td>
<td></td>
</tr>
</tbody>
</table>

7.1.2 Multiaxial loading conditions

The set of multiaxial loading cases presented in the following is inspired by the work of [104] and consists in the application of velocity boundary conditions. All outer faces of the RVEs are independently subjected to uniform and time-constant velocities; the loading might be tensile or compressive, see Figure 7.1. In order to ensure a uniform initial strain rate within the RVE, a linear velocity distribution along the loading direction is prescribed in the RVE at \( t=0 \).
Figure 7.1: Geometric representation of 121 sets of boundary velocity components employed in multiaxial mesoscale simulations. Each dot represents a specific loading case. Red dots denote tensile loading, blue ones compressive loading and green ones mixed loading involving both tension and compression. \( U_{\text{max}} \) is the maximum velocity component that can be defined in any direction.

By convention, the performance of a series of 121 loading cases at a fixed value \( U_{\text{max}} \) will be associated to one unique strain rate defined by \( \dot{\varepsilon} = \frac{U_{\text{max}}}{L_{\text{RVE}}} \), where \( L_{\text{RVE}} \) is the RVE initial length.

### 7.2 Identification of yield and failure surfaces

Each loading path represents a specific stress history in the principal stress space. Depending on the relative ratios of the three boundary velocity components, the material might be dominantly subjected to tension, shear or compression. A well-known descriptor of the confining state of a material is the pressure \( P \). Usually, the higher the confining pressure in a granular material is, the more resistant it is against failure. This feature is e.g. the basis of the Mohr-Coulomb and Drucker-Prager yield criteria, see again subsection 2.2.3. An additional factor that notably influences the likelihood for a material to yield or fail is the meridian plane containing the stress state, see again Figure 2.2 for a graphical representation of the different meridian planes. In standard porous materials, a stress loading along the tensile meridian plane induces an earlier onset of yielding or failure than if it were along the compressive meridian plane [104]. It will
be shown in the following subsections to which extent these empirically-known properties are valid for quartzite and sandstone.

7.2.1 Assessment of macroscopic stress-strain profiles

In the following, loading categories will be discriminated from each other depending on the nature of the stress state they call forth.

The first loading category considers that all three boundary velocity components are of tensile nature. Accordingly, the material is subjected to a three-dimensional tensile stress state for which failure mechanisms prevail. Figure 7.2 shows a collection of macroscopic stress-strain profiles for quartzite and sandstone under different 3D tensile loading configurations at a strain rate $\dot{\varepsilon} = 150 \text{ s}^{-1}$, for which $U_x \geq U_y \geq U_z > 0$. Stresses and strains are here regarded as effective quantities. The legend indicates for each loading configuration the three values that are adopted by the velocity vector and that are normalized by the maximum velocity $U_{\text{max}}$. See again Figure 7.1.

![Figure 7.2: Macroscopic stress-strain profile for a selection of three-dimensional tensile loading configurations at a strain rate $\dot{\varepsilon} = 150 \text{ s}^{-1}$. Left: quartzite. Right: sandstone. Velocity components are all positive and obey the inequation $U_x \geq U_y \geq U_z > 0$. The legend indicates the three normalized velocity components with respect to $U_{\text{max}}$.](image)

All stress-strain curves exhibit a maximum stress value which stands for the macroscopic failure stress. The post-peak behavior is characterized by
a gentle stress decrease which is attributed to the ongoing decohesion process of cohesive zone elements. The post-peak behavior, which shall provide information about macroscopic fracture energy depending on the applied loading configuration, is a relevant aspect that will be studied in future work.

The second loading category considers mixed tensile-compressive modes for which at least one velocity component is negative. In that case, the decohesion process that would naturally develop in the tensile-loaded directions is counterbalanced by the compressive deformation. Accordingly, the confining effect engendered by the compressive-loaded direction prevents the material from failing from a macroscopic point of view. Rather than achieving a maximum stress value, the mixed tensile-compressive mode is characterized by a kink in the stress-strain curve. This is evidenced by Figure 7.3 where macroscopic stress-strain curves are represented for quartz and sandstone for a selected set of mixed loading configurations.

Figure 7.3: Macroscopic stress-strain profiles for a selection of mixed tensile-compressive loading configurations at a strain rate $\dot{\varepsilon} = 150 \text{ s}^{-1}$. Left: quartzite. Right: sandstone. At least one velocity component is negative. The legend indicates the three normalized velocity components with respect to $U_{\text{max}}$.

The curve flattening produced by the observable kink is typical for material yielding and flowing (see again Figure 2.5). Although not explicitly investigated here, it is expected that the removal of the boundary conditions beyond the kink point leaves residual strains. In this regard, the
von Mises stress at the inflexion point can be reasonably identified as the yield stress.

The last loading category addresses configurations for which all velocities are of compressive nature, i.e. $0 > U_x \geq U_y \geq U_z$. There, the three-dimen-
sional confining process forbids any failure since compressive fracturing is not modeled. Figure 7.4 gives a representation of some macroscopic stress-strain curves for quartzite and sandstone in this compressive regime.

![Figure 7.4: Macroscopic stress-strain profiles over time for a selection of three-dimen-
sional compressive loading configurations at a strain rate $\dot{\varepsilon} = 150$ s$^{-1}$. Left: quartzite. Right: sandstone. Velocity components are all negative and obey the inequation $0 > U_x \geq U_y \geq U_z$. The legend indicates the three normalized velocity components with respect to $U_{\text{max}}$.](image)

Quartzite, due to its compact nature, shows a linear elastic behavior whereas sandstone exhibits a flattening in the stress-strain curve. The latter, as in the mixed tensile-compressive mode, testifies to material plasticity. The physical phenomenon involved here is the irreversible compac-
tion of pore spaces which tends to attenuate the macroscopic resistance of the material against the macroscopic confining process.
7.2.2 Derivation of a mixed yield-failure criterion

In the previous subsection, it has been evidenced that the predisposition of quartzite or sandstone to either yield or fail depends on the loading. Here, macroscale failure initiation is identified when the von Mises stress starts to decrease while the effective strain increases. The macroscopic yield stress is defined according to the following numerical criterion. It is the stress at which the slope of the stress-strain curve drops by more than 10% compared to the initial elastic slope. From the analysis of macroscopic stress-strain curves, it turns out that failure might set in without any precursory yielding and that yielding is often not terminated by any failure process. In this regard, a unified mixed yield-failure criterion for quartzite and sandstone is elaborated. Nevertheless, some critical analysis needs to be conducted about the transition from failure to yield relatively to the confining nature of applied velocities. Whereas the set of loading cases cover a large spectrum of the main stress space, the application of a compressive loading in at least one direction prevents the specimen from failing in that the material is capable of resisting high compressive strains. This way, the macroscopic stresses keep growing in amplitude even if grains are disaggregated from each other. As a result, yield states may hide internal failure processes and thus should not be strictly dissociated from failure states. The main purpose of the unified yield-failure criterion is to ascertain a stress threshold beyond which the material gets irreversibly deteriorated. In the following, all loadings have been applied at a fixed strain rate \( \dot{\varepsilon} = 150 \text{ s}^{-1} \).

7.2.2.1 Quartzite

For the sake of convenience, a representation of the yield-failure surface of quartzite is provided in a two-dimensional \((\sigma_{vM} - P)\) diagram at two different scales, see Figure 7.5. The left diagram sets a zoom into the vicinity of the failure loci while the right diagram sketches the complete set of failure and yield loci. In order to discriminate failure and yield loci in terms of Lode angles, a color coding is performed depending on the Lode angle interval in which a failing or yielding stress state is comprised. These intervals are the three regular subdivisions of the first sextant, namely \([0^\circ, 20^\circ]\), \([20^\circ, 40^\circ]\) and \([40^\circ, 60^\circ]\), which represent approximations to tensile, shear and compressive meridians, respectively. On each yield-failure surface, an additional stress point, corresponding to the macroscopic dynamic tensile strength \( T_{\text{macro}}^{\text{crit}} = 16.7 \text{ MPa} \) in quartzite, is repre-
Multiaxial mesoscale simulations

This value has been derived from simulated Split-Hopkinson-Bar-Tests, see again Table 5.4. Since the Hopkinson configuration involves a one-dimensional stress state, the von Mises stress at failure directly mirrors the dynamic tensile strength. Moreover, it can be easily shown that the mean stress is proportional to the von Mises stress via a factor of one third that is called triaxiality. In this regard, the dynamic tensile strength is represented by the point (-5.57 MPa, 16.7 MPa).

Figure 7.5: Two-dimensional representation of failure and yield loci in a $(\sigma_{vM} - P)$ diagram for quartzite under a strain rate $\dot{\varepsilon} = 150 \, \text{s}^{-1}$. Failure and yield loci are color-coded according to three Lode angle intervals, corresponding to three regular subdivisions of the first sextant. The macroscopic dynamic tensile strength in quartzite is highlighted by a star symbol. Left: zoom into the failure loci. Right: overall view of failure and yield loci.

The color coding makes it clear that loading states associated to higher Lode angles, i.e. in the vicinity of the compressive meridian plane, postpone the onset of yielding or failure compared to lower Lode angles close to the tensile meridian plane. This observation is in accordance with empirically-based models such as the RHT model [81][82][41]. The dynamic tensile strength, although related to failure per nature, shows to lie in the yield domain of the $(\sigma_{vM} - P)$ diagram. This mismatch is presumably attributed to the biased definition of yielding due to the confinement effects imparted by the boundary conditions. As can be observed, the dynamic tensile strength lies on the shear meridian that slightly surpasses the tensile meridian. At this point, it can be reasonably hypothesized that if failure could be captured at low negative pressures, the three failure meridians at high negative pressures would be prolonged such that
they would outreach the three yield meridians represented in Figure 7.5. From this point of view, the locus of the dynamic tensile strength in quartzite would probably cross the tensile meridian of the virtual failure surface, as has to be the case for one-dimensional stress states. In this frame of hypotheses, some consistency can be stated between the macroscopic dynamic tensile strength, determined in Split-Hopkinson-Bar simulations, and the macroscopic yield-failure surface for quartzite, which bases upon a separate set of mesoscopic loading cases.

In order to summarize yield and failure data into a unique analytical model, interpolating functions, catching the yield or failure function for each of the three Lode angle intervals, are defined. Yield and failure data are separately interpolated due to their different physical nature. Interpolants are second-order polynomials and are separately set up for yield data and failure data. For practical reasons, Lode angle intervals are reduced to a single value, namely $0^\circ$, $30^\circ$, and $60^\circ$. These angles are representative for the tensile, shear and compressive meridians, respectively. Owing to this interpolation method, three yield or failure point values are provided for any considered deviatoric plane, in which the confining pressure is fixed. To derive a yield or failure surface over a local deviatoric plane sextant $[0^\circ, 60^\circ]$, a second-order polynomial interpolation is again proposed, though with respect to the Lode angle. According to the isotropy hypothesis, the yield or failure surface pattern in a sextant can be symmetrized with respect to the principal stress axes such that a complete $360^\circ$ yield or failure surface can be derived. By combining both polynomial interpolations with respect to pressure and Lode angle, an analytical, extrapolated yield-failure surface can be eventually derived from discrete yield and failure data, see Figure 7.6.
Figure 7.6: Representation of the failure surface (blue) and yield surface (red) of quartzite under a strain rate $\dot{\varepsilon} = 150$ s$^{-1}$ in the principal stress space (a) and cross-sectional view thereof in three different deviatoric planes, defined by $P=\pm 5$ MPa (b), $P=0$ MPa (c) and $P=5$ MPa (d). The color coding in the deviatoric cross-sections stands for the intensity level of the mean stress $\bar{\sigma}$.

The yield-failure surface exhibits a pseudo-conic shape expanding towards compressive stresses. In the tensile stress domain, the yield cone is terminated by a failure cap, as already suggested by the $(\sigma_{\text{YM}} - P)$ in Figure 7.5. The cross-sectional views of the yield surface in the different deviatoric planes point out that, with increasing pressure, the Lode angle dependency intensifies. In particular, the yield surface on the compressive meridian at higher pressures significantly stretches out compared to the tensile meridian.
7.2.2.2 Sandstone
A similar analysis is conducted for sandstone, see Figure 7.7. In contrast to the funnel-shaped yield surface in quartzite, the yield surface of sandstone is terminated by a cap located in the positive pressure domain. This feature is attributed to the irreversible pore compaction phenomenon in sandstone that has been pointed out in the previous subsection. Accordingly, yielding is even likely to occur if a pure confining pressure without any shear contribution is applied to the material. Again, the dynamic tensile strength from Split-Hopkinson-Bar-Tests is represented by the point (-1.83 MPa, 5.5 MPa).

Figure 7.7: Two-dimensional representation of failure and yield loci in a $(\sigma_{vM} - P)$ diagram for sandstone under a strain rate $\dot{\varepsilon} = 150$ s$^{-1}$. Failure and yield loci are color-coded according to three Lode angle intervals, namely the three regular subdivisions of the first sextant. The macroscopic dynamic tensile strength in sandstone is highlighted by a star symbol. Left: zoom into the failure loci. Right: overall view of failure and yield loci.

The dynamic tensile strength $T_{macro}^{crit}$ of sandstone fits to the shear meridian curve very well as for quartzite. Again, by assuming that, at a fixed triaxiality, failure states surpass yield states in the $(\sigma_{vM} - P)$ representation, a consistency between the macroscopic tensile strength and the macroscopic yield-failure surface for sandstone can be found. By the use of the interpolation methodology, a yield-failure surface for sandstone is determined, see Figure 7.8.
Figure 7.8: Representation of the failure surface (blue) and yield surface (red) of sandstone under a strain rate $\dot{\varepsilon} = 150 \text{ s}^{-1}$ in the principal stress space (a) and cross-sectional view thereof in three different deviatoric planes, defined by $P=-3 \text{ MPa}$ (b), $P=0 \text{ MPa}$ (c) and $P=3 \text{ MPa}$ (d). The color coding in the deviatoric cross-sections stands for the intensity level of the mean stress $-P$.

Figure 7.8 evidences again both failure and yield caps in sandstone. Accordingly, cross-sectional views of the yield surface in three deviatoric planes show, as in quartzite, an expansion of the yield surface from negative pressures to moderate positive pressures. At further increasing pressures, however, the yield surface contracts back due to the yield cap phenomenon. The Lode angle dependency of the yield surface is not as straightforward as in the case of quartzite. While the compressive meridian exhibits, compared to the tensile meridian, higher yield stresses at negative pressures and at small positive pressures, this tendency is inverted at further increasing pressures.
7.2.3 Strain rate effects

In this subsection, strain rate effects on yield and failure states are investigated. The underlying purpose therewith is to permit the development of an enriched macroscopic material model that accounts for the strain rate as a macroscopic variable. Three strain rates, namely $15 \text{ s}^{-1}$, $150 \text{ s}^{-1}$ and $1500 \text{ s}^{-1}$ have been investigated.

In quartzite, no strain rate effects could be observed. As a plausible explanation, it can be conjectured that inertial effects in granular structures are preponderantly driven by porosity reduction mechanisms, which are naturally absent in compact quartzite. In sandstone, by contrast, strain rate effects are noticeable. The homogenized $(\sigma_{vM} - P)$ diagram, see Figure 7.9, demonstrates that stress state discrepancies owing to strain rate effects are only observable at higher pressures in the yield cap region. In particular, higher strain rates are associated to higher yield stresses. This observation confirms that inertial effects are particularly perceptible at high confining pressures where pore collapsing is prominent.

![Figure 7.9: Two-dimensional representation of failure and yield loci in a $(\sigma_{vM} - P)$ diagram for sandstone. Color coding stands for three different strain rates, namely $15 \text{ s}^{-1}$ (blue), $150 \text{ s}^{-1}$ (red) and $1500 \text{ s}^{-1}$ (green). Left: zoom into the failure loci. Right: overall view of failure and yield loci.](image)

In the yield cap region, the higher strain rate case $\dot{\varepsilon} = 1500 \text{ s}^{-1}$ exhibits a somewhat more scattered collection of stress points than the lower strain rate cases, thus impeding a precise assessment of the yield cap. This
phenomenon is presumably attributed to high inertial effects in sandstone which tend to introduce some variability in the onset of yielding.

7.3 On the way to macroscale models

The knowledge of homogenized yield and failure data for quartzite and sandstone sets the course for the development of a macroscale plasticity and failure model. A variety of macroscale models devoted to geologic materials have been put forward in subsection 1.2.1. A further macroscale model, namely the RHT model, is briefly presented in the following and is intended to give perspectives for parameter calibration in the future.

The RHT model is historically motivated by the need of modeling concrete under a wide spectrum of loading configurations. Not only multi-axis stress states, but also strain rate effects have to be accounted for in order to model the observed macroscale material response. The macroscale behavior is described in terms of strain rate dependent yield and failure surfaces and a post-failure softening law, characterized by shear strength degradation while damage increases. All these features are briefly exposed in the following subsections and their applicability to the homogenized response of quartzite and sandstone will be appraised.

7.3.1 Failure surface

The failure surface corresponds to the maximum admissible shear stress $\sigma_f$ in the material as a function of pressure $P$, lode angle $\theta$ and effective plastic strain rate $\dot{\varepsilon}_{eff}^{pl}$. It is expressed by:

$$\sigma_f = \sigma_f(P, \theta, \dot{\varepsilon}_{eff}^{pl}) = f_c \sigma_f^*(P^*, F_R(\dot{\varepsilon}_{eff}^{pl})) R_S(P^*, \theta) \quad (7.1)$$

where $\sigma_f^*$ is the failure stress in the tensile meridian, i.e. at $\theta = 0$, normalized by the compressive failure stress $f_c$ achieved in a one-dimensional stress state. In the following, all variables outfitted with an asterisk are normalized by $f_c$. The function $F_R$ describes the strain rate dependency of the failure stress and is neglected in this subsection for the sake
of clarity. $R_3$ is a pressure and a Lode angle-dependent function and will be described in more detail in the next subsection.

The function $\sigma_f^*$ is defined over three pressure intervals. At negative pressures, a linear branch initiates from the normalized volumetric tensile limit $P_t^*$ and crosses the normalized tensile failure stress $f_t^*/Q_2$ on the compressive meridian and the normalized shear failure stress $f_s^*/Q_1$ on the compressive meridian. The quantity $f_t^*$ is the normalized tensile failure stress achieved in a one-dimensional stress state, i.e. on the tensile meridian, and is divided by factor $Q_2$ to match the compressive meridian. Analogously, the quantity $f_s^*$ is the normalized shear failure stress achieved under pure shear loading, i.e. on the shear meridian, and is divided by the factor $Q_1$ to match the compressive meridian. At positive pressures, though below the one-dimensional compressive stress threshold curve, a second linear branch runs from $f_s^*/Q_1$ to one. At higher pressures, a power law as sketched in Figure 7.10 governs the ascending behavior of the normalized failure stress.
Multiaxial mesoscale simulations

Figure 7.10: Normalized failure stress $\sigma_f^*$ on the compressive meridian over normalized pressure $P^*$. The mathematical principle, consisting of two linear branches and a power law function, is depicted in (a). Variations of the exponent $n$ of the power law (b), of the shear failure stress on the shear meridian $f_s^*/Q_1$ (c) and of the tensile failure stress on the tensile meridian $f_t^*/Q_2$ (d).

As macroscopic failure in quartzite and sandstone is identified to occur only in a negative pressure range, the first linear branch can be parameterized independently of the rest of the function. The linear branch at positive pressures and the power low function can then be set artificially high in order to prevent failure at higher pressures.

7.3.2 Lode angle dependency

The Lode angle-dependent function $R_3(P^*, \theta)$ was developed in [105] and describes, for any normalized pressure $P^*$, the ratio of failure stress at any Lode angle $\theta$ to the failure stress on the compressive meridian. On the tensile meridian, i.e. at $\theta = 0$, the function $R_3$ is reduced to a
pressure-dependent function $Q(P^*)$ which is defined to be linearly dependent on $P^*$ while remaining within the interval $[0.5, 1]$, see Figure 7.11. At lower pressures for which $Q(P^*) = 0.5$, the failure surface cross-section in a deviatoric plane exhibits a triangular shape. At higher pressures for which $Q(P^*) = 1$, the cross-section of the failure surface exhibits a circular shape since all meridians achieve the same failure stress value as the compressive meridian. Cross-sections of failure surfaces at any intermediate pressure are characterized by a transitional shape between the triangular and circular shapes. The transition from the triangular shape to the circular shape is known as the brittle-to-ductile transition. It can be incidentally remarked that the factors $Q_1$ and $Q_2$ defined in the previous subsection can be derived from $R_3$ at specific values $(P^*, \theta)$ by construction.

![Figure 7.11: Representation of the normalized failure surface for different superimposed deviatoric planes. The distance between any failure surface point and the hydrostatic axis is given by $R_3(P^*, \theta)$. A triangular shape is encountered at lower pressures and gradually transforms to a circular shape at increasing pressures.](image)

\[
Q = Q_0 + BP^*
\]

\[
\begin{align*}
Q &= 1 \\
Q &= 0.88 \\
Q &= 0.69 \\
Q &= 0.59 \\
Q &= 0.5
\end{align*}
\]

In quartzite and sandstone, failure and yield surfaces also exhibit a dependency on the Lode angle. In quartzite, the failure stress on the compressive meridian overrates its counterpart on the tensile meridian, even at high confining pressures. In this respect, cross-sectional views of failure surfaces in deviatoric planes tend to exhibit triangular shapes.
throughout the hydrostatic axis. In sandstone, the dominancy of the compressive meridian at negative pressures is inverted at positive pressures. Geometrically, this means that the triangle-like shapes encountered at low pressures gradually rotate by an angle of $60^\circ$ at increasing pressures.

### 7.3.3 Strain rate dependency

As already introduced at the beginning of this section, a strain rate dependency is imparted to the failure surface via the function $F_R(\dot{\varepsilon}_{\text{eff}}^{\text{pl}})$. In general, the function $F_R$ is governed by the concatenation of two user-defined power law functions joining at a common strain rate value $\dot{\varepsilon}_{\text{limit}}$, see Figure 7.12-left. Accordingly, the failure surface is scaled for any strain rate $\dot{\varepsilon}_{\text{eff}}^{\text{pl}}$ by the corresponding $F_R$ value, see Figure 7.12-right.

![Figure 7.12](image)

Figure 7.12: Left: typical evolution of the strain rate factor $F_R$ as a function of the effective plastic strain $\dot{\varepsilon}_{\text{eff}}^{\text{pl}}$. An intermediate strain rate value $\dot{\varepsilon}_{\text{limit}}$ marks the intersection point between two power laws. Right: Strain-rate enhanced failure stress $\sigma_f^*$ on the compressive meridian over normalized pressure $P^*$. All strain rates are normalized by a reference strain rate $\dot{\varepsilon}_0$ which generally amounts to $1 \text{ s}^{-1}$.

As a strain rate dependency of the yield-failure surface has been observed in sandstone, a function $F_R$ might be tailored for sandstone in the light of the investigated strain rate range.
7.3.4 Initial elastic and yield surfaces

In the RHT model, the initial elastic surface is derived from the failure surface via a downscaling factor. Intermediate expanding yield surfaces due to hardening effects are derived from linear interpolation between the initial yield surface and the failure surface, see Figure 7.13-left. The weighting rule to be applied on the two latter curves is monitored by the current effective plastic strain \( \varepsilon^{pl\ast} \) that is normalized by the maximum admissible plastic strain at the failure point. Besides, an additional cap function can be adjoined to the initial elastic surface in order to reflect yielding effects under pure volumetric compression. The evolution of the elastic cap is dictated by an Equation of State in which pressure is set in relation to porosity. Any intermediate yield surface, here denoted by \( \sigma^\ast \), is then obtained by linear interpolation between the current, capped elastic surface and the failure surface.

![Figure 7.13: Left: representation of the initial elastic, intermediate yield and failure surfaces. Right: Incorporation of a cap function into the initial elastic surface function. Dotted lines refer to the updated capped elastic surface at a fixed plastic strain. Solid lines stand for intermediate yield surfaces via interpolation between current capped elastic and failure surfaces.](image)

In quartzite, no yielding occurs under pure volumetric loading. This way, a yield description without cap is appropriate. The yield surface resulting from numerical simulations can be identified as the initial yield surface in the RHT model. Hardening effects and even failure states at positive confining pressures have not been investigated in the numerical study but may be modeled in the future via the mathematical formulation presented in this subsection. In sandstone, the capped yield surface can
be satisfactorily correlated to the RHT yield formulation by incorporating a pressure-dependent cap function. The hardening behavior of sandstone is, as for quartzite, open to further investigations.

7.3.5 Accumulated damage and residual surface

The last aspect to consider in the RHT model is the post-failure behavior. After achievement of the failure surface, the material subsequently softens and is subjected to a gradual stress decrease. The softening law is, analogously to the hardening law described in the previous subsection, monitored by an interpolation between the failure surface and a so-called residual surface. The residual surface is described by a user-defined power law. The weighting factor to be applied on the residual surface is given by the damage variable \( D = \sum \Delta \varepsilon_{\text{pl}} \varepsilon_{\text{eff}}^f \), where \( \sum \Delta \varepsilon_{\text{eff}} \) is the sum of plastic strain increments and \( \varepsilon_{\text{pl}}^f \) is the maximum allowable plastic strain. The latter quantity obeys a user-defined power law with respect to the normalized pressure \( P^* \). The normalized softening stress curve at a fixed damaged state is denoted by \( \sigma_D^* \). More details about the damage description can be found in [48].

![Figure 7.14: Left: typical evolution of the damage variable \( D \) as a function of the cumulated plastic strain increments \( \sum \Delta \varepsilon_{\text{eff}} \) for different normalized pressures values \( P^* \) relatively to \( -P^*_1 \). Right: representation of failure surface, intermediate damaged surface and residual surface over normalized pressure \( P^* \).](image)

In quartzite and sandstone, the post-failure behavior in the negative pressure range, as e.g. observable in Figure 7.2 via the stress decline, has
not been investigated numerically. Since the mesoscale model accounts for energy dissipation processes via the cohesive zone formulation, the softening behavior as suggested by the RHT model can be used in future investigations. Nevertheless, the strain-based softening behavior available in the RHT model may need to be reformulated into a displacement-based softening behavior, as suggested in [89]. This way, mesh dependency effects might be limited as has been already the case in the mesoscale modeling owing to the cohesive zone formulation.
This work has been motivated by the long-term striving of the geoscientific community to enrich the comprehension and prediction of meteorite impact cratering scenarios from a modeling point of view. Impact cratering physics is dominated by a multitude of interacting mechanical phenomena. In this regard, the setup of a genuine, predictive material model is not straightforward. In this work, and for pragmatic reasons, partitioning of physical phenomena has been used to facilitate the problem resolution. For this purpose, the focus has been set on two key physical phenomena contributing to cratering. The first one is compressive shock loading which is mainly associated to the contact and compression stages following impact. The second one concerns dynamic fracture loading which is mostly encountered in the subsurface area in the form of spallation plates. The modeling of the latter phenomenon has been especially encouraged by strength-dominated crater formations. There, the appraisal of spallation effects allows geologists to trace back the interpretable transient crater from the final crater with good approximation.

In a preliminary step, Representative Volume Elements have been devised for quartzite and sandstone and have been meshed with tetrahedral finite elements. In order to ensure a good representativeness of the real rock microstructures, the RVEs have been generated on the basis of measured grain size distributions. The quartzite RVE has been set up using a Voronoi diagram, in which polygonal quartz grains with clearly-resolved grain boundaries could be aggregated to a compact structure. For sandstone, an improved version of the structure generator GEOSTAT, randomly seeding ellipsoidal grains into a cubic box while achieving a prescribed porosity, has been successfully employed. Since quartzite and sandstone are of isotropic nature, the choice for the generation of random grain geometries and orientations has been considered legitimate.

A key physical process driving the spallation behavior of quartzite and sandstone is inter-granular failure. Due to the high strength of quartz grains compared to the inter-granular strength, intra-granular failure has not been considered. An improved cohesive zone formulation has been developed in order to ensure a consistent and robust modeling of inter-granular failure. The general idea of cohesive zone models is that a
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process zone, located at the forefront of a crack, is initiated once a critical traction is reached. This process zone then gradually develops through the interfacial region in a physical way. An advantage offered by the cohesive zone formulation over continuum-based failure models, when applied to a Finite Element scheme, is the energy-based decohesion behavior following failure initiation, thus reducing mesh size effects. The use of an initially rigid cohesive law has proven to be the most suitable solution for modeling quartzite and sandstone. Indeed, no artificial degradation of the bulk stiffness due to premature activation of cohesive zone elements, as would be encountered in an initially elastic approach, has had to be dealt with. Nevertheless, the sudden formation of cohesive zones has caused some robustness issues, especially in the very first decohesion steps. The first issue has been concerned with cohesive force jumps arising in multi-branched failure paths, for which multiple node splits occur. This issue has been successfully solved by enforcing a time-continuous description of node accelerations. The second issue has been related to extremely large stiffness in cohesive zone elements that undergo an elastic release subsequently to small decohesion. This issue has been fixed by the application of corrective node accelerations taking into account the mutual internal forces of paired nodes.

The availability of an efficient and robust cohesive zone formulation has been crucial for this work as it represents the baseline for an accurate and robust model for tensile failure in quartzite and sandstone. For this purpose, a mesoscale setup has been generated on the basis of Split-Hopkinson-Bar-Tests in spallation configuration with an adapted geometry and revised boundary conditions. For each rock type, the RVE has been geometrically extended to the experimental specimen length via the insertion of an equivalent homogeneous material. A compressive velocity wave signal, indirectly derived from experimental measurements, has been applied on the free end of the modeled specimen. Lateral borders have been kept stress-free to ensure a macroscopic one-dimensional stress state comparable to the experiments. The purpose of Split-Hopkinson-Bar-Tests in spallation configuration has been to determine the dynamic tensile strength and dynamic fracture energy of the specimen. To achieve this, an equivalent numerical instrumentation has been implemented in order to deliver macroscopic quantities on the same basis as the experimental instrumentation. The natural mesoscale parameters describing tensile failure have been those associated with the cohesive zone parameters, namely the mesoscale critical traction and the
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mesoscale fracture energy. For sandstone and quartzite, the values of these parameters were not known before and could not be determined directly from experiments. Accordingly, a parameter study has been conducted on the mesoscale to identify mesoscale parameters that reproduce, after homogenization, the tensile strength and fracture energy observed on the macroscale. This way, separate sets of mesoscale parameters have been calibrated for quartzite and sandstone owing to their different geological formation. Furthermore, limitations of the experimental instrumentation have been pointed out and enhanced, physically-based analysis methodologies have been proposed and applied to the numerical modeling. Modeling of dynamic fracture in quartzite and sandstone has required the use of simplified geometries in order to keep the computational effort reasonable. Concomitantly, the crack location has been enforced, meaning that no secondary cracks have been modeled. In spite of these limitations, microstructural features have been successfully transported to the macroscale. In a nutshell, the main finding of the Split-Hopkinson-Bar simulations has been the determination, for each rock type, of values for the mesoscale critical traction and the mesoscale fracture energy that describe inter-granular strength reliably. The indirect calibration of mesoscale parameters to experimental data has been successfully conducted using variable homogenization.

Shock compression is the second key loading case that has been addressed in mesoscale modeling. For this purpose, two different discretization schemes have been employed. While the meshfree Smoothed Particle Hydrodynamics (SPH) scheme has been devoted to idealized sandstone geometries, in which porosity and pore content have been varied, the Finite Element (FE) method has been employed to model more realistic quartzite and sandstone geometries, in which grain shapes and orientations could be explicitly resolved. A parameter study has been conducted to assess the influence of impact velocity, porosity, pore content and the constitutive model for quartz on pore collapse dynamics and macroscopic shock Hugoniot data. In the SPH simulations, jetting and shrinking mechanisms relative to pore collapse have been observed, which are in good agreement with experimental observations in the literature. Furthermore, the impact of both, porosity and water content, on shock velocity and compressive longitudinal stresses have been quantified. Porosity weakens the propagation and pressure level of the shock wave whereas water-filling enhances them. The flattening of Hugoniot curves at intermediate particle velocities is caused by the quartz
phase transition prescribed by the Analytical Equation of State (ANEOS). This characteristic kink compares well with literature shock data and confirms the need for incorporating phase transitions into the quartz Equation of State in the shock loading regime. In the FE simulations, the focus has been set on quartz shear strength variations to quantify quartz strength effects on shock Hugonions. In particular, the enhancing effect of quartz stiffness on shock velocity in the lower shock regime has been observed and corroborated by experimental shock data in the literature. Slight effects of quartz anisotropy on shock Hugonions have been observed for sandstone only, whilst for quartzite, they are negligible. Some features such as the ANEOS model could not be incorporated in the FE formulation, especially due to contact issues. Similarly, quartz anisotropy has not been considered in the SPH formulation since grain boundaries cannot be explicitly resolved. As a result, the unification of material properties into a single mesoscale model has not been achieved yet. To summarize, the main finding of the shock compression simulations has been to identify the mechanisms relating mesoscale properties, such as porosity, water-filling, anisotropy, shear strength, to macroscale properties, such as pore closure, shock wave propagation, shock pressure, shock velocity. Via the analysis of literature-based shock data on quartzite and sandstone, promising suggestions for enhanced mesoscale modeling have been given. Amongst others, the incorporation of the ANEOS Equation of State, pressure-dependent stiffness and plasticity into a single quartz model is a goal to pursue. With the achievement of such a complex mesoscale model, detailed macroscale shock Equations of State can be elaborated using homogenization. Besides, deeper investigations about the influence of mesoscale parameters on micromechanical features such as Planar Deformation Features (PDFs) or pore collapse dynamics can be envisaged in future research.

The last step of this work has consisted in extending the collection of homogenized relationships for quartzite and sandstone in order to generate homogenized strength data for the development of macroscale models. To achieve this, different loading paths, defined via three independent velocity components, have been applied to quartzite and sandstone RVEs at three different strain rates. Inter-granular strength has been modeled with the mesoscale failure parameters determined in Split-Hopkinson-Bar simulations. Triaxiality-dependent yield and failure surfaces have been derived for quartzite and sandstone. The conical, open-shaped yield surface of quartzite towards high pressures indicates the reversibility
of pure compressive loading, whereas the capped yield surface in sandstone represents irreversible pore crushing. Finally, a concept has been presented how the mesoscale simulation results may be transferred to macroscale models, in particular to the RHT model.

In summary, the key result of this work has been the determination of macroscale properties for quartzite and sandstone on the basis of realistic microstructural geometries and realistic material properties. There, strain rate regimes ranging from moderate dynamics up to the shock regime have been covered. A high added value of this work is that the methodologies that have been developed for quartzite and sandstone constitute a toolbox that can be extended to any other generic material, in particular to granular materials. This use of this toolbox naturally requires the availability of data from experiment or natural observation in order to provide a solid basis for mesoscale modeling and parameter calibration.
9 Outlook

As a suggestion for future research, a number of tasks, aimed at improving and broadening the outcomes of this thesis, are recommended.

The first task that should be taken is the elaboration of a macroscale material model using parameters which can be explicitly quantified from the simulated material response on the mesoscale. The capabilities of the RHT model have been shown in this thesis and can be used to parameterize the macroscale material model.

The second task is the indirect validation of the mesoscale model by laboratory cratering experiments. This step is essential since the parameter calibration conducted for each individual phenomenon in the mesoscale modeling is precisely aimed at reconstituting step by step the whole cratering mechanics via homogenization. This way, existing MEMIN cratering experiments on the laboratory scale offer an excellent opportunity to validate the mesoscale model indirectly by using the macroscale model generated in the first proposed task.

The third task is an extended mesoscale modeling of partially or completely water-filled sandstone. This has already been addressed for the case of idealized sandstone geometries under compressive shock loading using the SPH formulation. Extending the modeling of water-filled sandstone to dynamic tensile loading cases shall provide knowledge about water effects on failure initiation and energy dissipation that can be compared with dry sandstone. Yield and failure surfaces of water-filled sandstone can then be derived and a new macroscopic variable, standing for the water-filling degree of the material, may be defined.

The last recommended enhancement of the mesoscale model is the incorporation of intra-granular failure in quartz [57], depicted by grain comminution in [16], into mesoscale modeling of high compressive and shear loading scenarios. This is, however, a challenging task as the very diffuse and random nature of failure paths all over the geometric mesh may compromise the robustness of the required combination of contact and cohesive zone formulations.
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All these improvements are aimed at developing a predictive macroscale model capable of replicating impact cratering scenarios from the laboratory scale to the natural scale with the help of scaling laws.

Finally, and probably most interesting for the geoscience community, the mesoscale simulation should be used to support the analysis of microstructural phenomena found in real, impacted rocks such as Planar Deformation Features. Due to the new level of detail that could be realized in the mesoscale modeling of quartzite and sandstone, quantitative estimates, e.g. on the level of pressures reached in grain-to-grain contacts, are now possible.
Bibliography

10 Bibliography


11 Appendix: mesostructure generator GEOSTAT

The structure generator GEOSTAT creates cubic voxel-based material distributions with controlled statistics and porosity. From the original GEOSTAT program, some improvements have been realized. Amongst others, the granular spheres to be seeded have been replaced by volume-equivalent ellipsoids with three independent semi-axes. Besides, the treatment of overlapping objects has been refined. The course of action of GEOSTAT can be split in three phases, namely seeding, voxel filling and growing-shrinking.

11.1 The seeding phase

Departing from a statistic grain size distribution, ellipsoids are seeded via their centroids into a cubic box. Their semi-axis lengths and orientations are randomly defined with the requirement that the seeded volumes conform to the grain size distribution. A condition on the aspect ratio of ellipsoids can also be imposed, e.g. the largest semi-axis length shall not exceed the smallest one by a factor two. To ensure a successful placement of ellipsoids, two criteria must be met:

a) An ellipsoid cannot overlap with already placed ellipsoids, unless an overlapping tolerance criterion is defined, see section 11.4 in this appendix. In order to optimize the placement of all prescribed ellipsoids, ellipsoids with the highest volumes are placed first, followed by decreasing volumes. This facilitates the insertion of smaller ellipsoids in available interstitial spaces. If the GEOSTAT program, after a user-defined number of trials, fails to find a convenient centroid position satisfying the overlapping criterion, the ongoing tentative volume is skipped and the process is repeated for the next lower volume.

b) The crossing tolerance of ellipsoids beyond box boundaries must be clearly defined by the user. Ellipsoids may be allowed to cross the box boundaries without any restriction, up to a limited amount, or not at all. In each case, the reference cubic box of interest remains unchanged, thus meaning that ellipsoids might get cut off at the
box boundaries. If periodic boundaries are prescribed, the outside part of an ellipsoid crossing a boundary surface is transferred to the opposite boundary surface. Any operation on spatial coordinates, and especially overlapping checks, must accordingly be performed modulo the cube edge length. Periodization can be very useful when a row of RVEs need to be appended to each other. A periodized sandstone RVE generated with GEOSTAT is exemplarily depicted in Figure 11.1.

Figure 11.1: Exemplary GEOSTAT-generated sandstone RVE with periodic boundaries.

11.2 The voxel filling phase

The purpose of this phase is to place a voxel grid with user-defined coarseness on the cubic box and to register for each grain the whole set of voxels it encompasses. This way, the volume percentage of the cubic box effectively filled with matter can be gauged. The finer the voxel mesh is, the more accurate is the voxel attribution to grains. Due to potential grain overlaps, the volume of the resulting material volume generally underrates the sum of individual raw volumes seeded into the box. In practice, the voxel filling process shall evaluate whether voxel centroids belong to at least one ellipsoid, i.e. satisfy at least one ellipsoid equation, see Inequation (11.1).
Let $E_i$ be an ellipsoid centered on the origin for which the semi-axes, of lengths $a_i, b_i, c_i$, respectively, are aligned with the vectors of the canonic base $B = (\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$. If a point $M$, represented by the coordinate vector $X = (x, y, z)^T|_B$, is located inside the volume of $E_i$, it must satisfy the ellipsoid inequation:

$$\frac{x^2}{a_i^2} + \frac{y^2}{b_i^2} + \frac{z^2}{c_i^2} \leq 1 \quad (11.1)$$

Let $A_i$ be the matrix defined by:

$$A_i = \begin{pmatrix} 
\frac{1}{a_i^2} & 0 & 0 \\
0 & \frac{1}{b_i^2} & 0 \\
0 & 0 & \frac{1}{c_i^2} 
\end{pmatrix}$$

$A_i$ represents the quadratic form of the ellipsoid and Inequation (11.1) can be rewritten as $X^T A_i X \leq 1$. If the ellipsoid $E_i$ is now oriented along arbitrary coordinate axes, as given by a new cartesian base $B^{(i)} = (\mathbf{e}'_x, \mathbf{e}'_y, \mathbf{e}'_z)$, the quadratic form can be expressed by:

$$X'^T A_i X' \leq 1 \quad (11.2)$$

where $X' = (x', y', z')^T|_{B^{(i)}}$ is the coordinate vector of $M$ in $B^{(i)}$. Let $P_i$ be the change base matrix from $B^{(i)}$ to $B$, it follows from the ellipsoid Inequation (11.1) and from $X' = P_i X$ a rotated inequation:

$$X^T A_i' X \leq 1 \quad (11.3)$$

where $A_i' = P_i^T A_i P_i$. If the centroid of $E_i$ is not at the origin but defined by the vector $X_{i0} = (x_{i0}, y_{i0}, z_{i0})^T|_B$, Inequation (11.3) can be generalized to:

$$(X^T - X_{i0}^T) A_i' (X - X_{i0}) \leq 1 \quad (11.4)$$
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The change base matrix $P_l$ expresses the canonic axes of $B$ with respect to the axes of $B^{(l)}$, along which $E_l$ is oriented. Thus, $P_l$ is an orthogonal matrix with the property $P_l^T = P_l^{-1}$ and is obtained by the multiplication of three orthogonal rotation matrices along each canonic axis, respectively. The transformation of $B$ to $B^{(l)}$ can be defined by the application of successive rotations along $e_x$ by an angle $\theta_1$, along $e_y$ by an angle $\theta_2$ and along $e_z$ by an angle $\theta_3$, respectively. Therefore, $P_l$ is given by the product of three rotation matrices:

\[
P_l = \begin{pmatrix}
    c_1 & s_1 & 0 \\
    -s_1 & c_1 & 0 \\
    0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
    c_2 & 0 & s_2 \\
    0 & 1 & 0 \\
    -s_2 & 0 & c_2
\end{pmatrix} \begin{pmatrix}
    1 & 0 & 0 \\
    0 & c_1 & s_1 \\
    0 & -s_1 & c_1
\end{pmatrix}
\]

where $c_k = \cos(\theta_k)$ and $s_k = \sin(\theta_k)$, for $k = 1, 2$ or $3$. After matrix multiplication, $P_l$ can be summarized into the expression:

\[
P_l = \begin{pmatrix}
    c_1c_3 - s_1c_2s_3 & s_1c_3 + c_1c_2s_3 & s_2s_3 \\
    -c_1s_3 - s_1c_2c_3 & c_1c_2c_3 - s_1s_3 & s_2c_3 \\
    s_1s_2 & -c_1s_2 & c_2
\end{pmatrix}
\] (11.5)

By browsing the voxels covered by each ellipsoidal grain, voxels, the centroids of which satisfy Inequation (11.4) are labeled with the corresponding grain ID. If further grains fulfill this criterion on already labeled voxels, a discriminating process is conducted such that voxels are eventually attributed to one single grain ID. Usually, it consists in seeking the minimum of the distance between the voxel center and each conflicting ellipsoid centroid. Alternatively, this distance can be normalized by the equivalent radius of the ellipsoid before being minimized. The single or multiple grain presence in voxels can also be the consequence of growth or shrinking phases, as portrayed in the following section.

11.3 The growth-shrinking phase

This growth-shrinking phase is intended to control the porosity of the whole structure. Basing on the voxel grid from the previous phase, porosity can be calculated as the ratio of void voxels, i.e. voxels without grain attribution, over the total number of voxels. If the user-defined target porosity is higher than the current one, ellipsoid volumes are
reduced by a user-defined shrinking factor. If, in contrast, the target porosity is lower than the current one, ellipsoids grow via an enlargement factor and may thus overlap. Optionally, the shrinking or enlargement factor can be defined in an adaptive way such that isolated ellipsoids undergo larger volume variations than tighter ellipsoids. By recourse to the voxel grid, the voxel filling phase, including grain discrimination, is performed again, followed by porosity reevaluation and if necessary, the application of a new shrinking or enlargement factor. This double process is iteratively operated until the porosity approaches the target porosity within a certain tolerance interval.

11.4 Overlapping tolerance

The introduction of a user-defined overlapping tolerance in GEOSTAT is motivated by two reasons. First, grain overlapping breaks up with ideal ellipsoidal shapes in that arbitrariness is introduced into grain shapes, thus making the mesostructure geometry closer to nature. Second, grain overlapping enhances the population of inter-granular surfaces, which is an essential feature when inter-granular failure is modeled, e.g. via the use of cohesive zone elements.

In the ideal case of spheres, the overlapping tolerance definition is trivial. Given two spheres of centers $O_i$ and $O_j$ and of radii $r_i$ and $r_j$, respectively, the overlapping length $l_{ij}$ is defined as the part of the center-to-center segment $O_iO_j$ that lies in the sphere overlapping volume, see Figure 11.2. This overlapping length should not exceed a user-defined percentage $p_{tol}$ of each sphere radius.
Mathematically, the overlapping criterion can be summarized as follows:

\[ l_{ij} \leq p_{tot} \cdot r_i \text{ and } l_{ij} \leq p_{tot} \cdot r_j \]  

(11.6)

By introducing the inter-centroid distance \( o_i o_j \), Inequalities (11.6) can be rewritten into:

\[ o_i o_j \geq (1 - p_{tot}) r_i + r_j \text{ and } o_i o_j \geq (1 - p_{tot}) r_j + r_i \]  

(11.7)

Whereas the overlapping criterion for spheres can be easily defined via the inter-centroid distance and the sphere radii, overlapping in ellipsoids is more delicate to define. Given two ellipsoids \( E_i \) and \( E_j \), interpenetration is prevented if, for any point \( M_i \) inside \( E_i \) and represented by the vector \( X_i \), the following inequation is satisfied:

\[ (X_i^T - X_{j0}^T)A_j'(X_i - X_{j0}) > 1 \]  

(11.8)

Inequality (11.8) is the negation of Inequality (11.4) by taking \( E_j \) as the reference ellipsoid. By introducing an overlapping tolerance \( p_{tot} \) such that \( 0 \leq p_{tot} \leq 1 \), Inequality (11.8) can be softened to:
\begin{align}
(X_i^T - X_{j0}^T)A_j'(X_i - X_{j0}) &\geq p_{tol}^2 \tag{11.9}
\end{align}

$p_{tol} = 0$ allows for full volume interpenetration whereas $p_{tol} = 1$ forbids any interpenetration. Graphically, $p_{tol}$ represents the scaling factor of a homothetic ellipsoid with respect to $E_j$, see Figure 11.3-left.

Reversely, any point point $M_j$ inside $E_j$ and represented by the vector $X_j$ must satisfy the inequation:

\begin{align}
(X_j^T - X_{i0}^T)A_i'(X_j - X_{i0}) &\geq p_{tol}^2 \tag{11.10}
\end{align}

In the following, Inequation (11.9) will be taken as reference, i.e. the penetration condition of points of $E_i$ into $E_j$ will be investigated. The left member of Inequation (11.9) can be defined as a function of type $f_j(X_i) = (X_i^T - X_{j0}^T)A_j'(X_i - X_{j0})$, where $X_i$ can vary within $E_i$ and all terms indexed by $j$ are constant as $E_j$ is the reference ellipsoid. To fulfill the inequation $f_j(X_i) \geq p_{tol}^2$ for any $X_i$, it is sufficient to check if it is fulfilled for $X_i^{\min}$ which represents the global minimum of $f_j$. This global minimum is naturally located on the surface of $E_i$. To find it out, the surface of $E_i$ is parametrized by two independent variables $u$ and $v$ with $(u, v) \in [-\pi, \pi] \times [-\frac{\pi}{2}, \frac{\pi}{2}]$, such that any point $M_i$ on the surface of $E_i$ can be expressed in the local coordinate system $B^{(i)}$ of $E_i$ by the vector $X_i$ of coordinates:

\begin{align*}
    x_i' &= a_i \cos(v) \cos(u) \\
    y_i' &= b_i \cos(v) \sin(u) \\
    z_i' &= c_i \sin(v)
\end{align*}

The vector of $M_i$ in the canonic base is thus expressed by $X_i(u, v) = P_i^{T}X_i' + X_{i0}$. The function $f_j$ can be redefined as a function $F_j$ of two independent variables $u$ and $v$:

$$
[-\pi, \pi] \times [-\frac{\pi}{2}, \frac{\pi}{2}] \to \mathbb{R} \\
(u, v) \mapsto F_j(u, v) = f_j(X_i(u, v))
$$
Different numerical minimization methods exist to determine the minimum of a multi-variable function. The first issue encountered is the presence of several local minima of \( F_j \), as exemplarily illustrated in Figure 11.3-right.

![Figure 11.3](image)

Figure 11.3: Left: 2D projection of two interpenetrating ellipsoids. Right: graphical representation of the two-variable function \( F_j(u, v) \).

To ensure that the seeking of the global minimum is conducted in the right function valley, a prerequisite step, intended to eliminate other local minima of the research, is performed. By subdividing \([-\pi, \pi]^2\) into regular cells, the function \( F_j \) is evaluated at a finite number of \((u, v)\) pairs. Let \((u^0, v^0)\) be the \((u, v)\) pair that minimizes \( F_j \) in this discretization. Provided that the discretization is fine enough, \( F_j(u^0, v^0) \) is ensured to stand in the global valley and is thus labeled as the global discrete minimum of \( F_j \). For a finer minimization, the following loop algorithm is executed and initialized with the integer \( k = 0 \).

a) Calculate the direction of the steepest descent of \( F_j \) at the point \((u^k, v^k)\), given by the vector \(-\nabla F_j(u_k, v_k)\). The normalized gradient vector is defined by:

\[
e^k = \frac{-\nabla F_j(u_k, v_k)}{\|\nabla F_j(u_k, v_k)\|}
\]
where $e_k^\xi = \left( \frac{\partial F_j}{\partial u}(u_k, v_k), \frac{\partial F_j}{\partial v}(u_k, v_k) \right)^T$

b) The intent is to translate the point $(u^k, v^k)$ along the vector $e_k^\xi$ and to seek the minimum of $F_j$ along this one-dimensional path. For this purpose, one defines the mono-variable function:

$$[0, \infty] \rightarrow \mathbb{R}$$

$$t \mapsto g_k(t) = F_j(u^k - t \cdot e^k_{u}, v^k - t \cdot e^k_{v})$$

with $e^k_{u} = -\frac{\partial F_j(u^k, v^k)}{\|\nabla F_j(u_k, v_k)\|}$ and $e^k_{v} = -\frac{\partial F_j(u^k, v^k)}{\|\nabla F_j(u_k, v_k)\|}$

c) Finding the minimum of $g_k$ can be transposed into finding the zero point of its derivative $\frac{dg_k}{dt}$. By using the cascade derivation rule, $\frac{dg_k}{dt}$ is given by the following scalar product:

$$\frac{dg_k}{dt} = -e^k_\xi \cdot \nabla F_j(u^k - t \cdot e^k_{u}, v^k - t \cdot e^k_{v})$$

d) As the research of the minimum is performed in the global valley of $F_k$, the restricted function $g_k$ admits a single minimum for $t \geq 0$ and its derivative is monotonic. It can be easily shown that:

$$\frac{dg_k}{dt}(t = 0) = -\|\nabla F_j(u_k, v_k)\| < 0$$

Due to the monotonicity of $\frac{dg_k}{dt}$, there exists a value $t > 0$ from which $\frac{dg_k}{dt} > 0$. The variable $t$ is thus stepwise increased until $\frac{dg_k}{dt}$ becomes positive. As far as the zero point of $\frac{dg_k}{dt}$ is confined between two known bounds, a classical dichotomy method can be executed. Calling $t^p_{left}$ such that $\frac{dg_k}{dt}(t^p_{left}) < 0$ and $t^p_{right}$ such that $\frac{dg_k}{dt}(t^p_{right}) > 0$, the dichotomy is executed until a stop criterion is fulfilled, as summarized in the following sub-loop initialized with $p = 0$. 
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i) set $t_{mid}^p = \frac{t_{left}^p + t_{right}^p}{2}$ and evaluate $\frac{dg_k}{dt}(t_{mid}^p)$

ii) if $\frac{dg_k}{dt}(t_{mid}^p) > 0$, set $t_{left}^{p+1} = t_{left}^p$ and $t_{right}^{p+1} = t_{mid}^p$
dead if $\frac{dg_k}{dt}(t_{mid}^p) < 0$, set $t_{left}^{p+1} = t_{mid}^p$ and $t_{right}^{p+1} = t_{right}^p$

iii) Increment $p$ by 1

iv) if $|t_{mid}^p - t_{mid}^{p-1}| > t_{stop}$, iterate the sub-loop again.

e) Increment $k$ by 1 and set:

$$(u^k, v^k) = (u^{k-1} - t_{mid}^p \epsilon_{u}^{k-1}, v^{k-1} - t_{mid}^p \epsilon_{v}^{k-1})$$

f) If the cartesian distance between $(u^k, v^k)$ and $(u^{k-1}, v^{k-1})$ still exceeds a user-defined distance tolerance $d_{tol}$, iterate the main loop again.

Eventually, the evaluation of $f_j$ at the final $(u^k, v^k)$ pair can be used to check the fulfillment or not of Inequation (11.9). If the latter is fulfilled, a new ellipsoid can be seeded, otherwise the ellipsoid centroid is tentatively shifted to another location within the seeding box, and the whole interpenetration check procedure must be conducted again.

Defining an overlapping tolerance in GEOSTAT presents a double advantage. Not only does it break up with the original spherical shapes of grains to make them more arbitrary, i.e. more realistic, but it also eases the seeding process by offering more free space for the seeding. Nevertheless, the major disadvantage is that every overlapping volume between two or more spheres represents a volume loss. This way, the grain distribution resulting from the GEOSTAT process may be altered with regard to the prescribed grain size distribution.

To investigate how far the overlapping tolerance affects the final grain size distribution, a small parameter study is conducted. By departing from a grain size distribution in sandstone with a porosity of 23 %, three overlapping tolerance values have been defined: 40, 60 and 80 %. Due to the loss in volume induced by grain overlapping, the growth phase must be repeatedly called by the GEOSTAT program in order to catch up to the target porosity of 23 %. The raw grain size distribution and those
resulting from the overlapping tolerance criteria are plotted in Figure 11.4. Here, the cumulative frequency against the equivalent grain diameter is represented.

Figure 11.4: Cumulative grain frequency over equivalent grain diameter from a grain size distribution in sandstone (23 % porosity) before and after GEOSTAT processing, using three overlapping tolerance values: 40 %, 60 % and 80 %.

As can be observed in Figure 11.4, the grain size distributions after the GEOSTAT processing for overlapping tolerances of 40 %, 60 % and 80 % show an excellent accordance with the raw grain size distribution. As an explanation for this result, the volume loss of individual grains due to overlapping in the seeding phase seems to be compensated by the subsequent grain expansion in the iterative growth phase. In this regard, the GEOSTAT program proves to be a powerful and efficient tool for generating granular structures on the basis of grain size distributions.