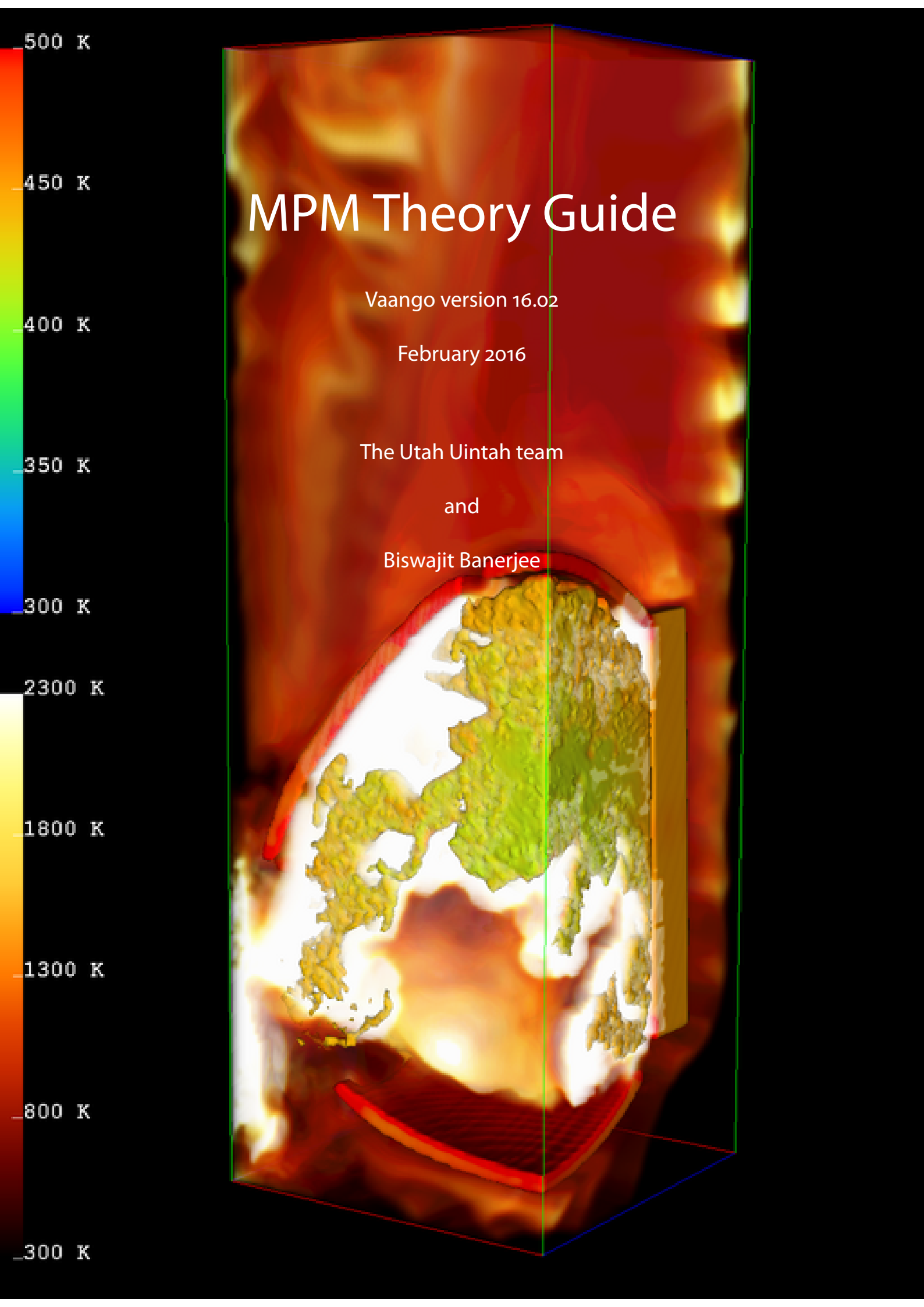

MPM Theory Guide

Vaango version 16.02

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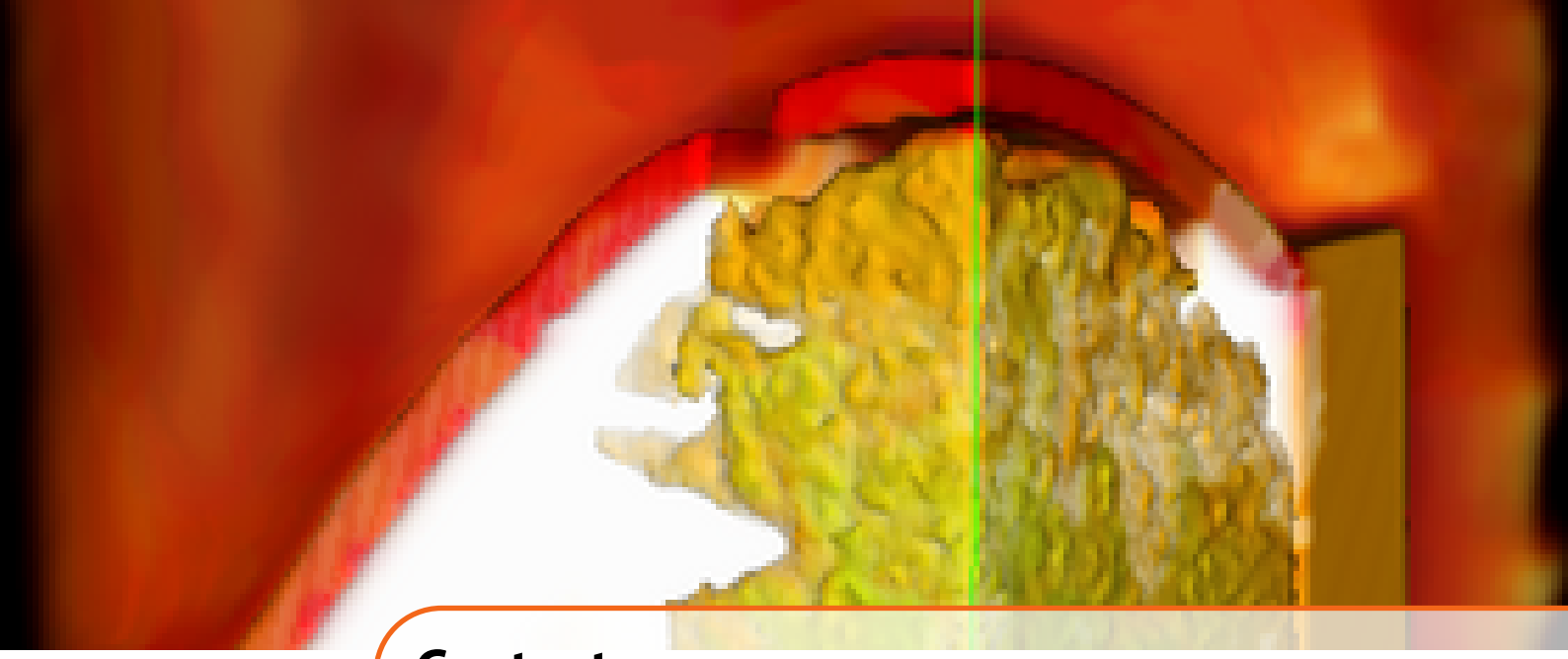
The Utah Uintah team

and

Biswajit Banerjee

The contents of this manual can and will change significantly over time. Please make sure that all the information is up to date.



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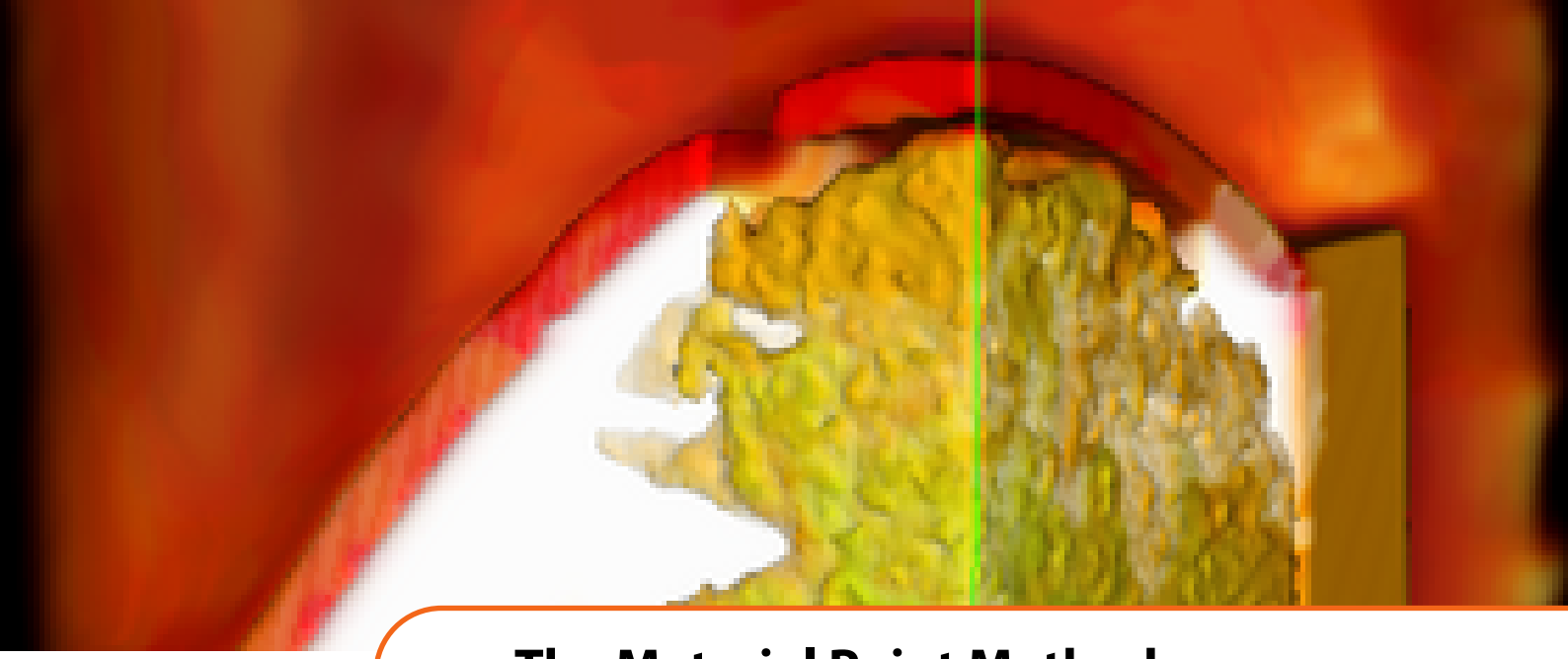


1 — The Material Point Method

1.1 Introduction

The Material Point Method (MPM) as described by Sulsky, et al. [SCS94; SZS95] is a particle method for structural mechanics simulations. Solid objects are represented by a collection of particles, or "material points." Each of these particles carries with it information for that part of the solid object that it represents. This includes the mass, volume, position, velocity and stress of that material. MPM differs from other so called "mesh-free" particle methods in that, while each object is primarily represented by a collection of particles, a computational mesh is also an important part of the calculation. Particles do not interact with each other directly, rather the particle information is interpolated to the grid, where the equations of motion are integrated forward in time. This time advanced solution is then used to update the particle state. An example of two disks initially approaching each other represented by material points on an overlying mesh is show in Figure 1.1.

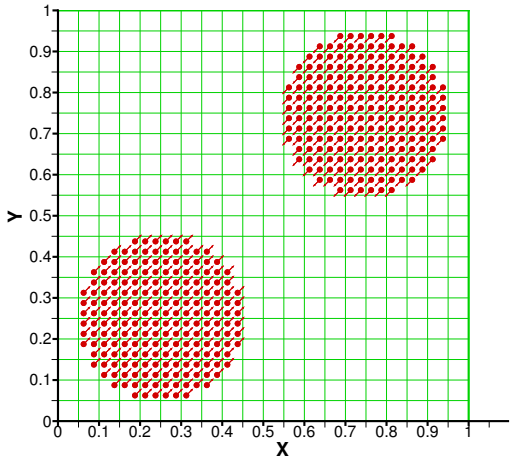


Figure 1.1: Initial particle representation of two colliding disks on an overlying mesh.

The method usually uses a regular structured grid as a computational mesh. While this grid, in principle, deforms as the material that it is representing deforms, at the end of each timestep, it is reset to it's original undeformed position, in effect providing a new computational grid for each timestep. The use of

a regular structured grid for each time step has a number of computational advantages. Computation of spatial gradients is simplified. Mesh entanglement, which can plague fully Lagrangian techniques, such as the Finite Element Method (FEM), is avoided. MPM has also been successful in solving problems involving contact between colliding objects, having an advantage over FEM in that the use of the regular grid eliminates the need for doing costly searches for contact surfaces[BBS00].

The choice of MPM over FEM as the C-SAFE structural mechanics method was only in small part for the above mentioned criteria. The primary motivation was the ability to use MPM together with a multimaterial CFD algorithm for solving tightly coupled fluid-structure interaction problems. This capability was first demonstrated in the CFDLIB codes from Los Alamos by Bryan Kashiwa and co-workers. There, as in Vaango, MPM serves as the Lagrangian description of the solid material in a multimaterial CFD code. Certain elements of the solution procedure are based in the Eulerian CFD algorithm, including intermaterial heat and momentum transfer as well as satisfaction of a multimaterial equation of state. The use of a Lagrangian method such as MPM to advance the solution of the solid material eliminates the diffusion typically associated with Eulerian methods.

1.2 Algorithm

While a more detailed description of MPM can be found in [SZS95], the algorithm is laid out here. The equations of motion are cast in the form:

$$\mathbf{M}_g \cdot \mathbf{a}_g = \mathbf{Fext}_g - \mathbf{Fint}_g \tag{1.1}$$

where $\mathbf{M}_g$ is the mass matrix, $\mathbf{a}_g$ is the acceleration vector, $\mathbf{Fext}_g$ is the external force vector (sum of the body forces and tractions), and $\mathbf{Fint}_g$ is the internal force vector resulting from the divergence of the material stresses. In general, $\mathbf{M}_g$ is a large, sparse matrix. In practice, and in what follows here, a "lumped" mass matrix is used, which only has entries on the diagonal, and is thus represented as a column matrix.

The solution procedure begins by interpolating the particle state to the grid, to form $\mathbf{M}_g$, $\mathbf{Fext}_g$, and to get a velocity on the grid $\mathbf{v}_g$. These quantities are calculated at each grid node by the following equations:

$$\mathbf{M}_i = \sum_p S_{ip} m_p \tag{1.2}$$

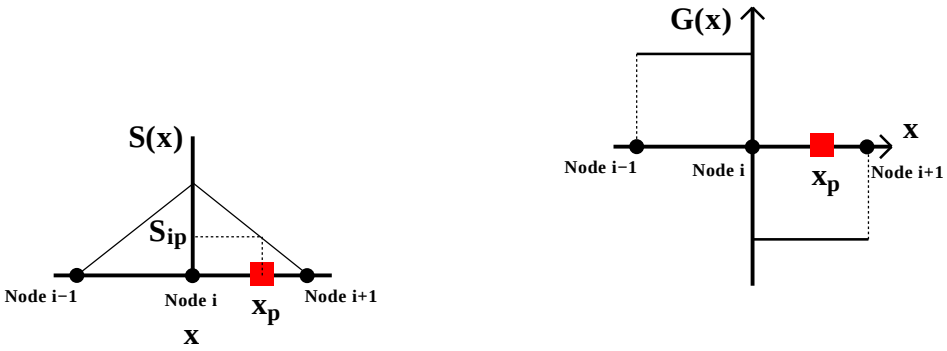
$$\mathbf{v}_i = \frac{\sum_p S_{ip} m_p \mathbf{v}_p}{\mathbf{M}_i} \tag{1.3}$$

$$\mathbf{Fext}_i = \sum_p S_{ip} \mathbf{Fext}_p. \tag{1.4}$$

m_p is the particle mass, $\mathbf{v}_p$ is the particle velocity, and $\mathbf{Fext}_p$ is the external force on the particle. The external force on the particle is generally an applied load of some type. In Equation 1.3, the numerator is the nodal momentum, which is then divided by the nodal mass to get a velocity. S_{ip} is a "shape function" for the ith node evaluated at $\mathbf{x}_p$. Traditionally, the shape functions are multiplicative combinations of one dimensional tent functions, as shown in Figure 1.2. The shape functions serve to distance weight the contribution of each particle to the grid nodes.

At this point, a velocity gradient, $\nabla \mathbf{v}_p$ is computed at each particle using the grid velocities $\mathbf{v}_g$:

$$\nabla \mathbf{v}_p = \sum_i \mathbf{G}_{ip} \mathbf{v}_I \tag{1.5}$$



$S(x) = (x - x_{i-1})/(x_i - x_{i-1})$ $\quad x_{i-1} < x < x_i$
$S(x) = (x_{i+1} - x)/(x_{i+1} - x_i)$ $\quad x_i < x < x_{i+1}$
$S(x) = 0$ $\quad x < x_{i-1} \quad x > x_{i+1}$

$G(x) = 1/(x_i - x_{i-1})$ $\quad x_{i-1} < x < x_i$
$G(x) = -1/(x_{i+1} - x_i)$ $\quad x_i < x < x_{i+1}$
$G(x) = 0$ $\quad x < x_{i-1} \quad x > x_{i+1}$

Figure 1.2: One dimensional linear shape function, $S(x)$ and its derivative, $G(x)$.

where $\mathbf{G}_{ip}$ is the gradient of the ith node's shape function, evaluated at $\mathbf{x}_p$. A one dimensional example of $\mathbf{G}_{ip}$ is shown in Figure 1.2. Note that in going to multiple dimensions, the $\mathbf{G}_{ip}$ are found by taking gradients of the multidimensional S_{ip} NOT by forming multiplicative combinations of the one-dimensional $\mathbf{G}_{ip}$.

This velocity gradient is used as input to a constitutive model (stress-strain relationship) which is evaluated at each particle. The specifics of this calculation are dependent on the constitutive model. An example of a simple elastic material model is described in the appendix. The result of this calculation is the Cauchy stress at each particle, $\boldsymbol{\sigma}_p$. With this, the internal force due to the divergence of the stress is calculated:

$$\mathbf{Fint}_g = \sum_p \mathbf{G}_{ip} \boldsymbol{\sigma}_p v_p \tag{1.6}$$

where v_p is the particle volume. The internal force can be thought of as the force that holds a material together. For a given deformation, this force is larger for stiffer materials.

Everything is now available to solve Equation 1.1 for $\mathbf{a}_g$. With that, the backward Euler method is used for all time integrations. A convective grid velocity $\mathbf{v}_g^L$ is computed:

$$\mathbf{v}_g^L = \mathbf{v}_g + \mathbf{a}_g dt \tag{1.7}$$

While the following calculation is never carried out, in principal, the nodes of the grid also move with that convective velocity:

$$\mathbf{x}_g^L = \mathbf{x}_g + \mathbf{v}_g^L dt \tag{1.8}$$

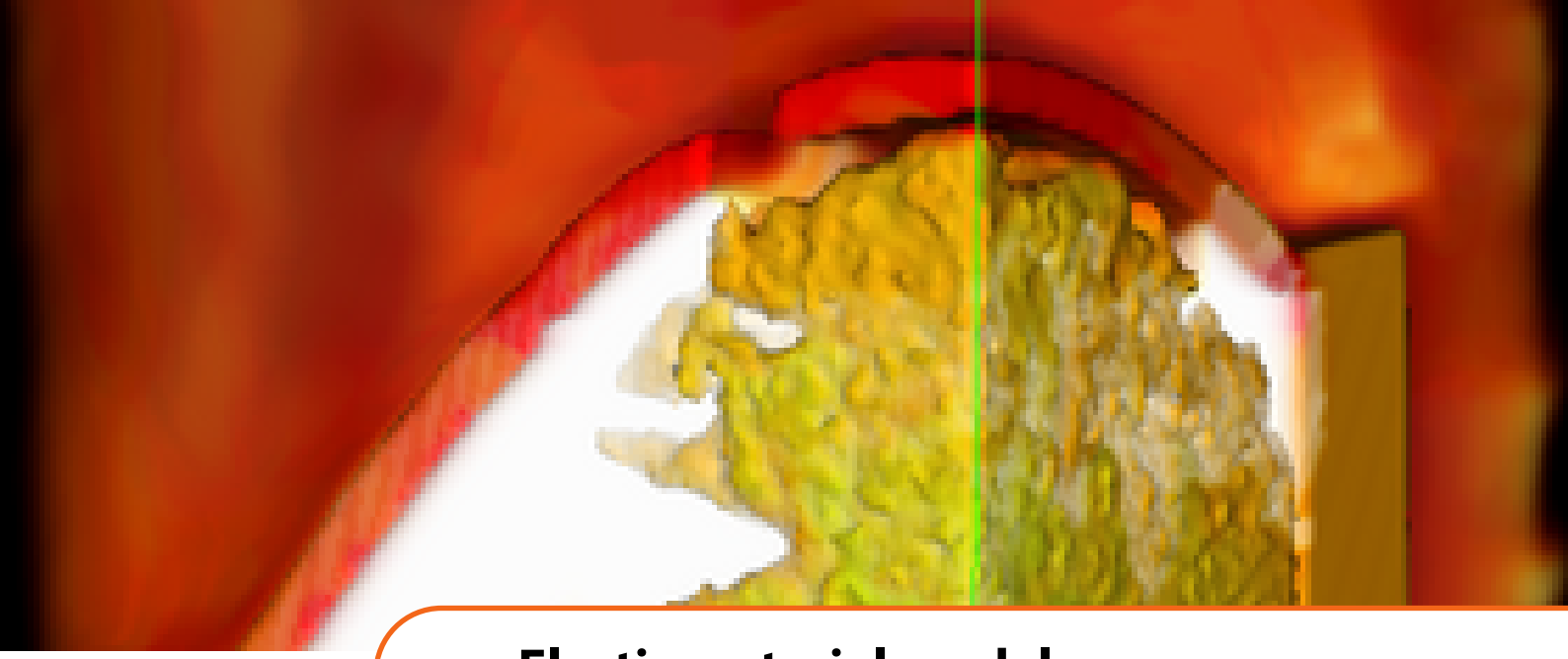
During this part of the computation, the particles move with the deforming grid. Their position and velocity is explicitly updated by:

$$\mathbf{v}_p(t + dt) = \mathbf{v}_p(t) + \sum_i S_{ip} \mathbf{a}_i dt \tag{1.9}$$

$$\mathbf{x}_p(t + dt) = \mathbf{x}_p(t) + \sum_i S_{ip} \mathbf{v}_i^L dt \tag{1.10}$$

This completes one timestep. Note that not carrying out the calculation in 1.8 explicitly has the effect of resetting the deformed grid to it's undeformed position at the end of the timestep cycle.

As with all explicit time integration methods, a timestep size limit must be enforced such that $dt < dx/(|\mathbf{v}_p| + c)$ for all particles, where dx is the computational grid spacing and c is the speed at which stress waves propagate through the material. Failure to adhere to this condition will cause the solution to become unstable and blow up. The material wavespeed depends on the material model used, as well as on the particular parameters chosen for that model. Specifics of calculating the wavespeed are given in the appendix.



2 — Elastic material models

2.1 Hyperelastic Material Models

The subject of modeling the response of materials to deformation is a subject that has filled numerous textbooks. Therefore, rather than attempt to condense these volumes, here the reader will be simply be given a simple material response model. Other more complex material response models can be interchanged in the framework discussed above quite readily.

The author has come to prefer a class of models known as hyperelastic models. What this means is that the stress response of these materials is derived from a strain energy function. A strain energy function gives a relationship between the state of deformation that a material is in, and the amount of stored strain energy that this material has. This is akin to the familiar relationship for the stored energy in a spring, $W = \frac{1}{2}kdx^2$ where k is the spring constant, and dx is the distance that the spring has been compressed or extended.

One such strain energy function is given by:

$$W = \frac{\lambda}{4}(J^2 - 1) - (\frac{\lambda}{2} + \mu)\ln J + \frac{\mu}{2}\mathrm{tr}(\mathbf{F}^T\mathbf{F} - 3) \tag{2.1}$$

from which the following relationship for the stress can be derived:

$$\boldsymbol{\sigma} = \frac{\lambda}{2}(J - \frac{1}{J})\mathbf{I} + \mu(\mathbf{F}\mathbf{F}^T) - \mathbf{I}) \tag{2.2}$$

where λ and μ are material constants, while J and $\mathbf{F}$ describe the state of deformation. These will be defined shortly.

In the Algorithm section, the calculation of the velocity gradient, $\nabla\mathbf{v}_p$ is given in Equation 1.5. Starting from there, we can then compute an increment in the deformation gradient, $\mathbf{F}(dt)$ by:

$$\mathbf{F}(dt) = \nabla\mathbf{v}_p dt + \mathbf{I}. \tag{2.3}$$

This increment in the deformation gradient can then be used to compute a new total deformation gradient using:

$$\mathbf{F}(t + dt) = \mathbf{F}(dt)\mathbf{F}(t). \tag{2.4}$$

Note that the initial (t=0) deformation gradient is simply the identity, i.e. $\mathbf{F}(0) = \mathbf{I}$. Now with the deformation gradient, one can compute J by:

$$J = \det(\mathbf{F}(t + dt)). \tag{2.5}$$

Note that J represents the volumetric part of the deformation. Specifically, it is the ratio of the current volume of an element of material to it's original volume. Similarly, we can define an increment in J as:

$$J_{inc} = \det(\mathbf{F}(dt)) \tag{2.6}$$

which is the ratio of the current volume of an element of material to it's volume at the previous timestep. Thus we can write:

$$v_p(t + dt) = J_{inc} v_p(t). \tag{2.7}$$

Elastic material properties are frequently given in terms of bulk and shear moduli, or κ and μ. The shear is sometimes denoted by G. The shear modulus μ appears in Equation 2.2 above. λ can be computed from κ and μ by:

$$\lambda = \kappa - \frac{2}{3}\mu. \tag{2.8}$$

Lastly, based on material properties λ and μ, a material wavespeed can be computed:

$$c^2 = (\lambda + 3\mu)\frac{m_p}{v_p}. \tag{2.9}$$

This wavespeed can be used in computing the timestep size as described above.

2.2 Other Material Models In the UCF

Other material models implemented into the Uintah-Vaango Computational Framework (UCF) have been chosen for three purposes:

- To verify the accuracy of the material point method (MPM) and to validate the coupling between the computational fluid dynamics code (ICE) and MPM.
- To model the elastic-plastic deformation of the steel container and the consequent damage in the regimes of both high and low strain rates and high and low temperatures.
- To model the polymer bonded explosive contained in the container under various strain rates and temperatures.

2.2.1 Material models for the validation of MPM

The models that have been implemented for the verification of MPM are:

- Isotropic hypoelastic model using the Jaumann rate of stress.
  1. MPM predictions have been compared with exact results for thick cylinders under internal pressure for small strains, three-point beam bending, etc.
  2. MPM predictions for the strain/stress contours for a set of disks in contact have been found to match experimental results.
- Isotropic hyperelastic material models for Mooney-Rivlin rubber and a modified compressible Neo-Hookean material. Isotropic strain hardening plasticity for the Neo-Hookean material.
  1. A billet compression problem has been simulated using MPM and the results have been found to closely match finite element simulations.
  2. MPM simulations for a thick cylinder under internal pressure with plastic deformation (perfect plasticity) compare well with the exact solution.

2.2.2 Material models for the container

The material model for the steel container is used to determine the state of stress in the container for an applied deformation rate and deformation gradient at each material point. The strain rates can vary from 10^{-3}/s to 10^{6}/s and temperatures in the container can vary from 250 K to 1000 K. Plasticity dominates the deformation of the container during the expansion of the explosive gases inside. At high strain rates the volumetric response of the container is best obtained using an equation of state. After the plastic strain in the container has reached a threshold value a damage/erosion model is required to rupture the container.

Two plasticity models with strain rate and temperature dependency are the Johnson-Cook and the Mechanical Threshold Stress (MTS) models. The volumetric response is calculated using a modified Mie-Gruneisen equation of state. A damage model that ties in well with the Johnson-Cook plasticity model is the Johnson-Cook damage model. The erosion algorithm either removes the contribution of the mass of the material point or forces the material point to undergo no tension or shear under further loading.

The stress update at each material point is performed using either of the two methods discussed below.

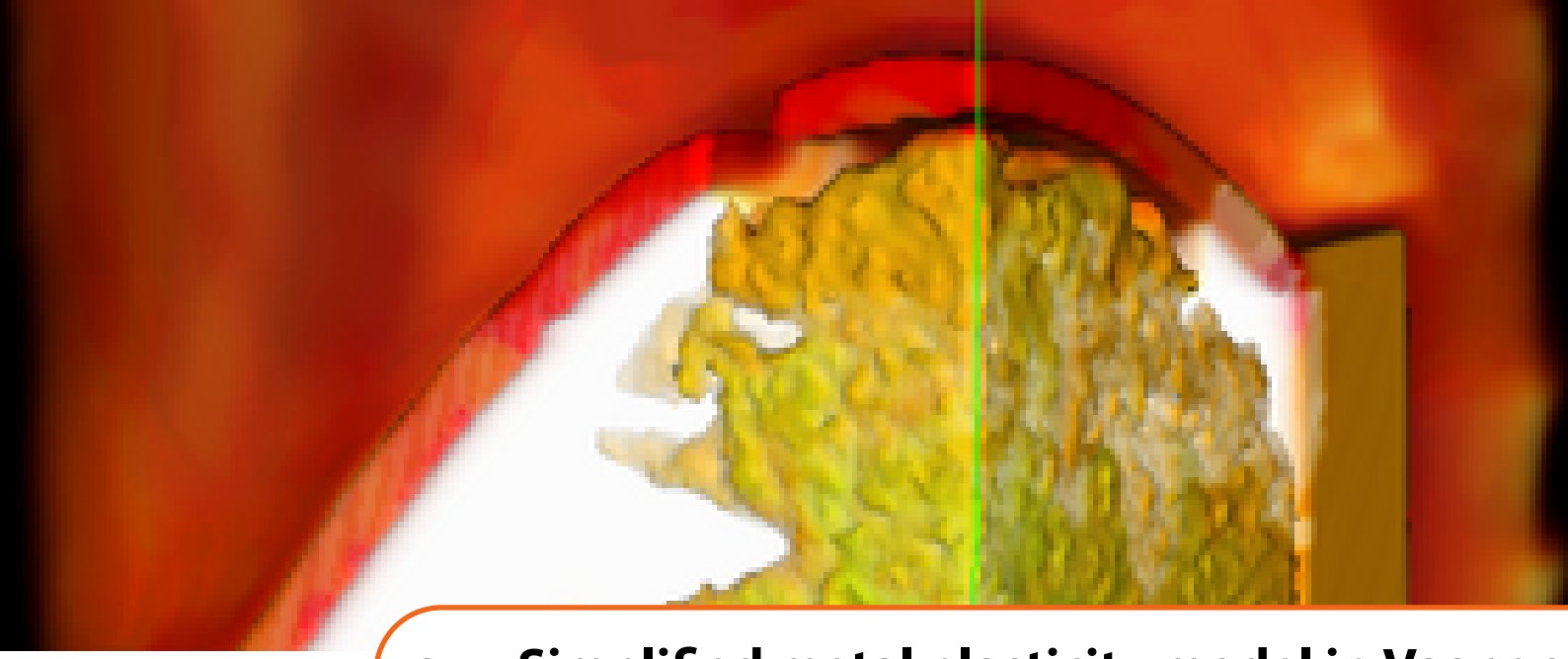
- Isotropic Hypoelastic-plastic material model using an additive decomposition of the rate of deformation tensor.
  1. The rate of deformation tensor a material point is calculated using the grid velocities.
  2. An incremental update of the left stretch and the rate of rotation tensors is calculated.
  3. The stress and the rate of deformation are rotated into the material coordinates.
  4. A trial elastic deviatoric stress state is calculated.
  5. The flow stress is calculated using the plasticity model and compared with the vonMises yield condition.
  6. If the stress state is elastic, an update of the stress is computed using the Mie-Gruneisen equation of state or the isotropic hypoelastic constitutive equation.
  7. If the stress state is plastic, all the strain rate is considered to the plastic and an elastic correction along with a radial return step move the stress state to the yield surface. The hydrostatic part of the stress is calculated using the equation of state or the hypoelastic constitutive equation.
  8. A scalar damage parameter is calculated and used to determine whether material points are to be eroded or not.
  9. Stresses and deformation rates are rotated back to the laboratory coordinates.
- Isotropic Hyperelastic-plastic material model using a multiplicative decomposition of the deformation gradient.
  1. The velocity gradient at a material point is calculated using the grid velocities.
  2. An incremental update of the deformation gradient and the left Cauchy-Green tensor is calculated.
  3. A trial elastic deviatoric stress state is calculated assuming a compressible Neo-Hookean elastic model.
  4. The flow stress is calculated using the plasticity model and compared with the vonMises yield condition.
  5. If the stress state is elastic, an update of the stress is computed using the Mie-Gruneisen equation of state or the compressible Neo-Hookean constitutive equation.
  6. If the stress state is plastic, all the strain rate is considered to the plastic and an elastic correction along with a radial return step move the stress state to the yield surface. The hydrostatic part of the stress state is calculated using the Mie-Gruneisen equation of state or the Neo-Hookean model.
  7. A scalar damage parameter is calculated and used to determine whether material points are to be eroded or not.

The implementations have been tested against Taylor impact test data for 4340 steel and HY 100 steel as well as one-dimensional problems which have been compared with experimental stress-strain data. At

large tensile strains, material points tend to separate from the main body. This issue is currently being explored and solutions are being sought in the framework of MPM.

2.2.3 Material models for the explosive

The explosive is modeled using the ViscoSCRAM constitutive model. Since large deformations or strains are not expected in the explosive, a small strain formulation has been implemented into the UCF. The model consists of five generalized Maxwell elements arranged in parallel, crack growth, friction at the crack interfaces and heating due to friction and reactions at the crack surfaces. The implementation has been verified with experimental data and found to be accurate.



3 — Simplified metal plasticity model in Vaango

3.1 Introduction

This document deals with some features of Vaango and some material models for solids that have been implemented in the Vaango Computational Framework (for use with the Material Point Method). The approach taken has been to separate the stress-strain relations from the numerical stress update algorithms as far as possible. A moderate rotation/small strain hypoelastic-plastic stress update algorithm is discussed and the manner in which plasticity flow rules, damage models and equations of state fit into the stress update algorithms are shown.

3.2 Stress Update Algorithms

The hypoelastic-plastic stress update is based on an additive decomposition of the rate of deformation tensor into elastic and plastic parts while the hyperelastic-plastic stress update is based on a multiplicative decomposition of the elastic and plastic deformation gradients. Incompressibility is assumed for plastic deformations. The volumetric response is therefore determined either by a bulk modulus and the trace of the rate of deformation tensor or using an equation of state. The deviatoric response is determined either by an elastic constitutive equation or using a plastic flow rule in combination with a yield condition.

The material models that can be varied in these stress update approaches are (not all are applicable to both hypo- and hyperelastic formulations nor is the list exhaustive):

1. The elasticity model, for example,
   - Isotropic linear elastic model.
   - Anisotropic linear elastic models.
   - Isotropic nonlinear elastic models.
   - Anisotropic nonlinear elastic models.
2. Isotropic hardening or Kinematic hardening using a back stress evolution rule, for example,
   - Ziegler evolution rule .
3. The flow rule and hardening/softening law, for example,
   - Perfect plasticity/power law hardening plasticity.
   - Johnson-Cook plasticity .
   - Mechanical Threshold Stress (MTS) plasticity .
   - Anand plasticity .
4. The yield condition, for example,

- von Mises yield condition.
- Drucker-Prager yield condition.
- Mohr-Coulomb yield condition.

5. A continuum or nonlocal damage model with damage evolution given by, for example,
   - Johnson-Cook damage model.
   - Gurson-Needleman-Tvergaard model.
   - Sandia damage model.
6. An equation of state to determine the pressure (or volumetric response), for example,
   - Mie-Gruneisen equation of state.

The currently implemented stress update algorithms in the Vaango Computational Framework do not allow for arbitrary elasticity models, kinematic hardening, arbitrary yield conditions and continuum or nonlocal damage (however the a damage parameter is updated and used in the erosion algorithm). The models that can be varied are the flow rule models, damage variable evolution models and the equation of state models.

Note that there are no checks in the Unitah Computational Framework to prevent users from mixing and matching inappropriate models.

This section describes the current implementation of the hypoelastic- plastic model. The stress update algorithm is a slightly modified version of the approach taken by Nemat-Nasser et al. (1991,1992) [Nem91; NC92], Wang (1994) [WA94], Maudlin (1996) [MS96], and Zocher et al. (2000) [Zoc+00].

3.2.1 Simplified theory for hypoelastic-plasticity

A simplified version of the theory behind the stress update algorithm (in the contex of von Mises plasticity) is given below.

Following [MS96], the rotated spatial rate of deformation tensor ($\boldsymbol{d}$) is decomposed into an elastic part ($\boldsymbol{d}^e$) and a plastic part ($\boldsymbol{d}^p$)

$$\boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p \tag{3.1}$$

If we assume plastic incompressibility ($\mathrm{tr}(\boldsymbol{d}^p) = 0$), we get

$$\boldsymbol{\eta} = \boldsymbol{\eta}^e + \boldsymbol{\eta}^p \tag{3.2}$$

where $\boldsymbol{\eta}$, $\boldsymbol{\eta}^e$, and $\boldsymbol{\eta}^p$ are the deviatoric parts of $\boldsymbol{d}$, $\boldsymbol{d}^e$, and $\boldsymbol{d}^p$, respectively. For isotropic materials, the hypoelastic constitutive equation for deviatoric stress is

$$\dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \boldsymbol{\eta}^p) \tag{3.3}$$

where $\mathbf{s}$ is the deviatoric part of the stress tensor and μ is the shear modulus. We assume that the flow stress obeys the Huber-von Mises yield condition

$$f := \sqrt{\frac{3}{2}}\,\|\mathbf{s}\| - \sigma_y \le 0 \quad \text{or,} \quad F := \frac{3}{2}\mathbf{s} : \mathbf{s} - \sigma_y^2 \le 0 \tag{3.4}$$

where σ_y is the flow stress. Assuming an associated flow rule, and noting that $\boldsymbol{d}^p = \boldsymbol{\eta}^p$, we have

$$\boldsymbol{\eta}^p = \boldsymbol{d}^p = \lambda\frac{\partial f}{\partial \boldsymbol{\sigma}} = \Lambda\frac{\partial F}{\partial \boldsymbol{\sigma}} = 3\Lambda\mathbf{s} \tag{3.5}$$

where $\boldsymbol{\sigma}$ is the stress. Let $\mathbf{u}$ be a tensor proportional to the plastic straining direction, and define γ as

$$\mathbf{u} = \sqrt{3}\frac{\mathbf{s}}{\|\mathbf{s}\|}; \quad \gamma := \sqrt{3}\Lambda\,\|\mathbf{s}\| \quad \Longrightarrow \gamma\mathbf{u} = 3\Lambda\mathbf{s} \tag{3.6}$$

Therefore, we have

$$\boldsymbol{\eta}^p = \gamma \mathbf{u}; \quad \dot{\mathbf{s}} = 2\mu(\boldsymbol{\eta} - \gamma \mathbf{u}) \tag{3.7}$$

From the consistency condition, if we assume that the deviatoric stress remains constant over a timestep, we get

$$\gamma = \frac{\mathbf{s} : \boldsymbol{\eta}}{\mathbf{s} : \mathbf{u}} \tag{3.8}$$

which provides an initial estimate of the plastic strain-rate. To obtain a semi-implicit update of the stress using equation (3.7), we define

$$\tau^2 := \frac{3}{2}\mathbf{s} : \mathbf{s} = \sigma_y^2 \tag{3.9}$$

Taking a time derivative of equation (3.9) gives us

$$\sqrt{2}\dot{\tau} = \sqrt{3}\frac{\mathbf{s} : \dot{\mathbf{s}}}{\|\mathbf{s}\|} \tag{3.10}$$

Plugging equation (3.10) into equation $(3.7)_2$ we get

$$\dot{\tau} = \sqrt{2}\mu(\mathbf{u} : \boldsymbol{\eta} - \gamma \mathbf{u} : \mathbf{u}) = \sqrt{2}\mu(d - 3\gamma) \tag{3.11}$$

where $d = \mathbf{u} : \boldsymbol{\eta}$. If the initial estimate of the plastic strain-rate is that all of the deviatoric strain-rate is plastic, then we get an approximation to γ, and the corresponding error (γ_{er}) given by

$$\gamma_{\text{approx}} = \frac{d}{3}; \quad \gamma_{\text{er}} = \gamma_{\text{approx}} - \gamma = \frac{d}{3} - \gamma \tag{3.12}$$

The incremental form of the above equation is

$$\Delta\gamma = \frac{d^* \Delta t}{3} - \Delta\gamma_{\text{er}} \tag{3.13}$$

Integrating equation (3.11) from time t_n to time $t_{n+1} = t_n + \Delta t$, and using equation (3.13) we get

$$\tau_{n+1} = \tau_n + \sqrt{2}\mu(d^* \Delta t - 3\Delta\gamma) = \tau_n + 3\sqrt{2}\mu\Delta\gamma_{\text{er}} \tag{3.14}$$

where d^* is the average value of d over the timestep. Solving for $\Delta\gamma_{\text{er}}$ gives

$$\Delta\gamma_{\text{er}} = \frac{\tau_{n+1} - \tau_n}{3\sqrt{2}\mu} = \frac{\sqrt{2}\sigma_y - \sqrt{3}\,\|\mathbf{s}_n\|}{6\mu} \tag{3.15}$$

The direction of the total strain-rate ($\mathbf{u}^\eta$) and the direction of the plastic strain-rate ($\mathbf{u}^s$) are given by

$$\mathbf{u}^\eta = \frac{\boldsymbol{\eta}}{\|\boldsymbol{\eta}\|}; \quad \mathbf{u}^s = \frac{\mathbf{s}}{\|\mathbf{s}\|} \tag{3.16}$$

Let θ be the fraction of the time increment that sees elastic straining. Then

$$\theta = \frac{d^* - 3\gamma_n}{d^*} \tag{3.17}$$

where $\gamma_n = d_n/3$ is the value of γ at the beginning of the timestep. We also assume that

$$d^* = \sqrt{3}\boldsymbol{\eta} : \left[(1-\theta)\mathbf{u}^\eta + \frac{\theta}{2}(\mathbf{u}^\eta + \mathbf{u}^s)\right] \tag{3.18}$$

Plugging equation (3.17) into equation (3.18) we get a quadratic equation that can be solved for d^* as follows

$$\frac{2}{\sqrt{3}}(d^*)^2 - (\boldsymbol{\eta} : \mathbf{u}^s + \|\boldsymbol{\eta}\|)d^* + 3\gamma_n(\boldsymbol{\eta} : \mathbf{u}^s - \|\boldsymbol{\eta}\|) = 0 \tag{3.19}$$

The real positive root of the above quadratic equation is taken as the estimate for d. The value of $\Delta\gamma$ can now be calculated using equations (3.13) and (3.15). A semi-implicit estimate of the deviatoric stress can be obtained at this stage by integrating equation $(3.7)_2$

$$\tilde{\mathbf{s}}_{n+1} = \mathbf{s}_n + 2\mu\left(\eta\Delta t - \sqrt{3}\Delta\gamma\frac{\tilde{\mathbf{s}}_{n+1}}{\|\mathbf{s}_{n+1}\|}\right) \tag{3.20}$$

$$= \mathbf{s}_n + 2\mu\left(\eta\Delta t - \frac{3}{\sqrt{2}}\Delta\gamma\frac{\tilde{\mathbf{s}}_{n+1}}{\sigma_y}\right) \tag{3.21}$$

Solving for $\tilde{\mathbf{s}}_{n+1}$, we get

$$\tilde{\mathbf{s}}_{n+1} = \frac{\mathbf{s}^{\text{trial}}_{n+1}}{1 + 3\sqrt{2}\mu\dfrac{\Delta\gamma}{\sigma_y}} \tag{3.22}$$

where $\mathbf{s}^{\text{trial}}_{n+1} = \mathbf{s}_n + 2\mu\Delta t\boldsymbol{\eta}$. A final radial return adjustment is used to move the stress to the yield surface

$$\mathbf{s}_{n+1} = \sqrt{\frac{2}{3}}\sigma_y\frac{\tilde{\mathbf{s}}_{n+1}}{\|\tilde{\mathbf{s}}_{n+1}\|} \tag{3.23}$$

A pathological situation arises if $\gamma_n = \mathbf{u}_n : \boldsymbol{\eta}_n$ is less than or equal to zero or $\Delta\gamma_{\text{er}} \geq \frac{d^*}{3}\Delta t$. This can occur is the rate of plastic deformation is small compared to the rate of elastic deformation or if the timestep size is too small (see [NC92]). In such situations, we use a locally implicit stress update that uses Newton iterations (as discussed in [SH98], page 124) to compute $\tilde{\mathbf{s}}$.

3.3 Models

Below are some of the strain-rate, strain, and temperature dependent models for metals that are implemented in Vaango.

3.3.1 Equation of State Models

The elastic-plastic stress update assumes that the volumetric part of the Cauchy stress can be calculated using an equation of state. There are three equations of state that are implemented in Vaango. These are

1. A default hypoelastic equation of state.
2. A neo-Hookean equation of state.
3. A Mie-Gruneisen type equation of state.

Default hypoelastic equation of state

In this case we assume that the stress rate is given by

$$\dot{\boldsymbol{\sigma}} = \lambda\,\text{tr}(\boldsymbol{d}^e)\,\mathbf{1} + 2\,\mu\,\boldsymbol{d}^e \tag{3.24}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress, $\boldsymbol{d}^e$ is the elastic part of the rate of deformation, and λ, μ are constants.

If $\boldsymbol{\eta}^e$ is the deviatoric part of $\boldsymbol{d}^e$ then we can write

$$\dot{\boldsymbol{\sigma}} = \left(\lambda + \frac{2}{3}\,\mu\right)\,\text{tr}(\boldsymbol{d}^e)\,\mathbf{1} + 2\,\mu\,\boldsymbol{\eta}^e = \kappa\,\text{tr}(\boldsymbol{d}^e)\,\mathbf{1} + 2\,\mu\,\boldsymbol{\eta}^e\,. \tag{3.25}$$

If we split $\boldsymbol{\sigma}$ into a volumetric and a deviatoric part, i.e., $\boldsymbol{\sigma} = p\,\mathbf{1} + \mathbf{s}$ and take the time derivative to get $\dot{\boldsymbol{\sigma}} = \dot{p}\,\mathbf{1} + \dot{\mathbf{s}}$ then

$$\dot{p} = \kappa\,\mathrm{tr}(\boldsymbol{d}^e)\ . \tag{3.26}$$

In addition we assume that $\boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p$. If we also assume that the plastic volume change is negligible, we can then write that

$$\dot{p} = \kappa\,\mathrm{tr}(\boldsymbol{d})\ . \tag{3.27}$$

This is the equation that is used to calculate the pressure p in the default hypoelastic equation of state, i.e.,

$$\boxed{p_{n+1} = p_n + \kappa\,\mathrm{tr}(\boldsymbol{d}_{n+1})\,\Delta t\ .} \tag{3.28}$$

To get the derivative of p with respect to J, where $J = \det(\boldsymbol{F})$, we note that

$$\dot{p} = \frac{\partial p}{\partial J}\,\dot{J} = \frac{\partial p}{\partial J}\,J\,\mathrm{tr}(\boldsymbol{d})\ . \tag{3.29}$$

Therefore,

$$\boxed{\frac{\partial p}{\partial J} = \frac{\kappa}{J}\,.} \tag{3.30}$$

This model is invoked in Vaango using

```
<equation_of_state type="default_hypo">
</equation_of_state>
```

The code is in `.../MPM/ConstitutiveModel/PlasticityModels/DefaultHypoElasticEOS.cc`.

Default hyperelastic equation of state

In this model the pressure is computed using the relation

$$p = \tfrac{1}{2}\,\kappa\left(J^e - \frac{1}{J^e}\right) \tag{3.31}$$

where κ is the bulk modulus and J^e is determinant of the elastic part of the deformation gradient.

We can also compute

$$\frac{dp}{dJ} = \tfrac{1}{2}\,\kappa\left(1 + \frac{1}{(J^e)^2}\right)\ . \tag{3.32}$$

This model is invoked in Vaango using

```
<equation_of_state type="default_hyper">
</equation_of_state>
```

The code is in `.../MPM/ConstitutiveModel/PlasticityModels/HyperElasticEOS.cc`. If an EOS is not specified then this model is the **default**.

Mie-Gruneisen equation of state

The pressure (p) is calculated using a Mie-Grüneisen equation of state of the form ([Wil99; Zoc+00])

$$\boxed{p_{n+1} = -\frac{\rho_o\, C_o^2\, (1 - J^e_{n+1})[1 - \Gamma_o(1 - J^e_{n+1})/2]}{[1 - S_\alpha(1 - J^e_{n+1})]^2} - \Gamma_o\, e_{n+1}\,; \quad J^e := \det \boldsymbol{F}^e} \tag{3.33}$$

where C_o is the bulk speed of sound, ρ_o is the initial mass density, Γ_o is the Grüneisen's gamma at the reference state, $S_\alpha = dU_s/dU_p$ is a linear Hugoniot slope coefficient, U_s is the shock wave velocity, U_p is the particle velocity, and e is the internal energy density (per unit reference volume), $\boldsymbol{F}^e$ is the elastic part of the deformation gradient. For isochoric plasticity,

$$J^e = J = \det(\boldsymbol{F}) = \frac{\rho_o}{\rho}\,.$$

The internal energy is computed using

$$E = \frac{1}{V_o}\int C_v dT \approx \frac{C_v(T - T_o)}{V_o} \tag{3.34}$$

where $V_o = 1/\rho_o$ is the reference specific volume at temperature $T = T_o$, and C_v is the specific heat at constant volume.

Also,

$$\boxed{\frac{\partial p}{\partial J^e} = \frac{\rho_o\, C_o^2\, [1 + (S_\alpha - \Gamma_o)\,(1 - J^e)]}{[1 - S_\alpha\,(1 - J^e)]^3} - \Gamma_o\,\frac{\partial e}{\partial J^e}.} \tag{3.35}$$

We neglect the $\frac{\partial e}{\partial J^e}$ term in our calculations.

This model is invoked in Vaango using

```
<equation_of_state type="mie_gruneisen">
  <C_0>5386</C_0>
  <Gamma_0>1.99</Gamma_0>
  <S_alpha>1.339</S_alpha>
</equation_of_state>
```

The code is in `.../MPM/ConstitutiveModel/PlasticityModels/MieGruneisenEOS.cc`.

3.3.2 Melting Temperature

Default model

The default model is to use a constant melting temperature. This model is invoked using

```
<melting_temp_model type="constant_Tm">
</melting_temp_model>
```

SCG melt model

We use a pressure dependent relation to determine the melting temperature (T_m). The Steinberg-Cochran-Guinan (SCG) melt model ([SCG80]) has been used for our simulations of copper. This model is based on a modified Lindemann law and has the form

$$T_m(\rho) = T_{mo}\exp\left[2a\left(1 - \frac{1}{\eta}\right)\right]\eta^{2(\Gamma_o - a - 1/3)}; \quad \eta = \frac{\rho}{\rho_o} \tag{3.36}$$

where T_{mo} is the melt temperature at $\eta = 1$, a is the coefficient of the first order volume correction to Grüneisen's gamma (Γ_o).

This model is invoked with

```
<melting_temp_model type="scg_Tm">
  <T_m0> 2310.0 </T_m0>
  <Gamma_0> 3.0 </Gamma_0>
  <a> 1.67 </a>
</melting_temp_model>
```

BPS melt model

An alternative melting relation that is based on dislocation-mediated phase transitions - the Burakovsky-Preston-Silbar (BPS) model ([BPSoo]) can also be used. This model has been used to determine the melt temperature for 4340 steel. The BPS model has the form

$$T_m(p) = T_m(0)\left[\frac{1}{\eta} + \frac{1}{\eta^{4/3}}\frac{\mu_0'}{\mu_0}p\right]; \quad \eta = \left(1 + \frac{K_0'}{K_0}p\right)^{1/K_0'} \tag{3.37}$$

$$T_m(0) = \frac{\kappa\lambda\mu_0 v_{WS}}{8\pi\ln(z-1)\,k_b}\ln\left(\frac{\alpha^2}{4\,b^2\rho_c(T_m)}\right) \tag{3.38}$$

where p is the pressure, $\eta = \rho/\rho_0$ is the compression, μ_0 is the shear modulus at room temperature and zero pressure, $\mu_0' = \partial\mu/\partial p$ is the derivative of the shear modulus at zero pressure, K_0 is the bulk modulus at room temperature and zero pressure, $K_0' = \partial K/\partial p$ is the derivative of the bulk modulus at zero pressure, κ is a constant, $\lambda = b^3/v_{WS}$ where b is the magnitude of the Burgers' vector, v_{WS} is the Wigner-Seitz volume, z is the coordination number, α is a constant, $\rho_c(T_m)$ is the critical density of dislocations, and k_b is the Boltzmann constant.

This model is invoked with

```
<melting_temp_model type="bps_Tm">
  <B0> 137e9 </B0>
  <dB_dp0> 5.48 <dB_dp0>
  <G0> 47.7e9 <G0>
  <dG_dp0> 1.4 <dG_dp0>
  <kappa> 1.25 <kappa>
  <z> 12 <z>
  <b2rhoTm> 0.64 <b2rhoTm>
  <alpha> 2.9 <alpha>
  <lambda> 1.41 <lambda>
  <a> 3.6147e-9<a>
  <v_ws_a3_factor> 1/4 <v_ws_a3_factor>
  <Boltzmann_Constant> <Boltzmann_Constant>
</melting_temp_model>
```

3.3.3 Shear Modulus

Three models for the shear modulus (μ) have been tested in our simulations. The first has been associated with the Mechanical Threshold Stress (MTS) model and we call it the MTS shear model. The second is the model used by Steinberg-Cochran-Guinan and we call it the SCG shear model while the third is a model developed by Nadal and Le Poac that we call the NP shear model.

Default model

The default model gives a constant shear modulus. The model is invoked using

```
<shear_modulus_model type="constant_shear">
</shear_modulus_model>
```

MTS Shear Modulus Model

The simplest model is of the form suggested by [Var70] ([CG96])

$$\mu(T) = \mu_0 - \frac{D}{exp(T_0/T) - 1} \tag{3.39}$$

where μ_0 is the shear modulus at 0K, and D, T_0 are material constants.

The model is invoked using

```
<shear_modulus_model type="mts_shear">
  <mu_0>28.0e9</mu_0>
  <D>4.50e9</D>
  <T_0>294</T_0>
</shear_modulus_model>
```

SCG Shear Modulus Model

The Steinberg-Cochran-Guinan (SCG) shear modulus model ([SCG80; Zoc+00]) is pressure dependent and has the form

$$\mu(p, T) = \mu_0 + \frac{\partial \mu}{\partial p}\frac{p}{\eta^{1/3}} + \frac{\partial \mu}{\partial T}(T - 300); \quad \eta = \rho/\rho_0 \tag{3.40}$$

where, μ_0 is the shear modulus at the reference state($T = 300$ K, $p = 0$, $\eta = 1$), p is the pressure, and T is the temperature. When the temperature is above T_m, the shear modulus is instantaneously set to zero in this model.

The model is invoked using

```
<shear_modulus_model type="scg_shear">
  <mu_0> 81.8e9 </mu_0>
  <A> 20.6e-12 </A>
  <B> 0.16e-3 </B>
</shear_modulus_model>
```

NP Shear Modulus Model

A modified version of the SCG model has been developed by [NL03] that attempts to capture the sudden drop in the shear modulus close to the melting temperature in a smooth manner. The Nadal-LePoac (NP) shear modulus model has the form

$$\mu(p, T) = \frac{1}{\mathcal{J}(\hat{T})}\left[\left(\mu_0 + \frac{\partial \mu}{\partial p}\frac{p}{\eta^{1/3}}\right)(1 - \hat{T}) + \frac{\rho}{Cm}\, k_b\, T\right]; \quad C := \frac{(6\pi^2)^{2/3}}{3} f^2 \tag{3.41}$$

where

$$\mathcal{J}(\hat{T}) := 1 + \exp\left[-\frac{1 + 1/\zeta}{1 + \zeta/(1 - \hat{T})}\right] \quad \text{for} \quad \hat{T} := \frac{T}{T_m} \in [0, 1 + \zeta], \tag{3.42}$$

μ_0 is the shear modulus at 0 K and ambient pressure, ζ is a material parameter, k_b is the Boltzmann constant, m is the atomic mass, and f is the Lindemann constant.

The model is invoked using

```
<shear_modulus_model type="np_shear">
  <mu_0>26.5e9</mu_0>
  <zeta>0.04</zeta>
  <slope_mu_p_over_mu0>65.0e-12</slope_mu_p_over_mu0>
  <C> 0.047 </C>
  <m> 26.98 </m>
</shear_modulus_model>
```

PTW Shear model

The PTW shear model is a simplified version of the SCG shear model. The inputs can be found in `.../MPM/ConstitutiveModel/PlasticityModel/PTWShear.h`.

3.3.4 Flow Stress

We have explored five temperature and strain rate dependent models that can be used to compute the flow stress:

1. the Johnson-Cook (JC) model
2. the Steinberg-Cochran-Guinan-Lund (SCG) model.
3. the Zerilli-Armstrong (ZA) model.
4. the Mechanical Threshold Stress (MTS) model.
5. the Preston-Tonks-Wallace (PTW) model.

JC Flow Stress Model

The Johnson-Cook (JC) model ([JC83]) is purely empirical and gives the following relation for the flow stress (σ_y)

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \left[A + B(\varepsilon_p)^n\right]\left[1 + C\ln(\dot{\varepsilon}_p^*)\right]\left[1 - (T^*)^m\right] \tag{3.43}$$

where ε_p is the equivalent plastic strain, $\dot{\varepsilon}_p$ is the plastic strain rate, A, B, C, n, m are material constants,

$$\dot{\varepsilon}_p^* = \frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{p0}}; \quad T^* = \frac{(T - T_0)}{(T_m - T_0)}, \tag{3.44}$$

$\dot{\varepsilon}_{p0}$ is a user defined plastic strain rate, T_0 is a reference temperature, and T_m is the melt temperature. For conditions where $T^* < 0$, we assume that $m = 1$.

The inputs for this model are

```
<plasticity_model type="johnson_cook">
  <A>792.0e6</A>
  <B>510.0e6</B>
  <C>0.014</C>
  <n>0.26</n>
  <m>1.03</m>
  <T_r>298.0</T_r>
  <T_m>1793.0</T_m>
  <epdot_0>1.0</epdot_0>
</plasticity_model>
```

SCG Flow Stress Model

The Steinberg-Cochran-Guinan-Lund (SCG) model is a semi-empirical model that was developed by [SCG80] for high strain rate situations and extended to low strain rates and bcc materials by [SL89]. The flow stress in this model is given by

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \left[\sigma_a f(\varepsilon_p) + \sigma_t(\dot{\varepsilon}_p, T)\right]\frac{\mu(p, T)}{\mu_0} \tag{3.45}$$

where σ_a is the athermal component of the flow stress, $f(\varepsilon_p)$ is a function that represents strain hardening, σ_t is the thermally activated component of the flow stress, $\mu(p, T)$ is the shear modulus, and μ_0 is the shear modulus at standard temperature and pressure. The strain hardening function has the form

$$f(\varepsilon_p) = \left[1 + \beta(\varepsilon_p + \varepsilon_{pi})\right]^n; \quad \sigma_a f(\varepsilon_p) \leq \sigma_{\max} \tag{3.46}$$

where β, n are work hardening parameters, and ε_{pi} is the initial equivalent plastic strain. The thermal component σ_t is computed using a bisection algorithm from the following equation (based on the work of [HM77])

$$\dot{\varepsilon}_p = \left[\frac{1}{C_1}\exp\left[\frac{2U_k}{k_b\,T}\left(1-\frac{\sigma_t}{\sigma_p}\right)^2\right]+\frac{C_2}{\sigma_t}\right]^{-1}; \quad \sigma_t \le \sigma_p \tag{3.47}$$

where $2U_k$ is the energy to form a kink-pair in a dislocation segment of length L_d, k_b is the Boltzmann constant, σ_p is the Peierls stress. The constants C_1, C_2 are given by the relations

$$C_1 := \frac{\rho_d L_d a b^2 \nu}{2w^2}; \quad C_2 := \frac{D}{\rho_d b^2} \tag{3.48}$$

where ρ_d is the dislocation density, L_d is the length of a dislocation segment, a is the distance between Peierls valleys, b is the magnitude of the Burgers' vector, ν is the Debye frequency, w is the width of a kink loop, and D is the drag coefficient.

The inputs for this model are of the form

```
<plasticity_model type="steinberg_cochran_guinan">
  <mu_0> 81.8e9 </mu_0>
  <sigma_0> 1.15e9 </sigma_0>
  <Y_max> 0.25e9 </Y_max>
  <beta> 2.0 </beta>
  <n> 0.50 </n>
  <A> 20.6e-12 </A>
  <B> 0.16e-3 </B>
  <T_m0> 2310.0 </T_m0>
  <Gamma_0> 3.0 </Gamma_0>
  <a> 1.67 </a>
  <epsilon_p0> 0.0 </epsilon_p0>
</plasticity_model>
```

ZA Flow Stress Model

The Zerilli-Armstrong (ZA) model ([Zero4; ZA87; ZA93]) is based on simplified dislocation mechanics. The general form of the equation for the flow stress is

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \sigma_a + B\exp(-\beta(\dot{\varepsilon}_p)T) + B_0\sqrt{\varepsilon_p}\exp(-\alpha(\dot{\varepsilon}_p)T) \tag{3.49}$$

where σ_a is the athermal component of the flow stress given by

$$\sigma_a := \sigma_g + \frac{k_h}{\sqrt{l}} + K\varepsilon_p^n, \tag{3.50}$$

σ_g is the contribution due to solutes and initial dislocation density, k_h is the microstructural stress intensity, l is the average grain diameter, K is zero for fcc materials, B, B_0 are material constants. The functional forms of the exponents α and β are

$$\alpha = \alpha_0 - \alpha_1\ln(\dot{\varepsilon}_p); \quad \beta = \beta_0 - \beta_1\ln(\dot{\varepsilon}_p); \tag{3.51}$$

where $\alpha_0, \alpha_1, \beta_0, \beta_1$ are material parameters that depend on the type of material (fcc, bcc, hcp, alloys). The Zerilli-Armstrong model has been modified by [AV05] for better performance at high temperatures. However, we have not used the modified equations in our computations.

The inputs for this model are of the form

```
<bcc_or_fcc> fcc </bcc_or_fcc>
<c2> </c2>
<c3> </c3>
<c4> </c4>
<n> </n>
```

MTS Flow Stress Model

The Mechanical Threshold Stress (MTS) model ([FK88; Got+00; Koc01]) gives the following form for the flow stress

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \sigma_a + (S_i\sigma_i + S_e\sigma_e)\frac{\mu(p,T)}{\mu_0} \tag{3.52}$$

where σ_a is the athermal component of mechanical threshold stress, μ_0 is the shear modulus at 0 K and ambient pressure, σ_i is the component of the flow stress due to intrinsic barriers to thermally activated dislocation motion and dislocation-dislocation interactions, σ_e is the component of the flow stress due to microstructural evolution with increasing deformation (strain hardening), (S_i, S_e) are temperature and strain rate dependent scaling factors. The scaling factors take the Arrhenius form

$$S_i = \left[1 - \left(\frac{k_b\ T}{g_{0i}b^3\mu(p,T)}\ln\frac{\dot{\varepsilon}_{poi}}{\dot{\varepsilon}_p}\right)^{1/q_i}\right]^{1/p_i} \tag{3.53}$$

$$S_e = \left[1 - \left(\frac{k_b\ T}{g_{0e}b^3\mu(p,T)}\ln\frac{\dot{\varepsilon}_{poe}}{\dot{\varepsilon}_p}\right)^{1/q_e}\right]^{1/p_e} \tag{3.54}$$

where k_b is the Boltzmann constant, b is the magnitude of the Burgers' vector, (g_{0i}, g_{0e}) are normalized activation energies, $(\dot{\varepsilon}_{poi}, \dot{\varepsilon}_{poe})$ are constant reference strain rates, and (q_i, p_i, q_e, p_e) are constants. The strain hardening component of the mechanical threshold stress (σ_e) is given by a modified Voce law

$$\frac{d\sigma_e}{d\varepsilon_p} = \theta(\sigma_e) \tag{3.55}$$

where

$$\theta(\sigma_e) = \theta_0[1 - F(\sigma_e)] + \theta_{IV}F(\sigma_e) \tag{3.56}$$

$$\theta_0 = a_0 + a_1\ln\dot{\varepsilon}_p + a_2\sqrt{\dot{\varepsilon}_p} - a_3T \tag{3.57}$$

$$F(\sigma_e) = \frac{\tanh\left(\alpha\frac{\sigma_e}{\sigma_{es}}\right)}{\tanh(\alpha)} \tag{3.58}$$

$$\ln\left(\frac{\sigma_{es}}{\sigma_{0es}}\right) = \left(\frac{kT}{g_{0es}b^3\mu(p,T)}\right)\ln\left(\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_{poes}}\right) \tag{3.59}$$

and θ_0 is the hardening due to dislocation accumulation, θ_{IV} is the contribution due to stage-IV hardening, $(a_0, a_1, a_2, a_3, \alpha)$ are constants, σ_{es} is the stress at zero strain hardening rate, σ_{0es} is the saturation threshold stress for deformation at 0 K, g_{0es} is a constant, and $\dot{\varepsilon}_{poes}$ is the maximum strain rate. Note that the maximum strain rate is usually limited to about 10^7/s.

The inputs for this model are of the form

```
<plasticity_model type="mts_model">
  <sigma_a>363.7e6</sigma_a>
  <mu_0>28.0e9</mu_0>
  <D>4.50e9</D>
  <T_0>294</T_0>
  <koverbcubed>0.823e6</koverbcubed>
  <g_0i>0.0</g_0i>
  <g_0e>0.71</g_0e>
  <edot_0i>0.0</edot_0i>
  <edot_0e>2.79e9</edot_0e>
  <p_i>0.0</p_i>
  <q_i>0.0</q_i>
```

```
    <p_e>1.0</p_e>
    <q_e>2.0</q_e>
    <sigma_i>0.0</sigma_i>
    <a_0>211.8e6</a_0>
    <a_1>0.0</a_1>
    <a_2>0.0</a_2>
    <a_3>0.0</a_3>
    <theta_IV>0.0</theta_IV>
    <alpha>2</alpha>
    <edot_es0>3.42e8</edot_es0>
    <g_0es>0.15</g_0es>
    <sigma_es0>1679.3e6</sigma_es0>
  </plasticity_model>
```

PTW Flow Stress Model

The Preston-Tonks-Wallace (PTW) model ([PTW03]) attempts to provide a model for the flow stress for extreme strain rates (up to 10^{11}/s) and temperatures up to melt. The flow stress is given by

$$\sigma_y(\varepsilon_p, \dot{\varepsilon}_p, T) = \begin{cases} 2\left[\tau_s + \alpha \ln\left[1 - \varphi \exp\left(-\beta - \dfrac{\theta \varepsilon_p}{\alpha \varphi}\right)\right]\right]\mu(p,T) & \text{thermal regime} \\ 2\tau_s \mu(p,T) & \text{shock regime} \end{cases} \tag{3.60}$$

with

$$\alpha := \frac{s_0 - \tau_y}{d}; \quad \beta := \frac{\tau_s - \tau_y}{\alpha}; \quad \varphi := \exp(\beta) - 1 \tag{3.61}$$

where τ_s is a normalized work-hardening saturation stress, s_0 is the value of τ_s at 0K, τ_y is a normalized yield stress, θ is the hardening constant in the Voce hardening law, and d is a dimensionless material parameter that modifies the Voce hardening law. The saturation stress and the yield stress are given by

$$\tau_s = \max\left\{s_0 - (s_0 - s_\infty)\operatorname{erf}\left[\kappa \hat{T} \ln\left(\frac{\gamma\dot{\xi}}{\dot{\varepsilon}_p}\right)\right], s_0\left(\frac{\dot{\varepsilon}_p}{\gamma\dot{\xi}}\right)^{s_1}\right\} \tag{3.62}$$

$$\tau_y = \max\left\{y_0 - (y_0 - y_\infty)\operatorname{erf}\left[\kappa \hat{T} \ln\left(\frac{\gamma\dot{\xi}}{\dot{\varepsilon}_p}\right)\right], \min\left\{y_1\left(\frac{\dot{\varepsilon}_p}{\gamma\dot{\xi}}\right)^{y_2}, s_0\left(\frac{\dot{\varepsilon}_p}{\gamma\dot{\xi}}\right)^{s_1}\right\}\right\} \tag{3.63}$$

where s_∞ is the value of τ_s close to the melt temperature, (y_0, y_∞) are the values of τ_y at 0K and close to melt, respectively, (κ, γ) are material constants, $\hat{T} = T/T_m$, (s_1, y_1, y_2) are material parameters for the high strain rate regime, and

$$\dot{\xi} = \frac{1}{2}\left(\frac{4\pi\rho}{3M}\right)^{1/3}\left(\frac{\mu(p,T)}{\rho}\right)^{1/2} \tag{3.64}$$

where ρ is the density, and M is the atomic mass.

The inputs for this model are of the form

```
  <plasticity_model type="preston_tonks_wallace">
    <theta> 0.025 </theta>
    <p> 2.0 </p>
    <s0> 0.0085 </s0>
    <sinf> 0.00055 </sinf>
    <kappa> 0.11 </kappa>
    <gamma> 0.00001 </gamma>
    <y0> 0.0001 </y0>
    <yinf> 0.0001 </yinf>
    <y1> 0.094 </y1>
```

```
    <y2> 0.575 </y2>
    <beta> 0.25 </beta>
    <M> 63.54 </M>
    <G0> 518e8 </G0>
    <alpha> 0.20 </alpha>
    <alphap> 0.20 </alphap>
  </plasticity_model>
```

3.3.5 Adiabatic Heating and Specific Heat

A part of the plastic work done is converted into heat and used to update the temperature of a particle. The increase in temperature (ΔT) due to an increment in plastic strain ($\Delta\epsilon_p$) is given by the equation

$$\Delta T = \frac{\chi\sigma_y}{\rho C_p}\Delta\epsilon_p \tag{3.65}$$

where χ is the Taylor-Quinney coefficient, and C_p is the specific heat. The value of the Taylor-Quinney coefficient is taken to be 0.9 in all our simulations (see [Rav+01] for more details on the variation of χ with strain and strain rate).

The Taylor-Quinney coefficient is taken as input in the ElasticPlastic model using the tags

```
<taylor_quinney_coeff> 0.9 </taylor_quinney_coeff>
```

Default specific heat model

The default model returns a constant specific heat and is invoked using

```
<specific_heat_model type="constant_Cp">
</specific_heat_model>
```

Specific heat model for copper

The specific heat model for copper is of the form

$$Cp = \begin{cases} A_0\ T^3 - B_0\ T^2 + C_0\ T - D_0 & \text{if } T < T_0 \\ A_1\ T + B_1 & \text{if } T \geq T_0\ . \end{cases} \tag{3.66}$$

The model is invoked using

```
<specific_heat_model type = "copper_Cp"> </specific_heat_model>
```

Specific heat model for steel

A relation for the dependence of C_p upon temperature is used for the steel ([LSS74]).

$$C_p = \begin{cases} A_1 + B_1\ t + C_1\ |t|^{-\alpha} & \text{if } T < T_c \\ A_2 + B_2\ t + C_2\ t^{-\alpha'} & \text{if } T > T_c \end{cases} \tag{3.67}$$

$$t = \frac{T}{T_c} - 1 \tag{3.68}$$

where T_c is the critical temperature at which the phase transformation from the α to the γ phase takes place, and $A_1, A_2, B_1, B_2, \alpha, \alpha'$ are constants.

The model is invoked using

```
<specific_heat_model type = "steel_Cp"> </specific_heat_model>
```

The heat generated at a material point is conducted away at the end of a time step using the transient heat equation. The effect of conduction on material point temperature is negligible (but non-zero) for the high strain-rate problems simulated using Vaango.

3.3.6 Adding new models

In the parallel implementation of the stress update algorithm, sockets have been added to allow for the incorporation of a variety of plasticity, damage, yield, and bifurcation models without requiring any change in the stress update code. The algorithm is shown in Algorithm 3.1. The equation of state, plasticity model, yield condition, damage model, and the stability criterion are all polymorphic objects created using a factory idiom in C++ ([Cop92]).

Addition of a new model requires the following steps (the example below is only for the flow stress model but the same idea applies to other models) :

1. Creation of a new class that encapsulates the plasticity model. The template for this class can be copied from the existing plasticity models. The data that is unique to the new model are specified in the form of
   - A structure containing the constants for the plasticity model.
   - Particle variables that specify the variables that evolve in the plasticity model.
2. The implementation of the plasticity model involves the following steps.
   - Reading the input file for the model constants in the constructor.
   - Adding the variables that evolve in the plasticity model appropriately to the task graph.
   - Adding the appropriate flow stress calculation method.
3. The `PlasticityModelFactory` is then modified so that it recognizes the added plasticity model.

3.3.7 Damage Models and Failure

Only the Johnson-Cook damage evolution rule has been added to the DamageModelFactory so far. The damage model framework is designed to be similar to the plasticity model framework. New models can be added using the approach described in the previous section.

A particle is tagged as "failed" when its temperature is greater than the melting point of the material at the applied pressure. An additional condition for failure is when the porosity of a particle increases beyond a critical limit and the strain exceeds the fracture strain of the material. Another condition for failure is when a material bifurcation condition such as the Drucker stability postulate is satisfied. Upon failure, a particle is either removed from the computation by setting the stress to zero or is converted into a material with a different velocity field which interacts with the remaining particles via contact. Either approach leads to the simulation of a newly created surface. More details of the approach can be found in [Bano4a; Bano4b; Bano5].

3.3.8 Yield conditions

When failure is to be simulated we can use the Gurson-Tvergaard-Needleman yield condition instead of the von Mises condition.

The von Mises yield condition

The von Mises yield condition is the default and is invoked using the tags

```
<yield_condition type="vonMises">
</yield_condition>
```

The Gurson-Tvergaard-Needleman (GTN) yield condition

The Gurson-Tvergaard-Needleman (GTN) yield condition [Gur77; TN84] depends on porosity. An associated flow rule is used to determine the plastic rate parameter in either case. The GTN yield condition can be written as

$$\Phi = \left(\frac{\sigma_{eq}}{\sigma_f}\right)^2 + 2q_1 f_* \cosh\left(q_2 \frac{Tr(\sigma)}{2\sigma_f}\right) - (1 + q_3 f_*^2) = 0 \tag{3.69}$$

Table 3.1: Stress Update Algorithm

Persistent:Initial moduli, temperature, porosity,
scalar damage, equation of state, plasticity model,
yield condition, stability criterion, damage model
Temporary:Particle state at time t
Output: Particle state at time $t + \Delta t$

For *all the patches in the domain*
Read the particle data and initialize updated data storage
For *all the particles in the patch*
Compute the velocity gradient and the rate of deformation tensor
Compute the deformation gradient and the rotation tensor
Rotate the Cauchy stress and the rate of deformation tensor
to the material configuration
Compute the current shear modulus and melting temperature
Compute the pressure using the equation of state,
update the hydrostatic stress, and
compute the trial deviatoric stress
Compute the flow stress using the plasticity model
Evaluate the yield function
If *particle is elastic*
Update the elastic deviatoric stress from the trial stress
Rotate the stress back to laboratory coordinates
Update the particle state
Else
Compute the elastic-plastic deviatoric stress
Compute updated porosity, scalar damage, and
temperature increase due to plastic work
Compute elastic-plastic tangent modulus and evaluate stability condition
Rotate the stress back to laboratory coordinates
Update the particle state
End If
If *Temperature* > *Melt Temperature* or *Porosity* > *Critical Porosity* or *Unstable*
Tag particle as failed
End If
Convert failed particles into a material with a different velocity field
End For
End For

where q_1, q_2, q_3 are material constants and f_* is the porosity (damage) function given by

$$f* = \begin{cases} f & \text{for } f \le f_c, \\ f_c + k(f - f_c) & \text{for } f > f_c \end{cases} \tag{3.70}$$

where k is a constant and f is the porosity (void volume fraction). The flow stress in the matrix material is computed using either of the two plasticity models discussed earlier. Note that the flow stress in the matrix material also remains on the undamaged matrix yield surface and uses an associated flow rule.

This yield condition is invoked using

```
<yield_condition type="gurson">
  <q1> 1.5 </q1>
  <q2> 1.0 </q2>
  <q3> 2.25 </q3>
  <k> 4.0 </k>
  <f_c> 0.05 </f_c>
</yield_condition>
```

3.3.9 Porosity model

The evolution of porosity is calculated as the sum of the rate of growth and the rate of nucleation [RA98b]. The rate of growth of porosity and the void nucleation rate are given by the following equations [CN80]

$$\dot{f} = \dot{f}_{\text{nucl}} + \dot{f}_{\text{grow}} \tag{3.71}$$

$$\dot{f}_{\text{grow}} = (1 - f)\text{Tr}(\boldsymbol{D}_p) \tag{3.72}$$

$$\dot{f}_{\text{nucl}} = \frac{f_n}{(s_n\sqrt{2\pi})} \exp\left[-\tfrac{1}{2}\frac{(\epsilon_p - \epsilon_n)^2}{s_n^2}\right]\dot{\epsilon}_p \tag{3.73}$$

where $\boldsymbol{D}_p$ is the rate of plastic deformation tensor, f_n is the volume fraction of void nucleating particles , ϵ_n is the mean of the distribution of nucleation strains, and s_n is the standard deviation of the distribution.

The inputs tags for porosity are of the form

```
<evolve_porosity> true </evolve_porosity>
<initial_mean_porosity>          0.005 </initial_mean_porosity>
<initial_std_porosity>           0.001 </initial_std_porosity>
<critical_porosity>              0.3   </critical_porosity>
<frac_nucleation>                0.1   </frac_nucleation>
<meanstrain_nucleation>          0.3   </meanstrain_nucleation>
<stddevstrain_nucleation>        0.1   </stddevstrain_nucleation>
<initial_porosity_distrib>       gauss </initial_porosity_distrib>
```

3.3.10 Damage model

After the stress state has been determined on the basis of the yield condition and the associated flow rule, a scalar damage state in each material point can be calculated using the Johnson-Cook model [JC85]. The Johnson-Cook model has an explicit dependence on temperature, plastic strain, ans strain rate.

The damage evolution rule for the Johnson-Cook damage model can be written as

$$\dot{D} = \frac{\dot{\epsilon_p}}{\epsilon_p^f}; \quad \epsilon_p^f = \left[D_1 + D_2 \exp\left(\frac{D_3}{3}\sigma^*\right)\right]\left[1 + D_4 \ln(\dot{\epsilon_p}^*)\right]\left[1 + D_5 T^*\right] \; ; \quad \sigma^* = \frac{\text{Tr}(\boldsymbol{\sigma})}{\sigma_{eq}}; \tag{3.74}$$

where D is the damage variable which has a value of 0 for virgin material and a value of 1 at fracture, ϵ_p^f is the fracture strain, D_1, D_2, D_3, D_4, D_5 are constants, $\boldsymbol{\sigma}$ is the Cauchy stress, and T^* is the scaled temperature as in the Johnson-Cook plasticity model.

The input tags for the damage model are :

```
<damage_model type="johnson_cook">
  <D1>0.05</D1>
  <D2>3.44</D2>
  <D3>-2.12</D3>
  <D4>0.002</D4>
  <D5>0.61</D5>
</damage_model>
```

An initial damage distribution can be created using the following tags

```
<evolve_damage>                 true   </evolve_damage>
<initial_mean_scalar_damage>    0.005   </initial_mean_scalar_damage>
<initial_std_scalar_damage>     0.001 </initial_std_scalar_damage>
<critical_scalar_damage>        1.0    </critical_scalar_damage>
<initial_scalar_damage_distrib> gauss </initial_scalar_damage_distrib>
```

3.3.11 Erosion algorithm

Under normal conditions, the heat generated at a material point is conducted away at the end of a time step using the heat equation. If special adiabatic conditions apply (such as in impact problems), the heat is accumulated at a material point and is not conducted to the surrounding particles. This localized heating can be used to determine whether a material point has melted.

The determination of whether a particle has failed can be made on the basis of either or all of the following conditions:

- The particle temperature exceeds the melting temperature.
- The TEPLA-F fracture condition [JA88] is satisfied. This condition can be written as

$$(f/f_c)^2 + (\epsilon_p/\epsilon_p^f)^2 = 1 \tag{3.75}$$

  where f is the current porosity, f_c is the maximum allowable porosity, ϵ_p is the current plastic strain, and ϵ_p^f is the plastic strain at fracture.
- An alternative to ad-hoc damage criteria is to use the concept of bifurcation to determine whether a particle has failed or not. Two stability criteria have been explored in this paper - the Drucker stability postulate [Dru59] and the loss of hyperbolicity criterion (using the determinant of the acoustic tensor) [Per98; RR75].

The simplest criterion that can be used is the Drucker stability postulate [Dru59] which states that time rate of change of the rate of work done by a material cannot be negative. Therefore, the material is assumed to become unstable (and a particle fails) when

$$\dot{\boldsymbol{\sigma}} : \boldsymbol{D}^p \leq 0 \tag{3.76}$$

Another stability criterion that is less restrictive is the acoustic tensor criterion which states that the material loses stability if the determinant of the acoustic tensor changes sign [Per98; RR75]. Determination of the acoustic tensor requires a search for a normal vector around the material point and is therefore computationally expensive. A simplification of this criterion is a check which assumes that the direction of instability lies in the plane of the maximum and minimum principal stress [Bec02]. In this approach, we assume that the strain is localized in a band with normal **n**, and the magnitude of the velocity difference across the band is **g**. Then the bifurcation condition leads to the relation

$$R_{ij}g_j = 0\,; \quad R_{ij} = M_{ikjl}n_k n_l + M_{ilkj}n_k n_l - \sigma_{ik}n_j n_k \tag{3.77}$$

where M_{ijkl} are the components of the co-rotational tangent modulus tensor and σ_{ij} are the components of the co-rotational stress tensor. If $\det(R_{ij}) \leq 0$, then g_j can be arbitrary and there is a possibility of strain localization. If this condition for loss of hyperbolicity is met, then a particle deforms in an unstable

manner and failure can be assumed to have occurred at that particle. We use a combination of these criteria to simulate failure.

Since the material in the container may unload locally after fracture, the hypoelastic-plastic stress update may not work accurately under certain circumstances. An improvement would be to use a hyperelastic-plastic stress update algorithm. Also, the plasticity models are temperature dependent. Hence there is the issue of severe mesh dependence due to change of the governing equations from hyperbolic to elliptic in the softening regime [BB85; HH75; TN90]. Viscoplastic stress update models or nonlocal/gradient plasticity models [HLQ00; RA98a] can be used to eliminate some of these effects and are currently under investigation.

The tags used to control the erosion algorithm are in two places. In the `<MPM> </MPM>` section the following flags can be set

```
<erosion algorithm = "ZeroStress"/>
<create_new_particles>           false      </create_new_particles>
<manual_new_material>            false      </manual_new_material>
```

If the erosion algorithm is `"none"` then no particle failure is done.

In the `<constitutive_model type="elastic_plastic">` section, the following flags can be set

```
<evolve_porosity>               true  </evolve_porosity>
<evolve_damage>                 true  </evolve_damage>
<do_melting>                    true  </do_melting>
<useModifiedEOS>                true  </useModifiedEOS>
<check_TEPLA_failure_criterion> true  </check_TEPLA_failure_criterion>
<check_max_stress_failure>      false </check_max_stress_failure>
<critical_stress>              12.0e9 </critical_stress>
```

3.4 Implementation

The elastic response is assumed to be isotropic. The material constants that are taken as input for the elastic response are the bulk and shear modulus. The flow rule is determined from the input and the appropriate plasticity model is created using the `PlasticityModelFactory` class. The damage evolution rule is determined from the input and a damage model is created using the `DamageModelFactory` class. The equation of state that is used to determine the pressure is also determined from the input. The equation of state model is created using the `MPMEquationOfStateFactory` class.

In addition, a damage evolution variable (D) is stored at each time step (this need not be the case and will be transfered to the damage models in the future). The left stretch and rotation are updated incrementally at each time step (instead of performing a polar decomposition) and the rotation tensor is used to rotate the Cauchy stress and rate of deformation to the material coordinates at each time step (instead of using a objective stress rate formulation).

Any evolution variables for the plasticity model, damage model or the equation of state are specified in the class that encapsulates the particular model.

The flow stress is calculated from the plasticity model using a function call of the form

```
double flowStress = d_plasticity->computeFlowStress(tensorEta, tensorS,
                                                    pTemperature[idx],
                                                    delT, d_tol, matl, idx)
                                                        ;
```

A number of plasticity models can be evaluated using the inputs in the `computeFlowStress` call. The variable `d_plasticity` is polymorphic and can represent any of the plasticity models that can be created by the plasticity model factory. The plastic evolution variables are updated using a polymorphic function along the lines of `computeFlowStress`.

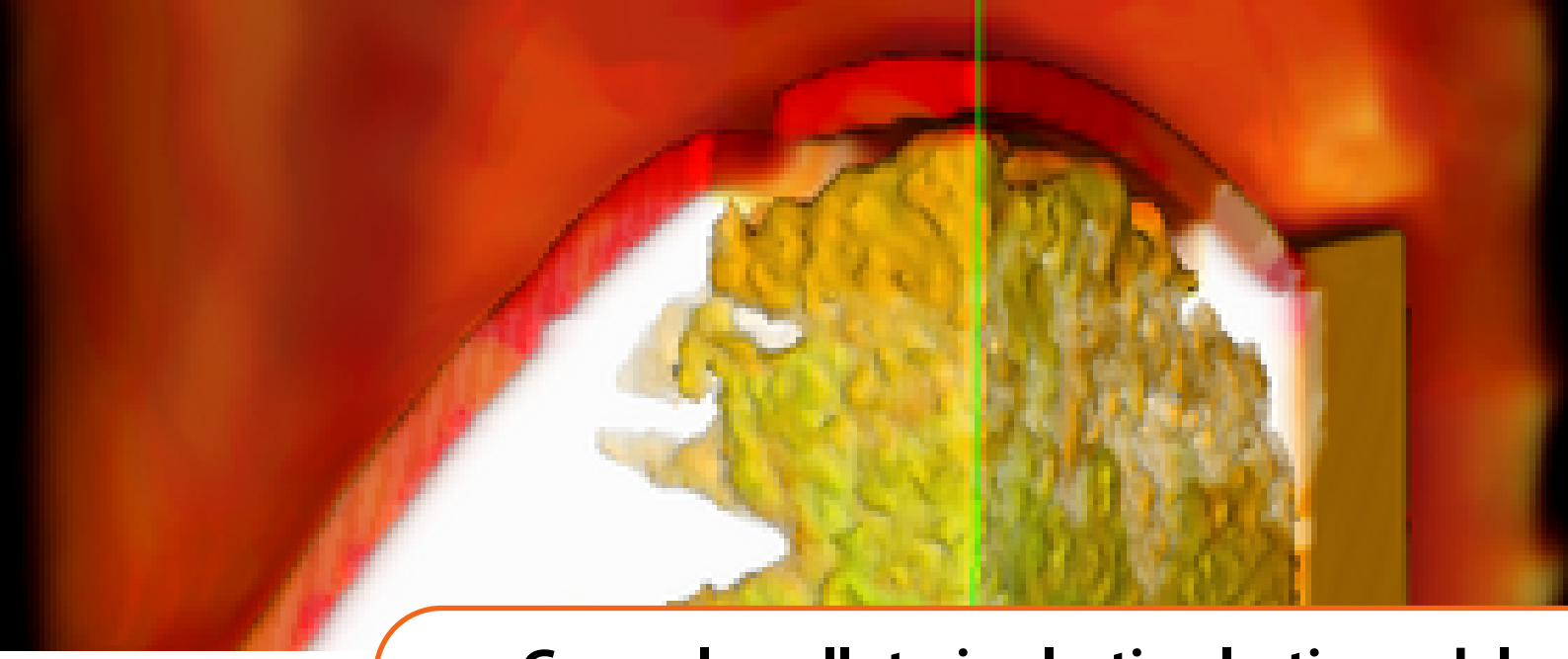
The equation of state is used to calculate the hydrostatic stress using a function call of the form

```
Matrix3 tensorHy = d_eos->computePressure(matl, bulk, shear,
                                          tensorF_new, tensorD,
                                          tensorP, pTemperature[idx],
                                          rho_cur, delT);
```

Similarly, the damage model is called using a function of the type

```
double damage = d_damage->computeScalarDamage(tensorEta, tensorS,
                                              pTemperature[idx],
                                              delT, matl, d_tol,
                                              pDamage[idx]);
```

Therefore, the plasticity, damage and equation of state models are easily be inserted into any other type of stress update algorithm without any change being needed in them as can be seen in the hyperelastic-plastic stress update algorithm discussed below.



4 — General small strain elastic-plastic model

4.1 Preamble

Let $\boldsymbol{F}$ be the deformation gradient, $\boldsymbol{\sigma}$ be the Cauchy stress, and $\boldsymbol{d}$ be the rate of deformation tensor. We first decompose the deformation gradient into a stretch and a rotations using $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$. The rotation $\boldsymbol{R}$ is then used to rotate the stress and the rate of deformation into the material configuration to give us

$$\hat{\boldsymbol{\sigma}} = \boldsymbol{R}^T \cdot \boldsymbol{\sigma} \cdot \boldsymbol{R} \,; \quad \hat{\boldsymbol{d}} = \boldsymbol{R}^T \cdot \boldsymbol{d} \cdot \boldsymbol{R} \tag{4.1}$$

This is equivalent to using a Green-Naghdi objective stress rate. In the following all equations are with respect to the hatted quantities and we drop the hats for convenience.

4.2 The model

4.2.1 Elastic relation

Let us split the Cauchy stress into a volumetric and a deviatoric part

$$\boldsymbol{\sigma} = p\,\boldsymbol{1} + \mathbf{s} \,; \quad p = \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma}) \,. \tag{4.2}$$

Taking the time derivative gives us

$$\dot{\boldsymbol{\sigma}} = \dot{p}\,\boldsymbol{1} + \dot{\mathbf{s}} \,. \tag{4.3}$$

We assume that the elastic response of the material is isotropic. The constitutive relation for a hypoelastic material of grade o can be expressed as

$$\dot{\boldsymbol{\sigma}} = \left[\lambda\,\mathrm{tr}(\boldsymbol{d}^e) - 3\,\kappa\,\alpha\,\frac{d}{dt}(T - T_o)\right]\boldsymbol{1} + 2\,\mu\,\boldsymbol{d}^e \,; \quad \boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p \tag{4.4}$$

where $\boldsymbol{d}^e$, $\boldsymbol{d}^p$ are the elastic and plastic parts of the rate of deformation tensor, λ, μ are the Lame constants, κ is the bulk modulus, α is the coefficient of thermal expansion, T_o is the reference temperature, and T is the current temperature. If we split $\boldsymbol{d}^e$ into volumetric and deviatoric parts as

$$\boldsymbol{d}^e = \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d}^e)\,\boldsymbol{1} + \boldsymbol{\eta}^e \tag{4.5}$$

we can write

$$\dot{\boldsymbol{\sigma}} = \left[\left(\lambda + \frac{2}{3}\mu\right)\,\mathrm{tr}(\boldsymbol{d}^e) - 3\,\kappa\,\alpha\,\frac{d}{dt}(T - T_0)\right]\boldsymbol{1} + 2\,\mu\,\boldsymbol{\eta}^e = \kappa\left[\mathrm{tr}(\boldsymbol{d}^e) - 3\,\alpha\,\frac{d}{dt}(T - T_0)\right]\boldsymbol{1} + 2\,\mu\,\boldsymbol{\eta}^e \quad (4.6)$$

Therefore, we have

$$\dot{\mathbf{s}} = 2\,\mu\,\boldsymbol{\eta}^e\,. \quad (4.7)$$

and

$$\dot{p} = \kappa\left[\mathrm{tr}(\boldsymbol{d}^e) - 3\,\alpha\,\frac{d}{dt}(T - T_0)\right]. \quad (4.8)$$

We will use a standard elastic-plastic stress update algorithm to integrate the rate equation for the deviatoric stress. However, we will assume that the volumetric part of the Cauchy stress can be computed using an equation of state. Then the final Cauchy stress will be given by

$$\boldsymbol{\sigma} = \left[p(J) - 3\,J\,\frac{dp(J)}{dJ}\,\alpha\,(T - T_0)\right]\boldsymbol{1} + \mathbf{s}\,;\quad J = \det(\boldsymbol{F})\,. \quad (4.9)$$

(Note that we assume that the plastic part of the deformation is volume preserving. This is not true for Gurson type models and will lead to a small error in the computed value of $\boldsymbol{\sigma}$.)

4.2.2 Flow rule

We assume that the flow rule is given by

$$\boldsymbol{d}^p = \dot{\gamma}\,\boldsymbol{r} \quad (4.10)$$

We can split $\boldsymbol{d}^p$ into a trace part and a trace free part, i.e.,

$$\boldsymbol{d}^p = \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d}^p)\,\boldsymbol{1} + \boldsymbol{\eta}^p \quad (4.11)$$

Then, using the flow rule, we have

$$\boldsymbol{d}^p = \tfrac{1}{3}\,\dot{\gamma}\,\mathrm{tr}(\boldsymbol{r})\,\boldsymbol{1} + \boldsymbol{\eta}^p\,. \quad (4.12)$$

Therefore we can write the flow rule as

$$\boldsymbol{\eta}^p = \dot{\gamma}\,\left(-\tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{r})\,\boldsymbol{1} + \boldsymbol{r}\right). \quad (4.13)$$

Note that

$$\boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p \quad\Longrightarrow\quad \mathrm{tr}(\boldsymbol{d}) = \mathrm{tr}(\boldsymbol{d}^e) + \mathrm{tr}(\boldsymbol{d}^p)\,. \quad (4.14)$$

Also,

$$\boldsymbol{d} = \boldsymbol{d}^e + \boldsymbol{d}^p \quad\Longrightarrow\quad \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d})\,\boldsymbol{1} + \boldsymbol{\eta} = \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d}^e)\,\boldsymbol{1} + \boldsymbol{\eta}^e + \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d}^p)\,\boldsymbol{1} + \boldsymbol{\eta}^p\,. \quad (4.15)$$

Therefore,

$$\boldsymbol{\eta} = \boldsymbol{\eta}^e + \boldsymbol{\eta}^p\,. \quad (4.16)$$

4.2.3 Isotropic and Kinematic hardening and porosity evolution rules

We assume that the strain rate, temperature, and porosity can be fixed at the beginning of a timestep and consider only the evolution of plastic strain and the back stress while calculating the current stress.

We assume that the plastic strain evolves according to the relation

$$\dot{\varepsilon^p} = \dot{\gamma}\, h^{\alpha} \tag{4.17}$$

We also assume that the back stress evolves according to the relation

$$\dot{\hat{\boldsymbol{\beta}}} = \dot{\gamma}\, \boldsymbol{h}^{\beta} \tag{4.18}$$

where $\hat{\boldsymbol{\beta}}$ is the back stress. If $\boldsymbol{\beta}$ is the deviatoric part of $\hat{\boldsymbol{\beta}}$, then we can write

$$\dot{\boldsymbol{\beta}} = \dot{\gamma}\, \mathrm{dev}(\boldsymbol{h}^{\beta})\,. \tag{4.19}$$

The porosity ϕ is assumed to evolve according to the relation

$$\dot{\phi} = \dot{\gamma}\, h^{\phi}\,. \tag{4.20}$$

4.2.4 Yield condition

The yield condition is assumed to be of the form

$$f(\mathbf{s}, \boldsymbol{\beta}, \varepsilon^p, \phi, \dot{\varepsilon}, T, \dots) = f(\boldsymbol{\xi}, \varepsilon^p, \phi, \dot{\varepsilon}, T, \dots) = 0 \tag{4.21}$$

where $\boldsymbol{\xi} = \mathbf{s} - \boldsymbol{\beta}$ and $\boldsymbol{\beta}$ is the deviatoric part of $\hat{\boldsymbol{\beta}}$. The Kuhn-Tucker loading-unloading conditions are

$$\dot{\gamma} \geq 0\,;\quad f \leq 0\,;\quad \dot{\gamma}\, f = 0 \tag{4.22}$$

and the consistency condition is $\dot{f} = 0$.

4.2.5 Temperature increase due to plastic dissipation

The temperature increase due to plastic dissipation is assume to be given by the rate equation

$$\dot{T} = \frac{\chi}{\rho\, C_p}\, \sigma_y\, \dot{\varepsilon^p}\,. \tag{4.23}$$

The temperature is updated using

$$T_{n+1} = T_n + \frac{\chi_{n+1}\, \Delta t}{\rho_{n+1}\, C_p}\, \sigma_y^{n+1}\, \dot{\varepsilon^p}_{n+1}\,. \tag{4.24}$$

4.2.6 Continuum elastic-plastic tangent modulus

To determine whether the material has undergone a loss of stability we need to compute the acosutic tensor which needs the computation of the continuum elastic-plastic tangent modulus.

To do that recall that

$$\boldsymbol{\sigma} = p\, \boldsymbol{1} + \mathbf{s} \quad \Longrightarrow \quad \dot{\boldsymbol{\sigma}} = \dot{p}\, \boldsymbol{1}\,. \tag{4.25}$$

We assume that

$$\dot{p} = J\, \frac{\partial p}{\partial J}\, \mathrm{tr}(\boldsymbol{d}) \qquad \text{and} \quad \dot{\mathbf{s}} = 2\, \mu\, \boldsymbol{\eta}^e\,. \tag{4.26}$$

Now, the consistency condition requires that

$$\dot{f}(\mathbf{s}, \boldsymbol{\beta}, \varepsilon^p, \phi, \dot{\varepsilon}, T, \dots) = 0 \,. \tag{4.27}$$

Keeping $\dot{\varepsilon}$ and T fixed over the time interval, we can use the chain rule to get

$$\dot{f} = \frac{\partial f}{\partial \mathbf{s}} : \dot{\mathbf{s}} + \frac{\partial f}{\partial \boldsymbol{\beta}} : \dot{\boldsymbol{\beta}} + \frac{\partial f}{\partial \varepsilon^p}\, \dot{\varepsilon^p} + \frac{\partial f}{\partial \phi}\, \dot{\phi} = 0 \,. \tag{4.28}$$

The needed rate equations are

$$\begin{aligned} \dot{\mathbf{s}} &= 2\,\mu\,\boldsymbol{\eta}^e = 2\,\mu\,(\boldsymbol{\eta} - \boldsymbol{\eta}^p) = 2\,\mu\,[\boldsymbol{\eta} - \dot{\gamma}\,\mathrm{dev}(\boldsymbol{r})] \\ \dot{\boldsymbol{\beta}} &= \dot{\gamma}\,\mathrm{dev}(\boldsymbol{h}^\beta) \\ \dot{\varepsilon^p} &= \dot{\gamma}\,h^\alpha \\ \dot{\phi} &= \dot{\gamma}\,h^\phi \end{aligned} \tag{4.29}$$

Plugging these into the expression for $\dot{f}$ gives

$$2\,\mu\,\frac{\partial f}{\partial \mathbf{s}} : [\boldsymbol{\eta} - \dot{\gamma}\,\mathrm{dev}(\boldsymbol{r})] + \dot{\gamma}\,\frac{\partial f}{\partial \boldsymbol{\beta}} : \mathrm{dev}(\boldsymbol{h}^\beta) + \dot{\gamma}\,\frac{\partial f}{\partial \varepsilon^p}\,h^\alpha + \dot{\gamma}\,\frac{\partial f}{\partial \phi}\,h^\phi = 0 \tag{4.30}$$

or,

$$\dot{\gamma} = \frac{2\,\mu\,\dfrac{\partial f}{\partial \mathbf{s}} : \boldsymbol{\eta}}{2\,\mu\,\dfrac{\partial f}{\partial \mathbf{s}} : \mathrm{dev}(\boldsymbol{r}) - \dfrac{\partial f}{\partial \boldsymbol{\beta}} : \mathrm{dev}(\boldsymbol{h}^\beta) - \dfrac{\partial f}{\partial \varepsilon^p}\,h^\alpha - \dfrac{\partial f}{\partial \phi}\,h^\phi} \,. \tag{4.31}$$

Plugging this expression for $\dot{\gamma}$ into the equation for $\dot{\mathbf{s}}$, we get

$$\dot{\mathbf{s}} = 2\,\mu\left[\boldsymbol{\eta} - \left(\frac{2\,\mu\,\dfrac{\partial f}{\partial \mathbf{s}} : \boldsymbol{\eta}}{2\,\mu\,\dfrac{\partial f}{\partial \mathbf{s}} : \mathrm{dev}(\boldsymbol{r}) - \dfrac{\partial f}{\partial \boldsymbol{\beta}} : \mathrm{dev}(\boldsymbol{h}^\beta) - \dfrac{\partial f}{\partial \varepsilon^p}\,h^\alpha - \dfrac{\partial f}{\partial \phi}\,h^\phi}\right)\mathrm{dev}(\boldsymbol{r})\right] \,. \tag{4.32}$$

At this stage, note that a symmetric $\boldsymbol{\sigma}$ implies a symmetric $\mathbf{s}$ and hence a symmetric $\boldsymbol{\eta}$. Also we assume that $\boldsymbol{r}$ is symmetric (and hence $\mathrm{dev}(\boldsymbol{r})$), which is true if the flow rule is associated. Then we can write

$$\boldsymbol{\eta} = \mathbf{I}^{4s} : \boldsymbol{\eta} \qquad \text{and} \qquad \mathrm{dev}(\boldsymbol{r}) = \mathbf{I}^{4s} : \mathrm{dev}(\boldsymbol{r}) \tag{4.33}$$

where $\mathbf{I}^{4s}$ is the fourth-order symmetric identity tensor. Also note that if $\boldsymbol{A}$, $\boldsymbol{C}$, $\boldsymbol{D}$ are second order tensors and $\mathbf{B}$ is a fourth order tensor, then

$$(\boldsymbol{A} : \mathbf{B} : \boldsymbol{C})\,(\mathbf{B} : \boldsymbol{D}) \equiv A_{ij}\,B_{ijkl}\,C_{kl}\,B_{mnpq}\,D_{pq} = (B_{mnpq}\,D_{pq})\,(A_{ij}\,B_{ijkl})\,C_{kl} \equiv [(\mathbf{B} : \boldsymbol{D}) \otimes (\boldsymbol{A} : \mathbf{B})] : \boldsymbol{C} \,. \tag{4.34}$$

Therefore we have

$$\dot{\mathbf{s}} = 2\,\mu\left[\mathbf{I}^{4s} : \boldsymbol{\eta} - \left(\frac{2\,\mu\,[\mathbf{I}^{4s} : \mathrm{dev}(\boldsymbol{r})] \otimes [\dfrac{\partial f}{\partial \mathbf{s}} : \mathbf{I}^{4s}]}{2\,\mu\,\dfrac{\partial f}{\partial \mathbf{s}} : \mathrm{dev}(\boldsymbol{r}) - \dfrac{\partial f}{\partial \boldsymbol{\beta}} : \mathrm{dev}(\boldsymbol{h}^\beta) - \dfrac{\partial f}{\partial \varepsilon^p}\,h^\alpha - \dfrac{\partial f}{\partial \phi}\,h^\phi}\right) : \boldsymbol{\eta}\right] \,. \tag{4.35}$$

Also,

$$\mathbf{I}^{4s} : \mathrm{dev}(\boldsymbol{r}) = \mathrm{dev}(\boldsymbol{r}) \qquad \text{and} \qquad \frac{\partial f}{\partial \mathbf{s}} : \mathbf{I}^{4s} = \frac{\partial f}{\partial \mathbf{s}} \,. \tag{4.36}$$

Hence we can write

$$\dot{\mathbf{s}} = 2\,\mu\left[\mathbf{I}^{4s} - \left(\frac{2\,\mu\,\mathrm{dev}(\boldsymbol{r})\otimes\frac{\partial f}{\partial \mathbf{s}}}{2\,\mu\,\frac{\partial f}{\partial \mathbf{s}}:\mathrm{dev}(\boldsymbol{r}) - \frac{\partial f}{\partial \boldsymbol{\beta}}:\mathrm{dev}(\boldsymbol{h}^{\beta}) - \frac{\partial f}{\partial \varepsilon^{p}}\,h^{\alpha} - \frac{\partial f}{\partial \phi}\,h^{\phi}}\right)\right]:\boldsymbol{\eta} \tag{4.37}$$

or,

$$\dot{\mathbf{s}} = \mathbf{B}^{ep}:\boldsymbol{\eta} = \mathbf{B}^{ep}:\left[\boldsymbol{d} - \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d})\,\boldsymbol{1}\right] \tag{4.38}$$

where

$$\mathbf{B}^{ep} := 2\,\mu\left[\mathbf{I}^{4s} - \left(\frac{2\,\mu\,\mathrm{dev}(\boldsymbol{r})\otimes\frac{\partial f}{\partial \mathbf{s}}}{2\,\mu\,\frac{\partial f}{\partial \mathbf{s}}:\mathrm{dev}(\boldsymbol{r}) - \frac{\partial f}{\partial \boldsymbol{\beta}}:\mathrm{dev}(\boldsymbol{h}^{\beta}) - \frac{\partial f}{\partial \varepsilon^{p}}\,h^{\alpha} - \frac{\partial f}{\partial \phi}\,h^{\phi}}\right)\right]. \tag{4.39}$$

Adding in the volumetric component gives

$$\begin{aligned}
\dot{\boldsymbol{\sigma}} &= \dot{p}\,\boldsymbol{1} + \dot{\mathbf{s}} \\
&= J\,\frac{\partial p}{\partial J}\,\mathrm{tr}(\boldsymbol{d})\,\boldsymbol{1} + \mathbf{B}^{ep}:\left[\boldsymbol{d} - \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{d})\,\boldsymbol{1}\right] \\
&= \left[3\,J\,\frac{\partial p}{\partial J}\,\boldsymbol{1} - \mathbf{B}^{ep}:\boldsymbol{1}\right]\frac{\boldsymbol{d}:\boldsymbol{1}}{3} + \mathbf{B}^{ep}:\boldsymbol{d} \\
&= J\,\frac{\partial p}{\partial J}\,(\boldsymbol{1}\otimes\boldsymbol{1}):\boldsymbol{d} - \tfrac{1}{3}\left[\mathbf{B}^{ep}:(\boldsymbol{1}\otimes\boldsymbol{1})\right]:\boldsymbol{d} + \mathbf{B}^{ep}:\boldsymbol{d}\,.
\end{aligned} \tag{4.40}$$

Therefore,

$$\dot{\boldsymbol{\sigma}} = \left[J\,\frac{\partial p}{\partial J}\,(\boldsymbol{1}\otimes\boldsymbol{1}) - \tfrac{1}{3}\left[\mathbf{B}^{ep}:(\boldsymbol{1}\otimes\boldsymbol{1})\right] + \mathbf{B}^{ep}\right]:\boldsymbol{d} = \mathbf{C}^{ep}:\boldsymbol{d}\,. \tag{4.41}$$

The quantity $\mathbf{C}^{ep}$ is the continuum elastic-plastic tangent modulus. We also use the continuum elastic-plastic tangent modulus in the implicit version of the code. However, for improved accuracy and faster convergence, an algorithmically consistent tangent modulus should be used instead. That tangent modulus can be calculated in the usual manner and is left for development and implementation as an additional feature in the future.

4.3 Stress update

A standard return algorithm is used to compute the updated Cauchy stress. Recall that the rate equation for the deviatoric stress is given by

$$\dot{\mathbf{s}} = 2\,\mu\,\boldsymbol{\eta}^{e}\,. \tag{4.42}$$

Integrating the rate equation using a Backward Euler scheme gives

$$\mathbf{s}_{n+1} - \mathbf{s}_{n} = 2\,\mu\,\Delta\,t\,\boldsymbol{\eta}^{e}_{n+1} = 2\,\mu\,\Delta\,t\,(\boldsymbol{\eta}_{n+1} - \boldsymbol{\eta}^{p}_{n+1}) \tag{4.43}$$

Now, from the flow rule, we have

$$\boldsymbol{\eta}^{p} = \dot{\gamma}\,\left(\boldsymbol{r} - \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{r})\,\boldsymbol{1}\right)\,. \tag{4.44}$$

Define the deviatoric part of $\boldsymbol{r}$ as

$$\mathrm{dev}(\boldsymbol{r}) := \boldsymbol{r} - \tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{r})\,\boldsymbol{1}\,. \tag{4.45}$$

Therefore,

$$\mathbf{s}_{n+1} - \mathbf{s}_n = 2\,\mu\,\Delta\,t\,\boldsymbol{\eta}_{n+1} - 2\,\mu\,\Delta\gamma_{n+1}\,\mathrm{dev}(\boldsymbol{r}_{n+1})\,. \tag{4.46}$$

where $\Delta\gamma := \dot{\gamma}\,\Delta t$. Define the trial stress

$$\mathbf{s}^{\mathrm{trial}} := \mathbf{s}_n + 2\,\mu\,\Delta\,t\,\boldsymbol{\eta}_{n+1}\,. \tag{4.47}$$

Then

$$\mathbf{s}_{n+1} = \mathbf{s}^{\mathrm{trial}} - 2\,\mu\,\Delta\gamma_{n+1}\,\mathrm{dev}(\boldsymbol{r}_{n+1})\,. \tag{4.48}$$

Also recall that the back stress is given by

$$\dot{\boldsymbol{\beta}} = \dot{\gamma}\,\mathrm{dev}\boldsymbol{h}^{\beta} \tag{4.49}$$

The evolution equation for the back stress can be integrated to get

$$\boldsymbol{\beta}_{n+1} - \boldsymbol{\beta}_n = \Delta\gamma_{n+1}\,\mathrm{dev}(\boldsymbol{h})^{\beta}_{n+1}\,. \tag{4.50}$$

Now,

$$\boldsymbol{\xi}_{n+1} = \mathbf{s}_{n+1} - \boldsymbol{\beta}_{n+1}\,. \tag{4.51}$$

Plugging in the expressions for $\mathbf{s}_{n+1}$ and $\boldsymbol{\beta}_{n+1}$, we get

$$\boldsymbol{\xi}_{n+1} = \mathbf{s}^{\mathrm{trial}} - 2\,\mu\,\Delta\gamma_{n+1}\,\mathrm{dev}(\boldsymbol{r}_{n+1}) - \boldsymbol{\beta}_n - \Delta\gamma_{n+1}\,\mathrm{dev}(\boldsymbol{h})^{\beta}_{n+1}\,. \tag{4.52}$$

Define

$$\boldsymbol{\xi}^{\mathrm{trial}} := \mathbf{s}^{\mathrm{trial}} - \boldsymbol{\beta}_n\,. \tag{4.53}$$

Then

$$\boldsymbol{\xi}_{n+1} = \boldsymbol{\xi}^{\mathrm{trial}} - \Delta\gamma_{n+1}(2\,\mu\,\mathrm{dev}(\boldsymbol{r}_{n+1}) + \mathrm{dev}(\boldsymbol{h})^{\beta}_{n+1})\,. \tag{4.54}$$

Similarly, the evolution of the plastic strain is given by

$$\varepsilon^p_{n+1} = \varepsilon^p_n + \Delta\gamma_{n+1}\,h^{\alpha}_{n+1} \tag{4.55}$$

and the porosity evolves as

$$\phi_{n+1} = \phi_n + \Delta\gamma_{n+1}\,h^{\phi}_{n+1}\,. \tag{4.56}$$

The yield condition is discretized as

$$f(\mathbf{s}_{n+1}, \boldsymbol{\beta}_{n+1}, \varepsilon^p_{n+1}, \phi_{n+1}, \dot{\varepsilon}_{n+1}, T_{n+1}, \dots) = f(\boldsymbol{\xi}_{n+1}, \varepsilon^p_{n+1}, \phi_{n+1}, \dot{\varepsilon}_{n+1}, T_{n+1}, \dots) = 0\,. \tag{4.57}$$

Important: We assume that the derivatives with respect to $\dot{\varepsilon}$ and T are small enough to be neglected.

4.3.1 Newton iterations

We now have the following equations that have to be solved for $\Delta\gamma_{n+1}$:

$$\begin{aligned}
\boldsymbol{\xi}_{n+1} &= \boldsymbol{\xi}^{\text{trial}} - \Delta\gamma_{n+1}(2\,\mu\,\text{dev}(\boldsymbol{r}_{n+1}) + \text{dev}(\boldsymbol{h})^{\beta}_{n+1}) \\
\varepsilon^{p}_{n+1} &= \varepsilon^{p}_{n} + \Delta\gamma_{n+1}\,h^{\alpha}_{n+1} \\
\phi_{n+1} &= \phi_{n} + \Delta\gamma_{n+1}\,h^{\phi}_{n+1} \\
f(\boldsymbol{\xi}_{n+1}, \varepsilon^{p}_{n+1}, \phi_{n+1}, \dot{\varepsilon}_{n+1}, T_{n+1}, \dots) &= 0\,.
\end{aligned} \tag{4.58}$$

Recall that if $g(\Delta\gamma) = 0$ is a nonlinear equation that we have to solve for $\Delta\gamma$, an iterative Newton method can be expressed as

$$\Delta\gamma^{(k+1)} = \Delta\gamma^{(k)} - \left[\frac{dg}{d\Delta\gamma}\right]^{-1}_{(k)} g^{(k)}\,. \tag{4.59}$$

Define

$$\delta\gamma := \Delta\gamma^{(k+1)} - \Delta\gamma^{(k)}\,. \tag{4.60}$$

Then, the iterative scheme can be written as

$$g^{(k)} + \left[\frac{dg}{d\Delta\gamma}\right]^{(k)} \delta\gamma = 0\,. \tag{4.61}$$

In our case we have

$$\begin{aligned}
\mathbf{a}(\Delta\gamma) &= 0 = -\boldsymbol{\xi} + \boldsymbol{\xi}^{\text{trial}} - \Delta\gamma(2\,\mu\,\text{dev}(\boldsymbol{r}) + \text{dev}(\boldsymbol{h})^{\beta}) \\
b(\Delta\gamma) &= 0 = -\varepsilon^{p} + \varepsilon^{p}_{n} + \Delta\gamma\,h^{\alpha} \\
c(\Delta\gamma) &= 0 = -\phi + \phi_{n} + \Delta\gamma\,h^{\phi} \\
f(\Delta\gamma) &= 0 = f(\boldsymbol{\xi}, \varepsilon^{p}, \phi, \dot{\varepsilon}, T, \dots)
\end{aligned} \tag{4.62}$$

Therefore,

$$\begin{aligned}
\frac{d\mathbf{a}}{d\Delta\gamma} &= -\frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} - (2\,\mu\,\text{dev}(\boldsymbol{r}) + \text{dev}(\boldsymbol{h})^{\beta}) - \Delta\gamma\left(2\,\mu\,\frac{\partial\text{dev}(\boldsymbol{r})}{\partial\Delta\gamma} + \frac{\partial\text{dev}(\boldsymbol{h})^{\beta}}{\partial\Delta\gamma}\right) \\
&= -\frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} - (2\,\mu\,\text{dev}(\boldsymbol{r}) + \text{dev}(\boldsymbol{h})^{\beta}) - \Delta\gamma\left(2\,\mu\,\frac{\partial\text{dev}(\boldsymbol{r})}{\partial\boldsymbol{\xi}} : \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} + 2\,\mu\,\frac{\partial\text{dev}(\boldsymbol{r})}{\partial\varepsilon^{p}}\,\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + 2\,\mu\,\frac{\partial\text{dev}(\boldsymbol{r})}{\partial\phi}\,\frac{\partial\phi}{\partial\Delta\gamma} + \right. \\
&\qquad \left. \frac{\partial\text{dev}(\boldsymbol{h})^{\beta}}{\partial\boldsymbol{\xi}} : \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} + \frac{\partial\text{dev}(\boldsymbol{h})^{\beta}}{\partial\varepsilon^{p}}\,\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + \frac{\partial\text{dev}(\boldsymbol{h})^{\beta}}{\partial\phi}\,\frac{\partial\phi}{\partial\Delta\gamma}\right) \\
\frac{db}{d\Delta\gamma} &= -\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + h^{\alpha} + \Delta\gamma\left(\frac{\partial h^{\alpha}}{\partial\boldsymbol{\xi}} : \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} + \frac{\partial h^{\alpha}}{\partial\varepsilon^{p}}\,\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + \frac{\partial h^{\alpha}}{\partial\phi}\,\frac{\partial\phi}{\partial\Delta\gamma}\right) \\
\frac{dc}{d\Delta\gamma} &= -\frac{\partial\phi}{\partial\Delta\gamma} + h^{\phi} + \Delta\gamma\left(\frac{\partial h^{\phi}}{\partial\boldsymbol{\xi}} : \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} + \frac{\partial h^{\phi}}{\partial\varepsilon^{p}}\,\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + \frac{\partial h^{\phi}}{\partial\phi}\,\frac{\partial\phi}{\partial\Delta\gamma}\right) \\
\frac{df}{d\Delta\gamma} &= \frac{\partial f}{\partial\boldsymbol{\xi}} : \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma} + \frac{\partial f}{\partial\varepsilon^{p}}\,\frac{\partial\varepsilon^{p}}{\partial\Delta\gamma} + \frac{\partial f}{\partial\phi}\,\frac{\partial\phi}{\partial\Delta\gamma}\,.
\end{aligned} \tag{4.63}$$

Now, define

$$\Delta\boldsymbol{\xi} := \frac{\partial\boldsymbol{\xi}}{\partial\Delta\gamma}\,\delta\gamma\,;\quad \Delta\varepsilon^{p} := \frac{\partial\varepsilon^{p}}{\partial\Delta\gamma}\,\delta\gamma\,;\quad \Delta\phi := \frac{\partial\phi}{\partial\Delta\gamma}\,\delta\gamma\,. \tag{4.64}$$

Then

$$\begin{aligned}
&\mathbf{a}^{(k)} - \Delta\boldsymbol{\xi} - \left[2\,\mu\,\mathrm{dev}(\boldsymbol{r}^{(k)}) + \mathrm{dev}(\boldsymbol{h})^{\beta(k)}\right]\delta\gamma \\
&\qquad - 2\,\mu\,\Delta\gamma\left(\frac{\partial \mathrm{dev}(\boldsymbol{r}^{(k)})}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial \mathrm{dev}(\boldsymbol{r}^{(k)})}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial \mathrm{dev}(\boldsymbol{r}^{(k)})}{\partial\phi}\,\Delta\phi\right) \\
&\qquad - \Delta\gamma\left(\frac{\partial \mathrm{dev}(\boldsymbol{h})^{\beta(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial \mathrm{dev}(\boldsymbol{h})^{\beta(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial \mathrm{dev}(\boldsymbol{h})^{\beta(k)}}{\partial\phi}\,\Delta\phi\right) = 0 \\
&b^{(k)} - \Delta\varepsilon^p + h^\alpha\,\delta\gamma + \Delta\gamma\left(\frac{\partial h^{\alpha(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial h^{\alpha(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial h^{\alpha(k)}}{\partial\phi}\,\Delta\phi\right) = 0 \\
&c^{(k)} - \Delta\phi + h^\phi\,\delta\gamma + \Delta\gamma\left(\frac{\partial h^{\phi(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial h^{\phi(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial h^{\phi(k)}}{\partial\phi}\,\Delta\phi\right) = 0 \\
&f^{(k)} + \frac{\partial f^{(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial f^{(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial f^{(k)}}{\partial\phi}\,\Delta\phi = 0
\end{aligned} \tag{4.65}$$

Because the derivatives of $\boldsymbol{r}^{(k)}, \boldsymbol{h}^{\alpha(k)}, \boldsymbol{h}^{\beta(k)}, \boldsymbol{h}^{\phi(k)}$ with respect to $\boldsymbol{\xi}, \varepsilon^p, \phi$ may be difficult to calculate, we instead use a semi-implicit scheme in our implementation where the quantities $\boldsymbol{r}$, h^α, $\boldsymbol{h}^\beta$, and h^ϕ are evaluated at t_n. Then the problematic derivatives disappear and we are left with

$$\begin{aligned}
\mathbf{a}^{(k)} - \Delta\boldsymbol{\xi} - \left[2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h})^\beta_n\right]\delta\gamma &= 0 \\
b^{(k)} - \Delta\varepsilon^p + h^\alpha_n\,\delta\gamma &= 0 \\
c^{(k)} - \Delta\phi + h^\phi_n\,\delta\gamma &= 0 \\
f^{(k)} + \frac{\partial f^{(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial f^{(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial f^{(k)}}{\partial\phi}\,\Delta\phi &= 0
\end{aligned} \tag{4.66}$$

We now force $\mathbf{a}^{(k)}$, $b^{(k)}$, and $c^{(k)}$ to be zero at all times, leading to the expressions

$$\begin{aligned}
\Delta\boldsymbol{\xi} &= -\left[2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h})^\beta_n\right]\delta\gamma \\
\Delta\varepsilon^p &= h^\alpha_n\,\delta\gamma \\
\Delta\phi &= h^\phi_n\,\delta\gamma \\
f^{(k)} + \frac{\partial f^{(k)}}{\partial\boldsymbol{\xi}} : \Delta\boldsymbol{\xi} + \frac{\partial f^{(k)}}{\partial\varepsilon^p}\,\Delta\varepsilon^p + \frac{\partial f^{(k)}}{\partial\phi}\,\Delta\phi &= 0
\end{aligned} \tag{4.67}$$

Plugging the expressions for $\Delta\boldsymbol{\xi}$, $\Delta\varepsilon^p$, $\Delta\phi$ from the first three equations into the fourth gives us

$$f^{(k)} - \frac{\partial f^{(k)}}{\partial\boldsymbol{\xi}} : \left[2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h})^\beta_n\right]\delta\gamma + h^\alpha_n\,\frac{\partial f^{(k)}}{\partial\varepsilon^p}\,\delta\gamma + h^\phi_n\,\frac{\partial f^{(k)}}{\partial\phi}\,\delta\gamma = 0 \tag{4.68}$$

or

$$\Delta\gamma^{(k+1)} - \Delta\gamma^{(k)} = \delta\gamma = \frac{f^{(k)}}{\frac{\partial f^{(k)}}{\partial\boldsymbol{\xi}} : \left[2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h}^\beta_n)\right] - h^\alpha_n\,\frac{\partial f^{(k)}}{\partial\varepsilon^p} - h^\phi_n\,\frac{\partial f^{(k)}}{\partial\phi}}\,. \tag{4.69}$$

4.3.2 Algorithm

The following stress update algorithm is used for each (plastic) time step:

1. Initialize:

$$k = 0\,;\quad (\varepsilon^p)^{(k)} = \varepsilon^p_n\,;\quad \phi^{(k)} = \phi_n\,;\quad \boldsymbol{\beta}^{(k)} = \boldsymbol{\beta}_n\,;\quad \Delta\gamma^{(k)} = 0\,;\quad \boldsymbol{\xi}^{(k)} = \boldsymbol{\xi}^{\mathrm{trial}}\,. \tag{4.70}$$

2. Check yield condition:

$$f^{(k)} := f(\boldsymbol{\xi}^{(k)}, (\varepsilon^p)^{(k)}, \phi^{(k)}, \dot{\varepsilon}_n, T_n, \dots) \tag{4.71}$$

If $f^{(k)} <$ tolerance then go to step 5 else go to step 3.

3. Compute updated $\delta\gamma^{(k)}$ using

$$\delta\gamma^{(k)} = \frac{f^{(k)}}{\dfrac{\partial f^{(k)}}{\partial \boldsymbol{\xi}} : [2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h}_n^{\beta})] - h_n^{\alpha}\,\dfrac{\partial f^{(k)}}{\partial \varepsilon^p} - h_n^{\phi}\,\dfrac{\partial f^{(k)}}{\partial \phi}}\,. \tag{4.72}$$

Compute

$$\begin{aligned} \Delta\boldsymbol{\xi}^{(k)} &= -[2\,\mu\,\mathrm{dev}(\boldsymbol{r}_n) + \mathrm{dev}(\boldsymbol{h}_n^{\beta})]\,\delta\gamma^{(k)} \\ (\Delta\varepsilon^p)^{(k)} &= h_n^{\alpha}\,\delta\gamma^{(k)} \\ \Delta\phi^{(k)} &= h_n^{\phi}\,\delta\gamma^{(k)} \end{aligned} \tag{4.73}$$

4. Update variables:

$$\begin{aligned} (\varepsilon^p)^{(k+1)} &= (\varepsilon^p)^{(k)} + (\Delta\varepsilon^p)^{(k)} \\ \phi^{(k+1)} &= \phi^{(k)} + \Delta\phi^{(k)} \\ \boldsymbol{\xi}^{(k+1)} &= \boldsymbol{\xi}^{(k)} + \Delta\boldsymbol{\xi}^{(k)} \\ \Delta\gamma^{(k+1)} &= \Delta\gamma^{(k)} + \delta\gamma^{(k)} \end{aligned} \tag{4.74}$$

Set $k \leftarrow k+1$ and go to step 2.

5. Update and calculate back stress and the deviatoric part of Cauchy stress:

$$\varepsilon^p_{n+1} = (\varepsilon^p)^{(k)}\;;\quad \phi_{n+1} = \phi^{(k)}\;;\quad \boldsymbol{\xi}_{n+1} = \boldsymbol{\xi}^{(k)}\;;\quad \Delta\gamma_{n+1} = \Delta\gamma^{(k)} \tag{4.75}$$

and

$$\begin{aligned} \hat{\boldsymbol{\beta}}_{n+1} &= \hat{\boldsymbol{\beta}}_n + \Delta\gamma_{n+1}\,\boldsymbol{h}^{\beta}(\boldsymbol{\xi}_{n+1}, \varepsilon^p_{n+1}, \phi_{n+1}) \\ \boldsymbol{\beta}_{n+1} &= \hat{\boldsymbol{\beta}}_{n+1} - \tfrac{1}{3}\,\mathrm{tr}(\hat{\boldsymbol{\beta}}_{n+1})\,\boldsymbol{1} \\ \mathbf{s}_{n+1} &= \boldsymbol{\xi}_{n+1} + \boldsymbol{\beta}_{n+1} \end{aligned} \tag{4.76}$$

6. Update the temperature and the Cauchy stress

$$\begin{aligned} T_{n+1} &= T_n + \frac{\chi_{n+1}\,\Delta t}{\rho_{n+1}\,C_p}\,\sigma_y^{n+1}\,\dot{\varepsilon^p}_{n+1} = T_n + \frac{\chi_{n+1}\,\Delta\gamma_{n+1}}{\rho_{n+1}\,C_p}\,\sigma_y^{n+1}\,h^{\alpha}_{n+1} \\ p_{n+1} &= p(J_{n+1}) \\ \kappa_{n+1} &= J_{n+1}\left[\frac{dp(J)}{dJ}\right]_{n+1} \\ \boldsymbol{\sigma}_{n+1} &= [p_{n+1} - 3\,\kappa_{n+1}\,\alpha\,(T_{n+1} - T_0)]\,\boldsymbol{1} + \mathbf{s}_{n+1} \end{aligned} \tag{4.77}$$

4.4 Examples

Let us now look at a few examples.

4.4.1 Example 1

Consider the case of J_2 plasticity with the yield condition

$$f := \sqrt{\frac{3}{2}}\,\|\mathbf{s}-\boldsymbol{\beta}\| - \sigma_y(\varepsilon^p, \dot{\varepsilon}, T, \dots) = \sqrt{\frac{3}{2}}\,\|\boldsymbol{\xi}\| - \sigma_y(\varepsilon^p, \dot{\varepsilon}, T, \dots) \le 0 \tag{4.78}$$

where $\|\boldsymbol{\xi}\| = \sqrt{\boldsymbol{\xi} : \boldsymbol{\xi}}$. Assume the associated flow rule

$$\boldsymbol{d}^p = \dot{\gamma}\,\boldsymbol{r} = \dot{\gamma}\,\frac{\partial f}{\partial \boldsymbol{\sigma}} = \dot{\gamma}\,\frac{\partial f}{\partial \boldsymbol{\xi}}\,. \tag{4.79}$$

Then

$$\boldsymbol{r} = \frac{\partial f}{\partial \boldsymbol{\xi}} = \sqrt{\frac{3}{2}}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|} \tag{4.80}$$

and

$$\boldsymbol{d}^p = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}\,;\quad \|\boldsymbol{d}^p\| = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,. \tag{4.81}$$

The evolution of the equivalent plastic strain is given by

$$\dot{\varepsilon^p} = \dot{\gamma}\,h^\alpha = \sqrt{\frac{2}{3}}\,\|\boldsymbol{d}^p\| = \dot{\gamma}\,. \tag{4.82}$$

This definition is consistent with the definition of equivalent plastic strain

$$\varepsilon^p = \int_0^t \dot{\varepsilon}^p\,d\tau = \int_0^t \sqrt{\frac{2}{3}}\,\|\boldsymbol{d}^p\|\;d\tau\,. \tag{4.83}$$

The evolution of porosity is given by (there is no evolution of porosity)

$$\dot{\phi} = \dot{\gamma}\,h^\phi = 0 \tag{4.84}$$

The evolution of the back stress is given by the Prager kinematic hardening rule

$$\dot{\hat{\boldsymbol{\beta}}} = \dot{\gamma}\,\boldsymbol{h}^\beta = \frac{2}{3}\,H'\,\boldsymbol{d}^p \tag{4.85}$$

where $\hat{\boldsymbol{\beta}}$ is the back stress and H' is a constant hardening modulus. Also, the trace of $\boldsymbol{d}^p$ is

$$\mathrm{tr}(\boldsymbol{d}^p) = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,\frac{\mathrm{tr}(\boldsymbol{\xi})}{\|\boldsymbol{\xi}\|}\,. \tag{4.86}$$

Since $\boldsymbol{\xi}$ is deviatoric, $\mathrm{tr}(\boldsymbol{\xi}) = 0$ and hence $\boldsymbol{d}^p = \boldsymbol{\eta}^p$. Hence, $\dot{\hat{\boldsymbol{\beta}}} = \dot{\boldsymbol{\beta}}$ (where $\boldsymbol{\beta}$ is the deviatoric part of $\hat{\boldsymbol{\beta}}$), and

$$\dot{\boldsymbol{\beta}} = \sqrt{\frac{2}{3}}\,H'\,\dot{\gamma}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}\,. \tag{4.87}$$

These relation imply that

$$\boxed{\begin{aligned} \boldsymbol{r} &= \sqrt{\frac{3}{2}}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|} \\ h^\alpha &= 1 \\ h^\phi &= 0 \\ \boldsymbol{h}^\beta &= \sqrt{\frac{2}{3}}\,H'\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|}\,. \end{aligned}} \tag{4.88}$$

We also need some derivatives of the yield function. These are

$$\begin{aligned}\frac{\partial f}{\partial \boldsymbol{\xi}} &= \boldsymbol{r}\\ \frac{\partial f}{\partial \varepsilon^p} &= -\frac{\partial \sigma_y}{\partial \varepsilon^p}\\ \frac{\partial f}{\partial \phi} &= 0\,.\end{aligned} \tag{4.89}$$

Let us change the kinematic hardening model and use the Armstrong-Frederick model instead, i.e.,

$$\dot{\boldsymbol{\beta}} = \dot{\gamma}\,\boldsymbol{h}^{\beta} = \frac{2}{3}\,H_1\,\boldsymbol{d}^p - H_2\,\boldsymbol{\beta}\,\left\|\boldsymbol{d}^p\right\|\,. \tag{4.90}$$

Since

$$\boldsymbol{d}^p = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|} \tag{4.91}$$

we have

$$\left\|\boldsymbol{d}^p\right\| = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,\frac{\|\boldsymbol{\xi}\|}{\|\boldsymbol{\xi}\|} = \sqrt{\frac{3}{2}}\,\dot{\gamma}\,. \tag{4.92}$$

Therefore,

$$\dot{\boldsymbol{\beta}} = \sqrt{\frac{2}{3}}\,H_1\,\dot{\gamma}\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|} - \sqrt{\frac{3}{2}}\,H_2\,\dot{\gamma}\,\boldsymbol{\beta}\,. \tag{4.93}$$

Hence we have

$$\boxed{\boldsymbol{h}^{\beta} = \sqrt{\frac{2}{3}}\,H_1\,\frac{\boldsymbol{\xi}}{\|\boldsymbol{\xi}\|} - \sqrt{\frac{3}{2}}\,H_2\,\boldsymbol{\beta}\,.} \tag{4.94}$$

4.4.2 Example 2

Let us now consider a Gurson type yield condition with kinematic hardening. In this case the yield condition can be written as

$$f := \frac{3\,\boldsymbol{\xi}:\boldsymbol{\xi}}{2\,\sigma_y^2} + 2\,q_1\,\phi^*\,\cosh\left(\frac{q_2\,\mathrm{tr}(\boldsymbol{\sigma})}{2\,\sigma_y}\right) - \left[1 + q_3\,(\phi^*)^2\right] \tag{4.95}$$

where ϕ is the porosity and

$$\phi^* = \begin{cases}\phi & \text{for } \phi \le \phi_c\\ \phi_c - \dfrac{\phi_u^* - \phi_c}{\phi_f - \phi_c}\,(\phi - \phi_c) & \text{for } \phi > \phi_c\end{cases} \tag{4.96}$$

Final fracture occurs for $\phi = \phi_f$ or when $\phi_u^* = 1/q_1$.

Let us use an associated flow rule

$$\boldsymbol{d}^p = \dot{\gamma}\,\boldsymbol{r} = \dot{\gamma}\,\frac{\partial f}{\partial \boldsymbol{\sigma}}\,. \tag{4.97}$$

Then

$$\boldsymbol{r} = \frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{3\,\boldsymbol{\xi}}{\sigma_y^2} + \frac{q_1\,q_2\,\phi^*}{\sigma_y}\,\sinh\left(\frac{q_2\,\mathrm{tr}(\boldsymbol{\sigma})}{2\,\sigma_y}\right)\boldsymbol{1}\,. \tag{4.98}$$

In this case

$$\operatorname{tr}(\boldsymbol{r}) = \frac{3\, q_1\, q_2\, \phi^*}{\sigma_y}\, \sinh\left(\frac{q_2\, \operatorname{tr}(\boldsymbol{\sigma})}{2\, \sigma_y}\right) \neq 0 \tag{4.99}$$

Therefore,

$$\boldsymbol{d}^p \neq \boldsymbol{\eta}^p\ . \tag{4.100}$$

For the evolution equation for the plastic strain we use

$$(\boldsymbol{\sigma} - \hat{\boldsymbol{\beta}}) : \boldsymbol{d}^p = (1-\phi)\, \sigma_y\, \dot{\varepsilon}^p \tag{4.101}$$

where $\dot{\varepsilon}^p$ is the effective plastic strain rate in the matrix material. Hence,

$$\dot{\varepsilon}^p = \dot{\gamma}\, h^\alpha = \dot{\gamma}\, \frac{(\boldsymbol{\sigma} - \hat{\boldsymbol{\beta}}) : \boldsymbol{r}}{(1-\phi)\, \sigma_y}\,. \tag{4.102}$$

The evolution equation for the porosity is given by

$$\dot{\phi} = (1-\phi)\, \operatorname{tr}(\boldsymbol{d}^p) + A\, \dot{\varepsilon^p} \tag{4.103}$$

where

$$A = \frac{f_n}{s_n\sqrt{2\pi}} \exp[-1/2(\varepsilon^p - \varepsilon_n)^2/s_n^2] \tag{4.104}$$

and f_n is the volume fraction of void nucleating particles, ε_n is the mean of the normal distribution of nucleation strains, and s_n is the standard deviation of the distribution.

Therefore,

$$\dot{\phi} = \dot{\gamma}\, h^\phi = \dot{\gamma}\, \left[(1-\phi)\, \operatorname{tr}(\boldsymbol{r}) + A\, \frac{(\boldsymbol{\sigma} - \hat{\boldsymbol{\beta}}) : \boldsymbol{r}}{(1-\phi)\, \sigma_y}\right]\ . \tag{4.105}$$

If the evolution of the back stress is given by the Prager kinematic hardening rule

$$\dot{\hat{\boldsymbol{\beta}}} = \dot{\gamma}\, \boldsymbol{h}^\beta = \frac{2}{3}\, H'\, \boldsymbol{d}^p \tag{4.106}$$

where $\hat{\boldsymbol{\beta}}$ is the back stress, then

$$\dot{\hat{\boldsymbol{\beta}}} = \frac{2}{3}\, H'\, \dot{\gamma}\, \boldsymbol{r}\ . \tag{4.107}$$

Alternatively, if we use the Armstrong-Frederick model, then

$$\dot{\hat{\boldsymbol{\beta}}} = \dot{\gamma}\, \boldsymbol{h}^\beta = \frac{2}{3}\, H_1\, \boldsymbol{d}^p - H_2\, \hat{\boldsymbol{\beta}}\ \left\|\boldsymbol{d}^p\right\|\ . \tag{4.108}$$

Plugging in the expression for $\boldsymbol{d}^p$, we have

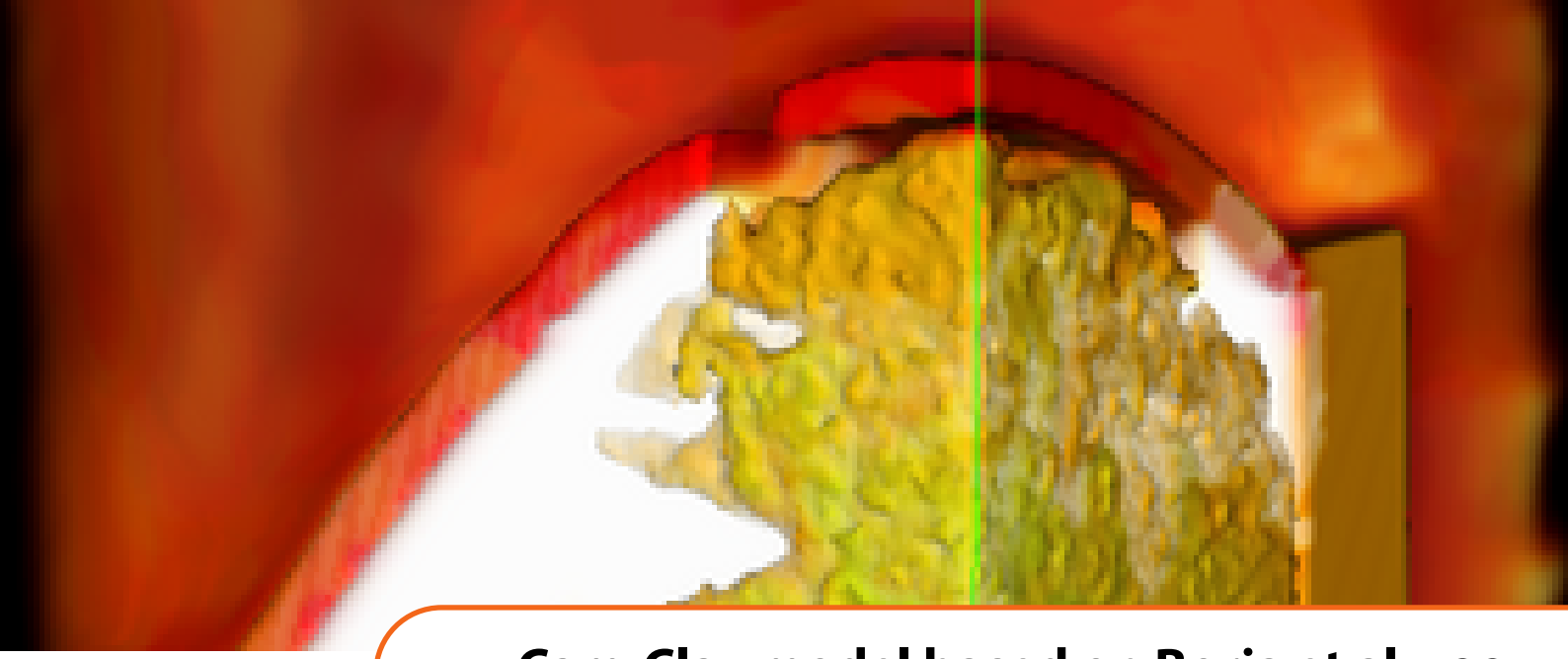
$$\dot{\hat{\boldsymbol{\beta}}} = \dot{\gamma}\, \left[\frac{2}{3}\, H_1\, \boldsymbol{r} - H_2\, \hat{\boldsymbol{\beta}}\ \|\boldsymbol{r}\|\right]\ . \tag{4.109}$$

Therefore, for this model,

$$\boxed{\begin{aligned} \boldsymbol{r} &= \frac{3\,\boldsymbol{\xi}}{\sigma_y^2} + \frac{q_1\,q_2\,\phi^*}{\sigma_y}\,\sinh\left(\frac{q_2\,\mathrm{tr}(\boldsymbol{\sigma})}{2\,\sigma_y}\right)\boldsymbol{1} \\ h^\alpha &= \frac{(\boldsymbol{\sigma}-\boldsymbol{\beta}):\boldsymbol{r}}{(1-\phi)\,\sigma_y} \\ h^\phi &= (1-\phi)\,\mathrm{tr}(\boldsymbol{r}) + A\,\frac{(\boldsymbol{\sigma}-\hat{\boldsymbol{\beta}}):\boldsymbol{r}}{(1-\phi)\,\sigma_y} \\ \boldsymbol{h}^\beta &= \frac{2}{3}\,H_1\,\boldsymbol{r} - H_2\,\hat{\boldsymbol{\beta}}\,\|\boldsymbol{r}\| \end{aligned}} \tag{4.110}$$

The other derivatives of the yield function that we need are

$$\begin{aligned} \frac{\partial f}{\partial \boldsymbol{\xi}} &= \frac{3\,\boldsymbol{\xi}}{\sigma_y^2} \\ \frac{\partial f}{\partial \varepsilon^p} &= \frac{\partial f}{\partial \sigma_y}\,\frac{\partial \sigma_y}{\partial \varepsilon^p} = -\left[\frac{3\,\boldsymbol{\xi}:\boldsymbol{\xi}}{\sigma_y^3} + \frac{q_1\,q_2\,\phi^*\,\mathrm{tr}(\boldsymbol{\sigma})}{\sigma_y^2}\,\sinh\left(\frac{q_2\,\mathrm{tr}(\boldsymbol{\sigma})}{2\,\sigma_y}\right)\right]\frac{\partial \sigma_y}{\partial \varepsilon^p} \\ \frac{\partial f}{\partial \phi} &= 2\,q_1\,\frac{d\phi^*}{d\phi}\,\cosh\left(\frac{q_2\,\mathrm{tr}(\sigma)}{2\,\sigma_y}\right) - 2\,q_3\,\phi^*\,\frac{d\phi^*}{d\phi}\,. \end{aligned} \tag{4.111}$$



5 — Cam-Clay model based on Borja et al. 1997

5.1 Introduction

The Cam-clay plasticity model and its modified ellipsoidal version [RB68; RS63; SW68; WH86] is widely considered to be an accurate model for the prediction of the compressive and shear behavior of clays. The Borja model [Bor91; BL90; BT98; BTA97] extends the original Cam-clay model to large deformations and uses a hyperelastic model and large strain elastic-plastic kinematics.

The Borja Cam-clay model and its implementation in Vaango are discussed in this chapter.

5.2 Quantities that are needed in a Vaango implementation

The implementation of a hyperelastic-plastic model in Vaango typically (but not always) involves the following:

1. an elasticity model factory that creates an elasticity model that provides the simulation with a pressure and a deviatoric stress for a given (elastic) deformation gradient.
2. a plasticity model factory that creates:
   (a) a yield condition factory that compute the yield function for a given stress and internal variable state,
   (b) a flow rule factory that gives the value of the plastic potential for a given state of stress/internal variables. The flow rule factory and yield condition factory are typically assumed to be identical (i.e., plastic flow is associated),
   (c) an internal variable factory that is used to update internal variables and compute hardening moduli.

The models returned by the various factories for Borja cam-clay are discussed below.

5.2.1 Elasticity

The elastic strain energy density in Borja's model has the form

$$W(\varepsilon_v^e, \varepsilon_s^e) = W_{\text{vol}}(\varepsilon_v^e) + W_{\text{dev}}(\varepsilon_v^e, Ve_s^e)$$

where

$$W_{\text{vol}}(\varepsilon_v^e) = -p_o\tilde{\kappa}\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right)$$
$$W_{\text{dev}}(\varepsilon_v^e, \varepsilon_s^e) = \tfrac{3}{2}\,\mu\,(\varepsilon_s^e)^2$$

where ε_{vo}^e is the volumetric strain corresponding to a mean normal compressive stress p_o (tension positive), $\tilde{\kappa}$ is the elastic compressibility index, and the shear modulus is given by

$$\mu = \mu_o + \frac{\alpha}{\tilde{\kappa}}\,W_{\text{vol}}(\varepsilon_v^e) = \mu_o - \alpha p_o\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right) = \mu_o - \mu_{\text{vol}}\,.$$

The parameter α determines the extent of coupling between the volumetric and deviatoric responses. For consistency with isotropic elasticity, Rebecca Brannon suggests that $\alpha = 0$ (citation?).

The stress invariants p and q are defined as

$$p = \frac{\partial W}{\partial \varepsilon_v^e} = p_o\left[1 + \tfrac{3}{2}\,\frac{\alpha}{\tilde{\kappa}}\,(\varepsilon_s^e)^2\right]\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right) = p_o\,\beta\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right)$$
$$q = \frac{\partial W}{\partial \varepsilon_s^e} = 3\left[\mu_o - \alpha p_o\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right)\right]\varepsilon_s^e = 3\mu\,\varepsilon_s^e\,.$$

The derivatives of the stress invariants are

$$\frac{\partial p}{\partial \varepsilon_v^e} = -\frac{p_o}{\tilde{\kappa}}\left[1 + \tfrac{3}{2}\,\frac{\alpha}{\tilde{\kappa}}\,(\varepsilon_s^e)^2\right]\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right) = -\frac{p}{\tilde{\kappa}}$$
$$\frac{\partial p}{\partial \varepsilon_s^e} = \frac{\partial q}{\partial \varepsilon_v^e} = \frac{3\alpha p_o \varepsilon_s^e}{\tilde{\kappa}}\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right) = \frac{3\alpha p}{\beta\tilde{\kappa}}\,\varepsilon_s^e = \frac{3\mu_{\text{vol}}}{\tilde{\kappa}}\,\varepsilon_s^e$$
$$\frac{\partial q}{\partial \varepsilon_s^e} = 3\left[\mu_o - \alpha p_o\,\exp\left(-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right)\right] = 3\mu\,.$$

5.2.2 Plasticity

For plasticity we use a Cam-Clay yield function of the form

$$f = \left(\frac{q}{M}\right)^2 + p(p - p_c)$$

where M is the slope of the critical state line and the consolidation pressure p_c is an internal variable that evolves according to

$$\frac{1}{p_c}\,\frac{dp_c}{dt} = \frac{1}{\tilde{\lambda} - \tilde{\kappa}}\,\frac{d\varepsilon_v^p}{dt}\,.$$

The derivatives of f that are of interest are

$$\frac{\partial f}{\partial p} = 2p - p_c$$
$$\frac{\partial f}{\partial q} = \frac{2q}{M^2}\,.$$

If we integrate the equation for p_c from t_n to t_{n+1}, we can show that

$$(p_c)_{n+1} = (p_c)_n\,\exp\left[\frac{(\varepsilon_v^e)_{\text{trial}} - (\varepsilon_v^e)_{n+1}}{\tilde{\lambda} - \tilde{\kappa}}\right].$$

The derivative of p_c that is of interest is

$$\frac{\partial p_c}{\partial (\varepsilon_v^e)_{n+1}} = -\frac{(p_c)_n}{\tilde{\lambda} - \tilde{\kappa}}\,\exp\left[\frac{(\varepsilon_v^e)_{\text{trial}} - (\varepsilon_v^e)_{n+1}}{\tilde{\lambda} - \tilde{\kappa}}\right].$$

5.3 Stress update based Rich Reguiero's notes

The volumetric and deviatoric components of the elastic strain $\boldsymbol{\epsilon}^e$ are defined as follows:

$$\boldsymbol{e}^e = \boldsymbol{\epsilon}^e - \tfrac{1}{3}\varepsilon_v^e\,\boldsymbol{1} = \boldsymbol{\epsilon}^e - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{\epsilon}^e)\,\boldsymbol{1} \quad \text{and} \quad \varepsilon_s^e = \sqrt{\tfrac{2}{3}}\,\|\boldsymbol{e}^e\| = \sqrt{\tfrac{2}{3}}\sqrt{\boldsymbol{e}^e : \boldsymbol{e}^e}\,.$$

The stress tensor is decomposed into a volumetric and a deviatoric component

$$\boldsymbol{\sigma} = p\,\boldsymbol{1} + \sqrt{\tfrac{2}{3}}\,q\,\boldsymbol{n} \quad \text{with} \quad \boldsymbol{n} = \frac{\boldsymbol{e}^e}{\|\boldsymbol{e}^e\|} = \sqrt{\tfrac{2}{3}}\,\frac{\boldsymbol{e}^e}{\varepsilon_s^e}\,.$$

The models used to determine p and q are

$$p = p_o\beta\exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}}\right] \quad \text{with} \quad \beta = 1 + \tfrac{3}{2}\,\frac{\alpha}{\tilde{\kappa}}\,(\varepsilon_s^e)^2$$
$$q = 3\mu\varepsilon_s^e\,.$$

The strains are updated using

$$\boldsymbol{\epsilon}^e = \boldsymbol{\epsilon}^e_{\text{trial}} - \Delta\gamma\,\frac{\partial f}{\partial \boldsymbol{\sigma}} \quad \text{where} \quad \boldsymbol{\epsilon}^e_{\text{trial}} = \boldsymbol{\epsilon}^e_n + \Delta\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^e_n + (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_n)\,.$$

Remark 1: The interface with MPMICE, among other things in Vaango, requires the computation of the quantity dp/dJ. Since J does not appear in the above equation we proceed as explained below.

$$J = \det(\boldsymbol{F}) = \det(\boldsymbol{1} + \nabla_o\mathbf{u}) = \det(\boldsymbol{1} + \boldsymbol{\epsilon})$$
$$= 1 + \mathrm{tr}\boldsymbol{\epsilon} + \tfrac{1}{2}\left[(\mathrm{tr}\boldsymbol{\epsilon})^2 - \mathrm{tr}(\boldsymbol{\epsilon}^2)\right] + \det(\boldsymbol{\epsilon})\,. \quad = 1 + \varepsilon_v + \tfrac{1}{2}\left[\varepsilon_v^2 - \mathrm{tr}(\boldsymbol{\epsilon}^2)\right] + \det(\boldsymbol{\epsilon})\,.$$

Also,

$$J = \frac{\rho_o}{\rho} = \frac{V}{V_o} \quad \text{and} \quad \varepsilon_v = \frac{V - V_o}{V_o} = \frac{V}{V_o} - 1 = J - 1\,.$$

We use the relation $J = 1 + \varepsilon_v$ while keeping in mind that this is *true only for infinitesimal strains and plastic incompressibility* for which ε_v^2, $\mathrm{tr}(\boldsymbol{\epsilon}^2)$, and $\det(\boldsymbol{\epsilon})$ are zero. Under these conditions

$$\frac{\partial p}{\partial J} = \frac{\partial p}{\partial \varepsilon_v}\,\frac{\partial \varepsilon_v}{\partial J} = \frac{\partial p}{\partial \varepsilon_v} \quad \text{and} \quad \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial \varepsilon_v}\,\frac{\partial \varepsilon_v}{\partial J}\,\frac{\partial J}{\partial \rho} = -\frac{J}{\rho}\,\frac{\partial p}{\partial \varepsilon_v}\,.$$

Remark 2: MPMICE also needs the density at a given pressure. For the Borja model, with $\varepsilon_v = J - 1 = \rho_o/\rho - 1$, we have

$$\rho = \rho_o\left[1 + \varepsilon_{vo} + \tilde{\kappa}\ln\left(\frac{p}{p_o\beta}\right)\right]^{-1}\,.$$

Remark 3: The quantity q is related to the deviatoric part of the Cauchy stress, $\boldsymbol{s}$ as follows:

$$q = \sqrt{3J_2} \quad \text{where} \quad J_2 = \tfrac{1}{2}\,\boldsymbol{s} : \boldsymbol{s}\,.$$

The shear modulus relates the deviatoric stress $\boldsymbol{s}$ to the deviatoric strain $\boldsymbol{e}^e$. We assume a relation of the form

$$\boldsymbol{s} = 2\mu\boldsymbol{e}^e\,.$$

Note that the above relation assumes a linear elastic type behavior. Then we get the Borja shear model:

$$q = \sqrt{\tfrac{3}{2}\,\boldsymbol{s} : \boldsymbol{s}} = \sqrt{\tfrac{3}{2}}\,(2\mu)\,\sqrt{\boldsymbol{e}^e : \boldsymbol{e}^e} = \sqrt{\tfrac{3}{2}}\,(2\mu)\,\sqrt{\tfrac{3}{2}}\,\varepsilon_s^e = 3\mu\varepsilon_s^e\,.$$

5.3.1 Elastic-plastic stress update

For elasto-plasticity we start with a yield function of the form

$$f = \left(\frac{q}{M}\right)^2 + p(p - p_c) \leq 0 \quad \text{where} \quad \frac{1}{p_c}\frac{dp_c}{dt} = \frac{1}{\tilde{\lambda} - \tilde{\kappa}}\frac{d\varepsilon_v^p}{dt}.$$

Integrating the ODE for p_c with the initial condition $p_c(t_n) = (p_c)_n$, at $t = t_{n+1}$,

$$(p_c)_{n+1} = (p_c)_n \exp\left[\frac{(\varepsilon_v^p)_{n+1} - (\varepsilon_v^p)_n}{\tilde{\lambda} - \tilde{\kappa}}\right].$$

From the additive decomposition of the strain into elastic and plastic parts, and if the elastic trial strain is defined as

$$(\varepsilon_v^e)_{\text{trial}} := (\varepsilon_v^e)_n + \Delta\varepsilon_v$$

we have

$$\varepsilon_v^p = \varepsilon_v - \varepsilon_v^e \quad \Longrightarrow \quad (\varepsilon_v^p)_{n+1} - (\varepsilon_v^p)_n = (\varepsilon_v)_{n+1} - (\varepsilon_v^e)_{n+1} - (\varepsilon_v)_n + (\varepsilon_v^e)_n = \Delta\varepsilon_v + (\varepsilon_v^e)_n - (\varepsilon_v^e)_{n+1} = (\varepsilon_v^e)_{\text{trial}} - (\varepsilon_v^e)_{n+1}.$$

Therefore we can write

$$(p_c)_{n+1} = (p_c)_n \exp\left[\frac{(\varepsilon_v^e)_{\text{trial}} - (\varepsilon_v^e)_{n+1}}{\tilde{\lambda} - \tilde{\kappa}}\right].$$

The flow rule is assumed to be given by

$$\frac{\partial \boldsymbol{\epsilon}^p}{\partial t} = \gamma \frac{\partial f}{\partial \boldsymbol{\sigma}}.$$

Integration of the PDE with backward Euler gives

$$\boldsymbol{\epsilon}_{n+1}^p = \boldsymbol{\epsilon}_n^p + \Delta t\, \gamma_{n+1} \left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1} = \boldsymbol{\epsilon}_n^p + \Delta\gamma \left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1}.$$

This equation can be expressed in terms of the trial elastic strain as follows.

$$\boldsymbol{\epsilon}_{n+1} - \boldsymbol{\epsilon}_{n+1}^e = \boldsymbol{\epsilon}_n - \boldsymbol{\epsilon}_n^e + \Delta\gamma \left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1}$$

or

$$\boldsymbol{\epsilon}_{n+1}^e = \Delta\boldsymbol{\epsilon} + \boldsymbol{\epsilon}_n^e - \Delta\gamma \left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1} = \boldsymbol{\epsilon}_{\text{trial}}^e - \Delta\gamma \left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1}.$$

In terms of the volumetric and deviatoric components

$$(\varepsilon_v^e)_{n+1} = \text{tr}(\boldsymbol{\epsilon}_{n+1}^e) = \text{tr}(\boldsymbol{\epsilon}_{\text{trial}}^e) - \Delta\gamma\, \text{tr}\left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1} = (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma\, \text{tr}\left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]_{n+1}$$

and

$$\boldsymbol{e}_{n+1}^e = \boldsymbol{e}_{\text{trial}}^e - \Delta\gamma \left[\left(\frac{\partial f}{\partial \boldsymbol{\sigma}}\right)_{n+1} - \tfrac{1}{3}\,\text{tr}\left(\frac{\partial f}{\partial \boldsymbol{\sigma}}\right)_{n+1} \boldsymbol{1}\right].$$

With $\boldsymbol{s} = \boldsymbol{\sigma} - p\boldsymbol{1}$, we have

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{\partial f}{\partial \boldsymbol{s}} : \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial \boldsymbol{\sigma}} = \frac{\partial f}{\partial \boldsymbol{s}} : \left[\mathbf{I}^{(s)} - \tfrac{1}{3}\boldsymbol{1} \otimes \boldsymbol{1}\right] + \frac{\partial f}{\partial p}\boldsymbol{1} = \frac{\partial f}{\partial \boldsymbol{s}} - \tfrac{1}{3}\,\text{tr}\left[\frac{\partial f}{\partial \boldsymbol{s}}\right]\boldsymbol{1} + \frac{\partial f}{\partial p}\boldsymbol{1}$$

and

$$\tfrac{1}{3}\,\mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]\boldsymbol{1} = \tfrac{1}{3}\left(\mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{s}}\right] - \mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{s}}\right] + 3\frac{\partial f}{\partial p}\right)\boldsymbol{1} = \frac{\partial f}{\partial p}\,\boldsymbol{1}\,.$$

Remark 4: Note that, because $\boldsymbol{\sigma} = \boldsymbol{\sigma}(p, q, p_c)$ the chain rule should contain a contribution from p_c:

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial p_c}\frac{\partial p_c}{\partial \boldsymbol{\sigma}}\,.$$

However, the Borja implementation does not consider that extra term. Also note that for the present model

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(p(\varepsilon_v^e, \varepsilon_s^e, \varepsilon_v^p, \varepsilon_s^p), \boldsymbol{s}(\varepsilon_v^e, \varepsilon_s^e, \varepsilon_v^p, \varepsilon_s^p), p_c(\varepsilon_v^p))$$

Therefore, for situations where $\mathrm{tr}(\partial f/\partial \boldsymbol{s}) = \mathbf{0}$, we have

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} - \tfrac{1}{3}\,\mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right]\boldsymbol{1} = \frac{\partial f}{\partial \boldsymbol{s}} - \tfrac{1}{3}\,\mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{s}}\right]\boldsymbol{1} = \frac{\partial f}{\partial \boldsymbol{s}}\,.$$

The deviatoric strain update can be written as

$$\boldsymbol{e}^e_{n+1} = \boldsymbol{e}^e_{\text{trial}} - \Delta\gamma\left(\frac{\partial f}{\partial \boldsymbol{s}}\right)_{n+1}$$

and the shear invariant update is

$$(\varepsilon_s^e)_{n+1} = \sqrt{\tfrac{2}{3}}\,\sqrt{\boldsymbol{e}^e_{n+1} : \boldsymbol{e}^e_{n+1}} = \sqrt{\tfrac{2}{3}}\,\sqrt{\boldsymbol{e}^e_{\text{trial}} : \boldsymbol{e}^e_{\text{trial}} - 2\Delta\gamma\left[\frac{\partial f}{\partial \boldsymbol{s}}\right]_{n+1} : \boldsymbol{e}^e_{\text{trial}} + (\Delta\gamma)^2\left[\frac{\partial f}{\partial \boldsymbol{s}}\right]_{n+1} : \left[\frac{\partial f}{\partial \boldsymbol{s}}\right]_{n+1}}$$

The derivative of f can be found using the chain rule (for smooth f):

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{\partial f}{\partial p}\frac{\partial p}{\partial \boldsymbol{\sigma}} + \frac{\partial f}{\partial q}\frac{\partial q}{\partial \boldsymbol{\sigma}} = (2p - p_c)\frac{\partial p}{\partial \boldsymbol{\sigma}} + \frac{2q}{M^2}\frac{\partial q}{\partial \boldsymbol{\sigma}}\,.$$

Now, with $p = 1/3\,\mathrm{tr}(\boldsymbol{\sigma})$ and $q = \sqrt{3/2\,\mathbf{s} : \mathbf{s}}$, we have

$$\frac{\partial p}{\partial \boldsymbol{\sigma}} = \frac{\partial}{\partial \boldsymbol{\sigma}}\left[\tfrac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})\right] = \tfrac{1}{3}\,\boldsymbol{1}$$
$$\frac{\partial q}{\partial \boldsymbol{\sigma}} = \frac{\partial}{\partial \boldsymbol{\sigma}}\left[\sqrt{\tfrac{3}{2}\,\boldsymbol{s} : \boldsymbol{s}}\right] = \sqrt{\tfrac{3}{2}}\,\frac{1}{\sqrt{\boldsymbol{s} : \boldsymbol{s}}}\,\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{\sigma}} : \boldsymbol{s} = \sqrt{\tfrac{3}{2}}\,\frac{1}{\|\boldsymbol{s}\|}\left[\mathbf{I}^{(s)} - \tfrac{1}{3}\boldsymbol{1}\otimes\boldsymbol{1}\right] : \boldsymbol{s} = \sqrt{\tfrac{3}{2}}\,\frac{\boldsymbol{s}}{\|\boldsymbol{s}\|}\,.$$

Therefore,

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{2p - p_c}{3}\,\boldsymbol{1} + \sqrt{\tfrac{3}{2}}\,\frac{2q}{M^2}\,\frac{\boldsymbol{s}}{\|\boldsymbol{s}\|}\,.$$

Recall that

$$\boldsymbol{\sigma} = p\,\boldsymbol{1} + \sqrt{\tfrac{2}{3}}\,q\,\boldsymbol{n} = p\,\boldsymbol{1} + \boldsymbol{s}\,.$$

Therefore,

$$\boldsymbol{s} = \sqrt{\tfrac{2}{3}}\,q\,\boldsymbol{n} \quad \text{and} \quad \|\boldsymbol{s}\| = \sqrt{\boldsymbol{s} : \boldsymbol{s}} = \sqrt{\tfrac{2}{3}\,q^2\,\boldsymbol{n} : \boldsymbol{n}} = \sqrt{\tfrac{2}{3}\,q^2\,\frac{\boldsymbol{e}^e : \boldsymbol{e}^e}{\|\boldsymbol{e}^e\|^2}} = \sqrt{\tfrac{2}{3}\,q^2} = \sqrt{\tfrac{2}{3}}\,q\,.$$

So we can write

$$\frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{2p - p_c}{3}\,\boldsymbol{1} + \sqrt{\tfrac{3}{2}}\,\frac{2q}{M^2}\,\boldsymbol{n}\,. \tag{5.1}$$

Using the above relation we have

$$\frac{\partial f}{\partial p} = \tfrac{1}{3}\,\mathrm{tr}\left[\frac{\partial f}{\partial \boldsymbol{\sigma}}\right] = 2p - p_c \quad \text{and} \quad \frac{\partial f}{\partial \boldsymbol{s}} = \frac{\partial f}{\partial \boldsymbol{\sigma}} - \frac{\partial f}{\partial p}\boldsymbol{1} = \sqrt{\tfrac{3}{2}}\,\frac{2q}{M^2}\,\boldsymbol{n}\,.$$

The strain updates can now be written as

$$\begin{aligned}
(\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma\,[2p_{n+1} - (p_c)_{n+1}] \\
\boldsymbol{e}^e_{n+1} &= \boldsymbol{e}^e_{\text{trial}} - \sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\boldsymbol{n}_{n+1} \\
(\varepsilon_s^e)_{n+1} &= \sqrt{\tfrac{2}{3}}\sqrt{\boldsymbol{e}^e_{\text{trial}} : \boldsymbol{e}^e_{\text{trial}} - \sqrt{6}\,(\Delta\gamma)^2\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\boldsymbol{n}_{n+1} : \boldsymbol{e}^e_{\text{trial}} + \tfrac{3}{2}\,(\Delta\gamma)^4\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)^2}\,.
\end{aligned}$$

From the second equation above,

$$\boldsymbol{n}_{n+1} : \boldsymbol{e}^e_{\text{trial}} = \boldsymbol{n}_{n+1} : \boldsymbol{e}^e_{n+1} + \sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\boldsymbol{n}_{n+1} : \boldsymbol{n}_{n+1} = \frac{\boldsymbol{e}^e_{n+1} : \boldsymbol{e}^e_{n+1}}{\|\boldsymbol{e}^e_{n+1}\|} + \sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right) = \|\boldsymbol{e}^e_{n+1}\| + \sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right).$$

Also notice that

$$\boldsymbol{e}^e_{\text{trial}} : \boldsymbol{e}^e_{\text{trial}} = \boldsymbol{e}^e_{n+1} : \boldsymbol{e}^e_{n+1} + 2\sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\boldsymbol{e}^e_{n+1} : \boldsymbol{n}_{n+1} + \left[\sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\right]^2$$

or,

$$\|\boldsymbol{e}^e_{\text{trial}}\|^2 = \left[\|\boldsymbol{e}^e_{n+1}\| + \sqrt{\tfrac{3}{2}}\,\Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\right]^2.$$

Therefore,

$$\boldsymbol{n}_{n+1} : \boldsymbol{e}^e_{\text{trial}} = \|\boldsymbol{e}^e_{\text{trial}}\|$$

and we have

$$(\varepsilon_s^e)_{n+1} = \sqrt{\tfrac{2}{3}}\sqrt{\|\boldsymbol{e}^e_{\text{trial}}\|^2 - \sqrt{6}\,(\Delta\gamma)^2\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)\|\boldsymbol{e}^e_{\text{trial}}\| + \tfrac{3}{2}\,(\Delta\gamma)^4\left(\frac{2q_{n+1}}{M^2_{n+1}}\right)^2} = \sqrt{\tfrac{2}{3}}\,\|\boldsymbol{e}^e_{\text{trial}}\| - \Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right).$$

The elastic strain can therefore be updated using

$$\begin{aligned}
(\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma\,[2p_{n+1} - (p_c)_{n+1}] \\
(\varepsilon_s^e)_{n+1} &= (\varepsilon_s^e)_{\text{trial}} - \Delta\gamma\left(\frac{2q_{n+1}}{M^2_{n+1}}\right).
\end{aligned}$$

The consistency condition is needed to close the above equations

$$f = \left(\frac{q_{n+1}}{M}\right)^2 + p_{n+1}[p_{n+1} - (p_c)_{n+1}] = 0\,.$$

The unknowns are $(\varepsilon_v^e)_{n+1}$, $(\varepsilon_s^e)_{n+1}$ and $\Delta\gamma$. Note that we can express the three equations as

$$\begin{aligned}
(\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma\left[\frac{\partial f}{\partial p}\right]_{n+1} \\
(\varepsilon_s^e)_{n+1} &= (\varepsilon_s^e)_{\text{trial}} - \Delta\gamma\left[\frac{\partial f}{\partial q}\right]_{n+1} \\
f_{n+1} &= 0\,.
\end{aligned} \tag{5.2}$$

5.3.2 Newton iterations

The three nonlinear equations in the three unknowns can be solved using Newton iterations for smooth yield functions. Let us define the residual as

$$\underline{\underline{r}}(\underline{\underline{x}}) = \begin{bmatrix} (\varepsilon_v^e)_{n+1} - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma \left[\dfrac{\partial f}{\partial p}\right]_{n+1} \\ (\varepsilon_s^e)_{n+1} - (\varepsilon_s^e)_{\text{trial}} + \Delta\gamma \left[\dfrac{\partial f}{\partial q}\right]_{n+1} \\ f_{n+1} \end{bmatrix} =: \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} \quad \text{where} \quad \underline{\underline{x}} = \begin{bmatrix} (\varepsilon_v^e)_{n+1} \\ (\varepsilon_s^e)_{n+1} \\ f_{n+1} \end{bmatrix} =: \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

The Newton root finding algorithm is :

Require: $\underline{\underline{x}}^0$

$k \leftarrow 0$

while $\underline{\underline{r}}(\underline{\underline{x}}^k) \neq 0$ **do**

$$\underline{\underline{x}}^{k+1} \Leftarrow \underline{\underline{x}}^k - \left[\left(\frac{\partial \underline{\underline{r}}}{\partial \underline{\underline{x}}}\right)^{-1}\right]_{\underline{\underline{x}}^k} \cdot \underline{\underline{r}}(\underline{\underline{x}}^k)$$

$k \leftarrow k + 1$

end while

To code the algorithm we have to find the derivatives of the residual with respect to the primary variables. Let's do the terms one by one. For the first row,

$$\begin{aligned}
\frac{\partial r_1}{\partial x_1} &= \frac{\partial}{\partial \varepsilon_v^e}\left[\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma\,(2p - p_c)\right] = 1 + \Delta\gamma\left(2\frac{\partial p}{\partial \varepsilon_v^e} - \frac{\partial p_c}{\partial \varepsilon_v^e}\right) \\
\frac{\partial r_1}{\partial x_2} &= \frac{\partial}{\partial \varepsilon_s^e}\left[\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma\,(2p - p_c)\right] = 2\Delta\gamma\frac{\partial p}{\partial \varepsilon_s^e} \\
\frac{\partial r_1}{\partial x_3} &= \frac{\partial}{\partial \Delta\gamma}\left[\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma\,(2p - p_c)\right] = 2p - p_c = \frac{\partial f}{\partial p}
\end{aligned}$$

where

$$\frac{\partial p}{\partial \varepsilon_v^e} = -\frac{p_0\,\beta}{\tilde{\kappa}}\exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\tilde{\kappa}}\right] = \frac{p}{\tilde{\kappa}} \quad , \quad \frac{\partial p_c}{\partial \varepsilon_v^e} = \frac{(p_c)_n}{\tilde{\kappa} - \tilde{\lambda}}\exp\left[\frac{\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}}}{\tilde{\kappa} - \tilde{\lambda}}\right] \quad \text{and}$$

$$\frac{\partial p}{\partial \varepsilon_s^e} = \frac{3\,p_0\,\alpha\,\varepsilon_s^e}{\tilde{\kappa}}\exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\tilde{\kappa}}\right].$$

For the second row,

$$\begin{aligned}
\frac{\partial r_2}{\partial x_1} &= \frac{\partial}{\partial \varepsilon_v^e}\left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta\gamma\,\frac{2q}{M^2}\right] = \frac{2\Delta\gamma}{M^2}\frac{\partial q}{\partial \varepsilon_v^e} \\
\frac{\partial r_2}{\partial x_2} &= \frac{\partial}{\partial \varepsilon_s^e}\left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta\gamma\,\frac{2q}{M^2}\right] = 1 + \frac{2\Delta\gamma}{M^2}\frac{\partial q}{\partial \varepsilon_s^e} \\
\frac{\partial r_2}{\partial x_3} &= \frac{\partial}{\partial \Delta\gamma}\left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta\gamma\,\frac{2q}{M^2}\right] = \frac{2q}{M^2} = \frac{\partial f}{\partial q}
\end{aligned}$$

where

$$\frac{\partial q}{\partial \varepsilon_v^e} = -\frac{3p_0\,\alpha\,\varepsilon_s^e}{\tilde{\kappa}}\exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\tilde{\kappa}}\right] = \frac{\partial p}{\partial \varepsilon_s^e} \quad \text{and} \quad \frac{\partial q}{\partial \varepsilon_s^e} = 3\mu_0 + 3p_0\,\alpha\exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\tilde{\kappa}}\right] = 3\mu\,.$$

For the third row,

$$\frac{\partial r_3}{\partial x_1} = \frac{\partial}{\partial \varepsilon_v^e}\left[\frac{q^2}{M^2} + p\,(p - p_c)\right] = \frac{2q}{M^2}\,\frac{\partial q}{\partial \varepsilon_v^e} + (2p - p_c)\,\frac{\partial p}{\partial \varepsilon_v^e} - p\,\frac{\partial p_c}{\partial \varepsilon_v^e} = \frac{\partial f}{\partial q}\,\frac{\partial q}{\partial \varepsilon_v^e} + \frac{\partial f}{\partial p}\,\frac{\partial p}{\partial \varepsilon_v^e} - p\,\frac{\partial p_c}{\partial \varepsilon_v^e}$$
$$\frac{\partial r_3}{\partial x_2} = \frac{\partial}{\partial \varepsilon_s^e}\left[\frac{q^2}{M^2} + p\,(p - p_c)\right] = \frac{2q}{M^2}\,\frac{\partial q}{\partial \varepsilon_s^e} + (2p - p_c)\,\frac{\partial p}{\partial \varepsilon_s^e} = \frac{\partial f}{\partial q}\,\frac{\partial q}{\partial \varepsilon_s^e} + \frac{\partial f}{\partial p}\,\frac{\partial p}{\partial \varepsilon_s^e}$$
$$\frac{\partial r_3}{\partial x_3} = \frac{\partial}{\partial \Delta\gamma}\left[\frac{q^2}{M^2} + p\,(p - p_c)\right] = 0\,.$$

We have to invert a matrix in the Newton iteration process. Let us see whether we can make this quicker to do. The Jacobian matrix has the form

$$\frac{\partial \underline{\underline{r}}}{\partial \underline{\underline{x}}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_1} & \frac{\partial r_1}{\partial x_2} & \frac{\partial r_1}{\partial x_3} \\ \frac{\partial r_2}{\partial x_1} & \frac{\partial r_2}{\partial x_2} & \frac{\partial r_2}{\partial x_3} \\ \frac{\partial r_3}{\partial x_1} & \frac{\partial r_3}{\partial x_2} & \frac{\partial r_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \underline{\underline{A}} & \underline{\underline{B}} \\ \underline{\underline{C}} & 0 \end{bmatrix}$$

where

$$\underline{\underline{A}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_1} & \frac{\partial r_1}{\partial x_2} \\ \frac{\partial r_2}{\partial x_1} & \frac{\partial r_2}{\partial x_2} \end{bmatrix}, \quad \underline{\underline{B}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_3} \\ \frac{\partial r_2}{\partial x_3} \end{bmatrix}, \quad \text{and} \quad \underline{\underline{C}} = \begin{bmatrix} \frac{\partial r_3}{\partial x_1} & \frac{\partial r_3}{\partial x_2} \end{bmatrix}.$$

We can also break up the $\underline{\underline{x}}$ and $\underline{\underline{r}}$ matrices:

$$\Delta\underline{\underline{x}} = \underline{\underline{x}}^{k+1} - \underline{\underline{x}}^{k} = \begin{bmatrix} \Delta\underline{\underline{x}}^{vs} \\ \Delta x_3 \end{bmatrix}, \quad \underline{\underline{r}} = \begin{bmatrix} \underline{\underline{r}}^{vs} \\ r_3 \end{bmatrix} \quad \text{where} \quad \underline{\underline{r}}^{vs} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} \quad \text{and} \quad \Delta\underline{\underline{x}}^{vs} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix}.$$

Then

$$\begin{bmatrix} \Delta\underline{\underline{x}}^{vs} \\ \Delta x_3 \end{bmatrix} = -\begin{bmatrix} \underline{\underline{A}} & \underline{\underline{B}} \\ \underline{\underline{C}} & 0 \end{bmatrix}^{-1} \begin{bmatrix} \underline{\underline{r}}^{vs} \\ r_3 \end{bmatrix} \quad \Longrightarrow \quad \begin{bmatrix} \underline{\underline{A}} & \underline{\underline{B}} \\ \underline{\underline{C}} & 0 \end{bmatrix} \begin{bmatrix} \Delta\underline{\underline{x}}^{vs} \\ \Delta x_3 \end{bmatrix} = -\begin{bmatrix} \underline{\underline{r}}^{vs} \\ r_3 \end{bmatrix}$$

or

$$\underline{\underline{A}}\,\Delta\underline{\underline{x}}^{vs} + \underline{\underline{B}}\,\Delta x_3 = -\underline{\underline{r}}^{vs} \quad \text{and} \quad \underline{\underline{C}}\,\Delta\underline{\underline{x}}^{vs} = -r_3\,.$$

From the first equation above,

$$\Delta\underline{\underline{x}}^{vs} = -\underline{\underline{A}}^{-1}\,\underline{\underline{r}}^{vs} - \underline{\underline{A}}^{-1}\,\underline{\underline{B}}\,\Delta x_3\,.$$

Plugging in the second equation gives

$$r_3 = \underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{r}}^{vs} + \underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{B}}\,\Delta x_3\,.$$

Rearranging,

$$\Delta x_3 = x_3^{k+1} - x_3^{k} = \frac{-\underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{r}}^{vs} + r_3}{\underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{B}}}\,.$$

Using the above result,

$$\Delta\underline{\underline{x}}^{vs} = -\underline{\underline{A}}^{-1}\,\underline{\underline{r}}^{vs} - \underline{\underline{A}}^{-1}\,\underline{\underline{B}}\left(\frac{-\underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{r}}^{vs} + r_3}{\underline{\underline{C}}\,\underline{\underline{A}}^{-1}\,\underline{\underline{B}}}\right).$$

We therefore have to invert only a 2×2 matrix.

5.3.3 Tangent calculation: elastic

We want to find the derivative of the stress with respect to the strain:

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} = \boldsymbol{1} \otimes \frac{\partial p}{\partial \boldsymbol{\epsilon}} + \sqrt{\tfrac{2}{3}}\, \boldsymbol{n} \otimes \frac{\partial q}{\partial \boldsymbol{\epsilon}} + \sqrt{\tfrac{2}{3}}\, q\, \frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}} \,. \tag{5.3}$$

For the first term above,

$$\frac{\partial p}{\partial \boldsymbol{\epsilon}} = p_{\text{o}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \frac{\partial \beta}{\partial \boldsymbol{\epsilon}} - p_{\text{o}}\, \frac{\beta}{\tilde{\kappa}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} = p_{\text{o}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \left(\frac{\partial \beta}{\partial \boldsymbol{\epsilon}} - \frac{\beta}{\tilde{\kappa}}\, \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}}\right) .$$

Now,

$$\frac{\partial \beta}{\partial \boldsymbol{\epsilon}} = \frac{3\alpha}{\tilde{\kappa}}\, \varepsilon_s^e\, \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} \,.$$

Therefore,

$$\frac{\partial p}{\partial \boldsymbol{\epsilon}} = \frac{p_{\text{o}}}{\tilde{\kappa}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \left(3\alpha\, \varepsilon_s^e\, \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} - \beta\, \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}}\right) .$$

We now have to figure out the other derivatives in the above expression. First,

$$\frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}}\, \frac{1}{\sqrt{\boldsymbol{e}^e : \boldsymbol{e}^e}}\, \frac{\partial \boldsymbol{e}^e}{\partial \boldsymbol{\epsilon}} : \boldsymbol{e}^e = \sqrt{\tfrac{2}{3}}\, \frac{1}{\|\boldsymbol{e}^e\|} \left(\frac{\partial \boldsymbol{e}^e}{\partial \boldsymbol{\epsilon}} - \tfrac{1}{3}\boldsymbol{1} \otimes \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}}\right) : \boldsymbol{e}^e \,.$$

For the special situation where all the strain is elastic, $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^e$, and (see Wikipedia article on tensor derivatives)

$$\frac{\partial \boldsymbol{\epsilon}^e}{\partial \boldsymbol{\epsilon}} = \frac{\partial \boldsymbol{\epsilon}}{\partial \boldsymbol{\epsilon}} = \mathbf{I}^{(s)} \quad \text{and} \quad \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} = \frac{\partial \varepsilon_v}{\partial \boldsymbol{\epsilon}} = \boldsymbol{1} \,.$$

That gives us

$$\frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}}\, \frac{1}{\|\boldsymbol{e}^e\|} \left(\mathbf{I}^{(s)} - \tfrac{1}{3}\boldsymbol{1} \otimes \boldsymbol{1}\right) : \boldsymbol{e}^e = \sqrt{\tfrac{2}{3}}\, \frac{1}{\|\boldsymbol{e}^e\|} \left[\boldsymbol{e}^e - \tfrac{1}{3}\text{tr}(\boldsymbol{e}^e)\boldsymbol{1}\right] .$$

But $\text{tr}(\boldsymbol{e}^e) = 0$ because this is the deviatoric part of the strain and we have

$$\boxed{\frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}}\, \frac{\boldsymbol{e}^e}{\|\boldsymbol{e}^e\|} = \sqrt{\tfrac{2}{3}}\, \boldsymbol{n}} \quad \text{and} \quad \boxed{\frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} = \boldsymbol{1} \,.}$$

Using these, we get

$$\frac{\partial p}{\partial \boldsymbol{\epsilon}} = \frac{p_{\text{o}}}{\tilde{\kappa}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \left(\sqrt{6}\, \alpha\, \varepsilon_s^e\, \boldsymbol{n} - \beta\, \boldsymbol{1}\right) . \tag{5.4}$$

The derivative of q with respect to $\boldsymbol{\epsilon}$ can be calculated in a similar way, i.e.,

$$\frac{\partial q}{\partial \boldsymbol{\epsilon}} = 3\mu\, \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} + 3\varepsilon_s^e\, \frac{\partial \mu}{\partial \boldsymbol{\epsilon}} = 3\mu\, \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} - 3\frac{p_{\text{o}}}{\tilde{\kappa}}\, \alpha\, \varepsilon_s^e\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} \,.$$

Using the expressions in the boxes above,

$$\frac{\partial q}{\partial \boldsymbol{\epsilon}} = \sqrt{6}\, \mu\, \boldsymbol{n} - 3\frac{p_{\text{o}}}{\tilde{\kappa}}\, \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{v\text{o}}^e}{\tilde{\kappa}}\right] \alpha\, \varepsilon_s^e\, \boldsymbol{1} \,. \tag{5.5}$$

Also,

$$\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}} \left[\frac{1}{\varepsilon_s^e} \frac{\partial \boldsymbol{e}^e}{\partial \boldsymbol{\epsilon}} - \frac{1}{(\varepsilon_s^e)^2} \boldsymbol{e}^e \otimes \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} \right] .$$

Using the previously derived expression, we have

$$\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}} \frac{1}{\varepsilon_s^e} \left[\mathbf{I}^{(s)} - \tfrac{1}{3} \boldsymbol{1} \otimes \boldsymbol{1} - \sqrt{\tfrac{2}{3}} \frac{1}{\varepsilon_s^e} \frac{\boldsymbol{e}^e \otimes \boldsymbol{e}^e}{\|\boldsymbol{e}^e\|} \right]$$

or

$$\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}} \frac{1}{\varepsilon_s^e} \left[\mathbf{I}^{(s)} - \tfrac{1}{3} \boldsymbol{1} \otimes \boldsymbol{1} - \boldsymbol{n} \otimes \boldsymbol{n} \right] . \tag{5.6}$$

Plugging the expressions for these derivatives in the original equation, we get

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} = \frac{p_o}{\tilde{\kappa}} \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] \left(\sqrt{6}\, \alpha\, \varepsilon_s^e\, \boldsymbol{1} \otimes \boldsymbol{n} - \beta\, \boldsymbol{1} \otimes \boldsymbol{1} \right) + 2\mu\, \boldsymbol{n} \otimes \boldsymbol{n} - \sqrt{6} \frac{p_o}{\tilde{\kappa}} \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] \alpha\, \varepsilon_s^e\, \boldsymbol{n} \otimes \boldsymbol{1} + \tfrac{2}{3} \frac{q}{\varepsilon_s^e} \left[\mathbf{I}^{(s)} - \tfrac{1}{3} \boldsymbol{1} \otimes \boldsymbol{1} - \boldsymbol{n} \otimes \boldsymbol{n} \right] .$$

Reorganizing,

$$\boxed{\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} = \frac{\sqrt{6}\, p_o\, \alpha\, \varepsilon_s^e}{\tilde{\kappa}} \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] (\boldsymbol{1} \otimes \mathbf{n} + \mathbf{n} \otimes \boldsymbol{1}) - \left(\frac{p_o \beta}{\tilde{\kappa}} \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] + \tfrac{2}{9} \frac{q}{\varepsilon_s^e} \right) \boldsymbol{1} \otimes \boldsymbol{1} + 2 \left(\mu - \tfrac{1}{3} \frac{q}{\varepsilon_s^e} \right) \boldsymbol{n} \otimes \boldsymbol{n} + \tfrac{2}{3} \frac{q}{\varepsilon_s^e} \mathbf{I}^{(s)} .} \tag{5.7}$$

5.3.4 Tangent calculation: elastic-plastic

From the previous section recall that

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\epsilon}} = \boldsymbol{1} \otimes \frac{\partial p}{\partial \boldsymbol{\epsilon}} + \sqrt{\tfrac{2}{3}}\, \boldsymbol{n} \otimes \frac{\partial q}{\partial \boldsymbol{\epsilon}} + \sqrt{\tfrac{2}{3}}\, q \frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}}$$

where

$$\frac{\partial p}{\partial \boldsymbol{\epsilon}} = \frac{p_o}{\tilde{\kappa}} \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] \left(3\alpha\, \varepsilon_s^e \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} - \beta \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} \right) , \qquad \frac{\partial q}{\partial \boldsymbol{\epsilon}} = 3\mu \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} - 3 \frac{p_o}{\tilde{\kappa}} \alpha\, \varepsilon_s^e \exp\left[-\frac{\varepsilon_v^e - \varepsilon_{vo}^e}{\tilde{\kappa}} \right] \frac{\partial \varepsilon_v^e}{\partial \boldsymbol{\epsilon}} \quad \text{and}$$

$$\frac{\partial \boldsymbol{n}}{\partial \boldsymbol{\epsilon}} = \sqrt{\tfrac{2}{3}} \left[\frac{1}{\varepsilon_s^e} \frac{\partial \boldsymbol{e}^e}{\partial \boldsymbol{\epsilon}} - \frac{1}{(\varepsilon_s^e)^2} \boldsymbol{e}^e \otimes \frac{\partial \varepsilon_s^e}{\partial \boldsymbol{\epsilon}} \right] .$$

The total strain is equal to the elastic strain for the purely elastic case and the tangent is relatively straightforward to calculate. For the elastic-plastic case we have

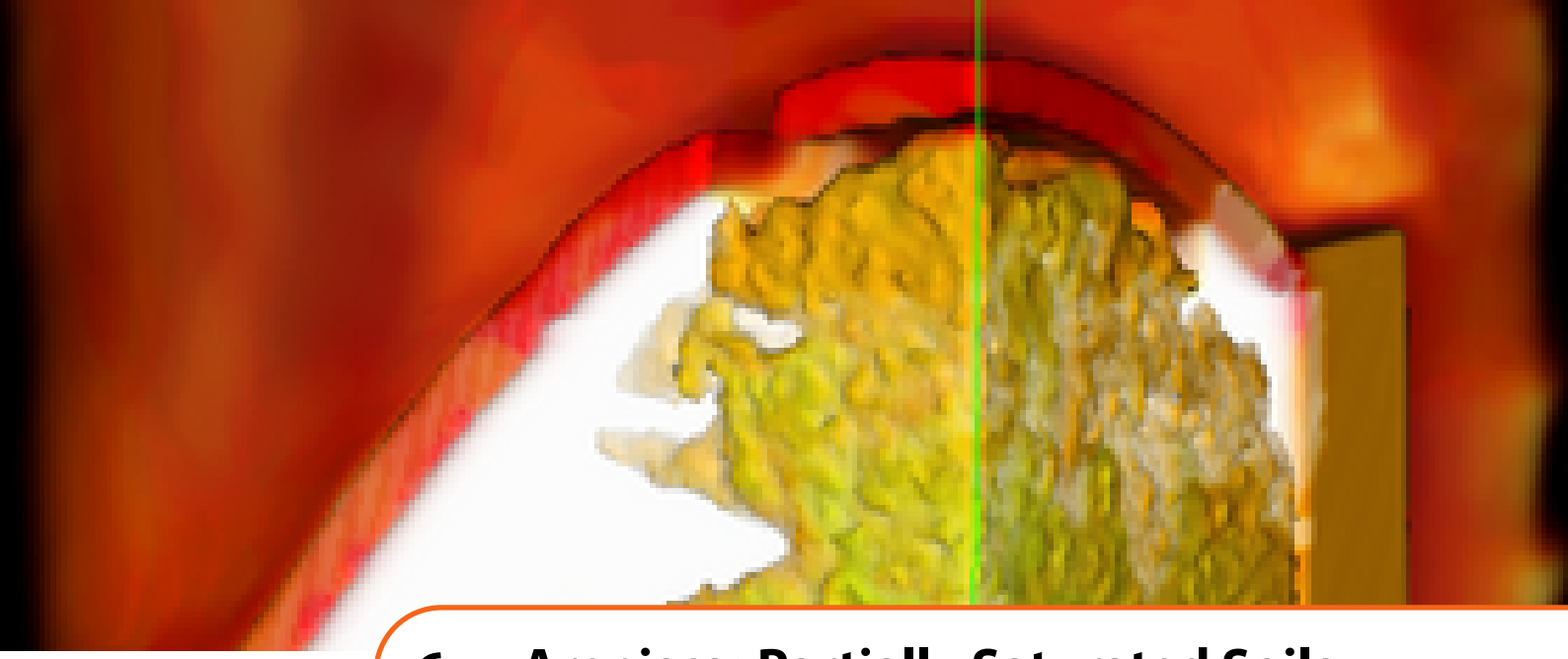
$$\boldsymbol{\epsilon}_{n+1}^e = \boldsymbol{\epsilon}_{\text{trial}}^e - \Delta\gamma \left[\frac{\partial f}{\partial \boldsymbol{\sigma}} \right]_{n+1} .$$

Dropping the subscript $n+1$ for convenience, we have

$$\frac{\partial \boldsymbol{\epsilon}^e}{\partial \boldsymbol{\epsilon}} = \frac{\partial \boldsymbol{\epsilon}_{\text{trial}}^e}{\partial \boldsymbol{\epsilon}} - \frac{\partial f}{\partial \boldsymbol{\sigma}} \otimes \frac{\partial \Delta\gamma}{\partial \boldsymbol{\epsilon}} - \Delta\gamma \frac{\partial}{\partial \boldsymbol{\epsilon}} \left[\frac{\partial f}{\partial \boldsymbol{\sigma}} \right] = \mathbf{I}^{(s)} - \left[\frac{2p - p_c}{3} \boldsymbol{1} + \sqrt{\tfrac{3}{2}} \frac{2q}{M^2} \boldsymbol{n} \right] \otimes \frac{\partial \Delta\gamma}{\partial \boldsymbol{\epsilon}} - \Delta\gamma \frac{\partial}{\partial \boldsymbol{\epsilon}} \left[\frac{2p - p_c}{3} \boldsymbol{1} + \sqrt{\tfrac{3}{2}} \frac{2q}{M^2} \boldsymbol{n} \right] .$$

5.4 Caveats

The Cam-Clay implementation in Vaango behaves reasonably for moderate strains but is known to fail to converge for high-rate applications that involve very large plastic strains.



6 — Arenisca: Partially Saturated Soils

The convention used in Vaango is that tension is positive and compression is negative. To keep the notation simple we define, for any x,

$$\bar{x} := -x\,, \quad \dot{x} := \frac{\partial x}{\partial t}\,. \tag{6.1}$$

6.1 Elasticity

The elasticity model used by Arenisca has the form

$$\dot{\boldsymbol{\sigma}}^{\text{eff}} = \dot{\boldsymbol{\sigma}} - \dot{\boldsymbol{\alpha}} = \mathbf{C}^{\text{e}}(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}^{\text{p}}, \phi, S_w) : \dot{\boldsymbol{\varepsilon}}^{\text{e}} - \dot{\lambda}\boldsymbol{Z} \tag{6.2}$$

where $\boldsymbol{\sigma}^{\text{eff}}$ is the effective stress, $\boldsymbol{\sigma}$ is the unrotated Cauchy stress, $\boldsymbol{\alpha}$ is the backstress, $\mathbf{C}^{\text{e}}$ is a tangent elastic modulus which depends on the stress (and also the plastic strain $\boldsymbol{\varepsilon}^{\text{p}}$, porosity ϕ, and water saturation S_w), the elastic strain is $\boldsymbol{\varepsilon}^{\text{e}}$, $\dot{\lambda}$ is the plastic flow rate, and $\boldsymbol{Z}$ in an elastic-plastic coupling tensor.

The model assumes that the tangent modulus tensor is isotropic and can be expressed as

$$\mathbf{C}^{\text{e}} = \left(K - \tfrac{2}{3}G\right)\boldsymbol{I}\otimes\boldsymbol{I} + 2G\,\mathbf{I} \tag{6.3}$$

where $K(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \boldsymbol{\varepsilon}^{\text{p}}, \phi, S_w)$ is the bulk modulus, $G(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \boldsymbol{\varepsilon}^{\text{p}}, \phi, S_w)$ is the shear modulus, $\boldsymbol{I}$ is rank-2 identity tensor, and $\mathbf{I}$ is the symmetric part of the rank-4 identity tensor.

If the effective stress is decomposed into volumetric and deviatoric parts:

$$\boldsymbol{\sigma}^{\text{eff}} = -\bar{p}\,\boldsymbol{I} + \mathbf{s}\,, \quad p := \tfrac{1}{3}\text{tr}(\boldsymbol{\sigma}^{\text{eff}})\,, \quad \mathbf{s} := \boldsymbol{\sigma}^{\text{eff}} - \tfrac{1}{3}\text{tr}(\boldsymbol{\sigma}^{\text{eff}})\boldsymbol{I} \tag{6.4}$$

and the elastic strain is also decomposed into volumetric and deviatoric parts

$$\boldsymbol{\varepsilon}^{\text{e}} = -\tfrac{1}{3}\bar{\varepsilon}^{\text{e}}_v\,\boldsymbol{I} + \boldsymbol{\gamma}^{\text{e}}\,, \quad \varepsilon^{\text{e}}_v := \text{tr}(\boldsymbol{\varepsilon}^{\text{e}})\,, \quad \boldsymbol{\gamma}^{\text{e}} := \boldsymbol{\varepsilon}^{\text{e}} - \tfrac{1}{3}\text{tr}(\boldsymbol{\varepsilon}^{\text{e}})\boldsymbol{I} \tag{6.5}$$

the elasticity model (without the coupling term), simplifies to

$$\dot{\bar{p}} = K(\boldsymbol{\sigma}, \alpha, \boldsymbol{\varepsilon}^{\text{p}}, \phi, S_w)\dot{\bar{\varepsilon}}^{\text{e}}_v\,, \quad \dot{\mathbf{s}} = 2G(\boldsymbol{\sigma}, \alpha, \boldsymbol{\varepsilon}^{\text{p}}, \phi, S_w)\,\dot{\boldsymbol{\gamma}}^{\text{e}}\,. \tag{6.6}$$

The partially saturated Arenisca model assumes the moduli depend only on

$$I_1 := \text{tr}(\boldsymbol{\sigma})\,, \quad \zeta = \text{tr}(\boldsymbol{\alpha})\,, \quad \varepsilon^{\text{p}}_v := \text{tr}(\boldsymbol{\varepsilon}^{\text{p}})\,, \quad \phi\,, \quad S_w\,. \tag{6.7}$$

6.1.1 Bulk modulus model: Solid matrix material

The pressure in the solid matrix is expressed as

$$\bar{p}_s = K_s \bar{\varepsilon}_v^s \; ; \quad \bar{\varepsilon}_v^s := \ln\left(\frac{V_{so}}{V_s}\right) \tag{6.8}$$

where $\bar{p}_s$ is the solid matrix pressure, K_s is the solid bulk modulus, $\bar{\varepsilon}_v^s$ is the volumetric strain, V_{so} is the initial volume of the solid, and V_s is the current volume of the solid. The solid bulk modulus is assumed to modeled by the Murnaghan equation:

$$K_s(\bar{p}_s) = K_{so} + n_s\,(\bar{p}_s - \bar{p}_{so}) \tag{6.9}$$

where K_{so} and n_s are material properties, and $\bar{p}_{so}$ is a reference pressure.

6.1.2 Bulk modulus model: Pore water

The equation of state of the pore water is

$$\bar{p}_w = K_w \bar{\varepsilon}_v^w + \bar{p}_o \; ; \quad \bar{\varepsilon}_v^w := \ln\left(\frac{V_{wo}}{V_w}\right) \tag{6.10}$$

where $\bar{p}_w$ is the water pressure, K_w is the water bulk modulus, V_{wo} is the initial volume of water, V_w is the current volume of water, $\bar{p}_o$ is the initial water pressure, and $\bar{\varepsilon}_v^w$ is the volumetric strain in the water. We use the isothermal Murnaghan bulk modulus model for water:

$$K_w(\bar{p}_w) = K_{wo} + n_w\,(\bar{p}_w - \bar{p}_{wo}) \tag{6.11}$$

where K_{wo} and n_w are material properties, and $\bar{p}_{wo}$ is a reference pressure.

6.1.3 Bulk modulus model: Pore air

The isentropic ideal gas equation of state for the pore air is

$$\bar{p}_a = \bar{p}_r\left[\exp(\gamma\,\bar{\varepsilon}_v^a) - 1\right] \; ; \quad \bar{\varepsilon}_v^a := \ln\left(\frac{V_{ao}}{V_a}\right) \tag{6.12}$$

where the quantities with subscript a represent quantities for the air model analogous to those for the water model in (6.10), $\bar{p}_r$ is a reference pressure (101325 Pa) and $\gamma = 1.4$. The bulk modulus of air (K_a) varies with the volumetric strain in the air:

$$K_a = \frac{d\bar{p}_a}{d\bar{\varepsilon}_v^a} = \gamma\,\bar{p}_r\,\exp(\gamma\,\bar{\varepsilon}_v^a) = \gamma\,(\bar{p}_a + \bar{p}_r)\,. \tag{6.13}$$

6.1.4 Bulk modulus model: Drained soil

The pressure model for drained soils has the form

$$\frac{\bar{p}^{\text{eff}}}{K_s(\bar{p}^{\text{eff}})} = b_0\,\bar{\varepsilon}_v^e + \frac{b_1(\bar{\varepsilon}_v^e)^{b_4}}{b_2(\bar{\varepsilon}_v^e)^{b_4} + b_3} \tag{6.14}$$

where the material parameters are $b_0 > 0, b_1 > 0, b_2 > 0, b_3 > 0, b_4 > 1$. Dependence on plastic strain can be added to the model if necessary.

The tangent bulk modulus is defined as

$$K_d(\bar{p}^{\text{eff}}) := \frac{d\bar{p}^{\text{eff}}}{d\bar{\varepsilon}_v^e}\,. \tag{6.15}$$

Then, using (6.14),

$$K_d(\bar{p}^{\text{eff}}) = \frac{[K_s(\bar{p}^{\text{eff}})]^2}{[K_s(\bar{p}^{\text{eff}}) - n_s\bar{p}^{\text{eff}}]}\left[b_0 + \frac{b_1 b_3 b_4 (\bar{\varepsilon}_v^e)^{b_4-1}}{\left[b_2(\bar{\varepsilon}_v^e)^{b_4} + b_3\right]^2}\right]. \tag{6.16}$$

To express (6.16) in closed-form in terms of $\bar{p}$ we have to eliminate $\bar{\varepsilon}_v^e$. But a closed form expression for the volumetric elastic strain cannot be derived from the pressure model. So we find an approximate form of (6.14) by assuming $b_0 \to 0$. This approximation is valid at moderate to large strains. Then, from (6.14) with $b_0 = 0$, we have

$$\bar{\varepsilon}_v^e \approx \left[\frac{b_3\bar{p}^{\text{eff}}}{b_1 K_s(\bar{p}^{\text{eff}}) - b_2\bar{p}^{\text{eff}}}\right]^{1/b_4} \tag{6.17}$$

and (6.16) can be expressed in terms of $\bar{p}$ as

$$K_d(\bar{p}^{\text{eff}}) = \frac{[K_s(\bar{p}^{\text{eff}})]^2}{[K_s(\bar{p}^{\text{eff}}) - n_s\bar{p}^{\text{eff}}]}\left[b_0 + \frac{b_1 b_3 b_4 \left(\frac{b_3\bar{p}^{\text{eff}}}{b_1 K_s(\bar{p}^{\text{eff}}) - b_2\bar{p}^{\text{eff}}}\right)^{1-1/b_4}}{\left[b_2\left(\frac{b_3\bar{p}^{\text{eff}}}{b_1 K_s(\bar{p}^{\text{eff}}) - b_2\bar{p}^{\text{eff}}}\right) + b_3\right]^2}\right]. \tag{6.18}$$

6.1.5 Bulk modulus model: Partially saturated soil

The pressure in the partially saturated soil ($\bar{p}$) is given by

$$\bar{p} = \int K(\bar{I}_1, \bar{\zeta}, \bar{\varepsilon}_v^p, \phi, S_w)\, \mathrm{d}\bar{\varepsilon}_v^e. \tag{6.19}$$

Note that

$$\bar{p}^{\text{eff}} = \tfrac{1}{3}(\bar{I}_1 - \bar{\zeta}). \tag{6.20}$$

The tangent bulk modulus of the partially saturated soil is found using a variation on the Grassman model for fully saturated rocks:

$$K(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w) = K_d(\bar{p}^{\text{eff}}) + \frac{\left(1 - \frac{K_d(\bar{p}^{\text{eff}})}{K_s(\bar{p}^{\text{eff}})}\right)^2}{\frac{1}{K_s(\bar{p}^{\text{eff}})}\left(1 - \frac{K_d(\bar{p}^{\text{eff}})}{K_s(\bar{p}^{\text{eff}})}\right) + \phi\left(\frac{1}{K_f(\bar{\zeta})} - \frac{1}{K_s(\bar{p}^{\text{eff}})}\right)} \tag{6.21}$$

where K is the effective bulk modulus of the partially saturated soil, K_d is the bulk modulus of the drained soil, K_f is the bulk modulus of the pore fluid, and K_s is the bulk modulus of the solid grains. At partial saturation, we compute the pore fluid bulk modulus using a harmonic mean (lower bound) on the air and water bulk moduli (K_a, K_f):

$$\frac{1}{K_f(\bar{\zeta})} = \frac{S_w}{K_w(\bar{\zeta})} + \frac{1 - S_w}{K_a(\bar{\zeta})}. \tag{6.22}$$

6.1.6 Shear modulus model: Drained soil

The shear modulus is typically assumed to be constant. However, a variable shear modulus may be needed to fit experimental data and to prevent negative values of Poisson's ratio in the simulations. In those situations a variable Poisson's ratio (ν) is defined as

$$\nu = \nu_1 + \nu_2 \exp\left[-\frac{K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)}{K_s(\bar{p}^{\text{eff}})}\right] \tag{6.23}$$

where ν_1 and ν_2 are material parameters. The shear modulus is computed using the Poisson's ratio and the drained bulk modulus:

$$G(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w) = \frac{3K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)(1 - 2\nu)}{2(1 + \nu)}. \tag{6.24}$$

6.2 Rate-independent plasticity

6.2.1 Yield function

The Arenisca yield function is

$$f = \sqrt{J_2} - F_f(\bar{I}_1, \zeta)\, F_c(\bar{I}_1, \bar{\zeta}, \overline{X}, \bar{\kappa}) = \sqrt{J_2} - F_f(\bar{p}^{\text{eff}})\, F_c(\bar{p}^{\text{eff}}, \overline{X}, \bar{\kappa}) \tag{6.25}$$

where

$$F_f(\bar{p}^{\text{eff}}) = a_1 - a_3 \exp[-3a_2\bar{p}^{\text{eff}})] + 3a_4\bar{p}^{\text{eff}} \tag{6.26}$$

and

$$F_c(\bar{p}^{\text{eff}}, \overline{X}, \bar{\kappa}) = \begin{cases} 1 & \text{for} \quad 3\bar{p}^{\text{eff}} \le \bar{\kappa} \\ \sqrt{1 - \left(\dfrac{3\bar{p}^{\text{eff}} - \bar{\kappa}}{\overline{X} - \bar{\kappa}}\right)^2} & \text{for} \quad 3\bar{p}^{\text{eff}} > \bar{\kappa}\,. \end{cases} \tag{6.27}$$

Here $\overline{X}$ is the hydrostatic compressive strength, $\bar{\kappa}$ is the branch point at which the cap function F_c starts decreasing until it reaches the hydrostatic strength point $(\overline{X}, 0)$, and

$$J_2 = \tfrac{1}{2}\mathbf{s} : \mathbf{s}\,. \tag{6.28}$$

Non-associativity is modeled using a parameter β that modifies $\sqrt{J_2}$ (see 6.8).

6.2.2 Hydrostatic compressive strength: Drained soil

The drained crush curve model is used to compute $\overline{X}$ and has the form

$$\overline{\varepsilon_v^p} - p_3 = \ln\left[1 - \frac{1 - \exp(-p_3)}{1 + \left(\frac{\overline{X}_d - p_0}{p_1}\right)^{p_2}}\right]. \tag{6.29}$$

where p_0, p_1, p_2, p_3 are model parameters and $\bar{\xi} = \overline{X} - \bar{p}_0$ where $\overline{X}$ is the hydrostatic compressive strength. The parameter p_3 is related to the initial porosity (ϕ_0) by $p_3 = -\ln(1 - \phi_0)$.

The drained hydrostatic compressive strength ($\overline{X}_d/3$) is found from the drained material crush curve using

$$\overline{X}_d(\overline{\varepsilon_v^p}, \phi_0) - p_0 = p_1\left[\frac{1 - \exp(-p_3)}{1 - \exp(-p_3 + \overline{\varepsilon_v^p})} - 1\right]^{1/p_2}, \quad p_3 := -\ln(1 - \phi_0)\,. \tag{6.30}$$

6.2.3 Hydrostatic compressive strength: Partially saturated soil

The elastic part of the volumetric strain at yield is defined in the model as

$$\varepsilon_v^{e,\text{yield}}(\overline{\varepsilon_v^p}) = \frac{\overline{X}_d(\overline{\varepsilon_v^p}, \phi_0)}{3\,K_d\left(\frac{1}{2}\frac{\overline{X}_d(\overline{\varepsilon_v^p}, \phi_0)}{3}\right)} \tag{6.31}$$

where X_d is found from the drained material crush curve.

The elastic volumetric strain at yield is assumed to be identical for drained and partially saturated materials. With this assumption, the compressive strength of a partially saturated sand is given by

$$\overline{X}(\overline{\varepsilon_v^p}) = 3K(\bar{p}^{\text{eff}}, \overline{\varepsilon_v^p}, \phi, S_w)\, \bar{\varepsilon}_v^{e,\text{yield}}(\overline{\varepsilon_v^p}) \tag{6.32}$$

where K is the bulk modulus of the partially saturated material.

6.2.4 Backstress: Pore pressure

The pore pressure as an isotropic backstress (ζ) that translates the Cauchy stress to the effective stress:

$$\boldsymbol{\sigma}^{\text{eff}} = \boldsymbol{\sigma} - \zeta \boldsymbol{I}\,, \quad \zeta := -\left[(1 - S_w)\bar{p}_a + S_w \bar{p}_w\right]. \tag{6.33}$$

In the elastically unloaded state (where the effective stress is zero) we assume that the pore pressure ($\bar{\zeta}$) is related to the volumetric plastic strain by

$$\exp(-\overline{\varepsilon_v^p}) = \phi_o\,(1 - S_o) \exp\left[-\frac{1}{\gamma} \ln\left(\frac{\bar{\zeta}}{\bar{p}_r} + 1\right)\right] + \phi_o\, S_o\, \exp\left(-\frac{\bar{\zeta} - \bar{p}_o}{K_w}\right) + (1 - \phi_o) \exp\left(-\frac{\bar{\zeta}}{K_s}\right). \tag{6.34}$$

This equation can be solved for $\bar{\zeta}(\overline{\varepsilon_v^p})$ using a root finding algorithm.

Alternatively, this equation can be converted into rate form and integrated using an explicit time stepping method if a Newton solve is too expensive or fails to converge:

$$\zeta = \int \frac{d\zeta}{d\varepsilon_v^p} \mathrm{d}\varepsilon_v^p\,. \tag{6.35}$$

where

$$\frac{d\zeta}{d\varepsilon_v^p} = \frac{\exp(-\overline{\varepsilon_v^p})}{\mathcal{B}}\,, \tag{6.36}$$

and

$$\mathcal{B} := \left[\frac{\phi_o\,(1 - S_o)}{\gamma(\bar{p}_r + \bar{\zeta})}\right] \exp\left[-\frac{1}{\gamma} \ln\left(\frac{\bar{\zeta}}{\bar{p}_r} + 1\right)\right] + \frac{\phi_o\, S_o}{K_w} \exp\left(\frac{\bar{p}_o - \bar{\zeta}}{K_w}\right) + \frac{1 - \phi_o}{K_s} \exp\left(-\frac{\bar{\zeta}}{K_s}\right). \tag{6.37}$$

6.3 Rate-dependent plasticity

6.4 Porosity and saturation

The total volumetric strain is given by

$$\exp(\varepsilon_v) = (1 - S_o)\phi_o \exp(\varepsilon_v^a) + S_o \phi_o \exp(\varepsilon_v^w) + (1 - \phi_o) \exp(\varepsilon_v^s) \tag{6.38}$$

where ϕ_o, S_o are the initial porosity and saturation, and

$$\varepsilon_v^w(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v) - \bar{p}_o}{K_w}\,, \quad \varepsilon_v^a(\varepsilon_v) = -\frac{1}{\gamma} \ln\left[1 + \frac{\bar{p}(\varepsilon_v)}{\bar{p}_r}\right], \quad \varepsilon_v^s(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v)}{K_s}\,. \tag{6.39}$$

We can combine (6.38) and (6.39) to solve for $\bar{p}(\varepsilon_v)$ and then compute the volumetric strain in the air in terms of the total volumetric strain.

6.4.1 Saturation

The saturation function $S_w(\varepsilon_v)$, is given by

$$S_w(\varepsilon_v) = \frac{\mathcal{C}(\varepsilon_v)}{1 + \mathcal{C}(\varepsilon_v)}\,, \quad \mathcal{C}(\varepsilon_v) := \left(\frac{S_o}{1 - S_o}\right) \exp(\varepsilon_v^w) \exp(-\varepsilon_v^a)\,. \tag{6.40}$$

6.4.2 Porosity

The porosity evolution equation (in the elastically unloaded state) for partially saturated sand has the form

$$\phi(\varepsilon_v) = \phi_o \left(\frac{1 - S_o}{1 - S_w(\varepsilon_v)} \right) \left[\frac{\exp(\varepsilon_v^a)}{\exp(\varepsilon_v)} \right] . \tag{6.41}$$

6.5 Summary of partially saturated soil model

Summary 6.5.1 ***Bulk modulus model***

Drained soil:
The equation of state of the drained soil is

$$K_d = \frac{[K_s]^2}{[K_s - n_s \bar{p}^{\text{eff}}]} \left[b_o + \frac{b_1 b_3 b_4 (\bar{\varepsilon}_v^e)^{b_4 - 1}}{\left[b_2 (\bar{\varepsilon}_v^e)^{b_4} + b_3 \right]^2} \right] , \quad \bar{\varepsilon}_v^e \approx \left[\frac{b_3 \bar{p}^{\text{eff}}}{b_1 K_s - b_2 \bar{p}^{\text{eff}}} \right]^{1/b_4} .$$

Partially saturated soil:
The bulk modulus model is

$$K = K_d + \frac{\left(1 - \dfrac{K_d}{K_s} \right)^2}{\dfrac{1}{K_s} \left(1 - \dfrac{K_d}{K_s} \right) + \phi \left(\dfrac{S_w}{K_w} + \dfrac{1 - S_w}{K_a} - \dfrac{1}{K_s} \right)}$$

where

$$K_s(\bar{p}) = K_{so} + n_s (\bar{p} - \bar{p}_{so}) , \quad K_w(\bar{p}) = K_{wo} + n_w (\bar{p} - \bar{p}_{wo}) , \quad K_a(\bar{p}) = \gamma (\bar{p} + \bar{p}_r)$$

Summary 6.5.2 ***Shear modulus model***

The shear modulus is either a constant (G_o) or determined using a variable Poisson's ratio (ν)

$$\nu = \nu_1 + \nu_2 \exp \left[- \frac{K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)}{K_s(\bar{p}^{\text{eff}})} \right]$$

$$G(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w) = \frac{3 K_d(\bar{p}^{\text{eff}}, \bar{\varepsilon}_v^p, \phi, S_w)(1 - 2\nu)}{2(1 + \nu)} .$$

Summary 6.5.3 ***Yield function***

The Arenisca yield function is

$$f = \sqrt{J_2} - F_f(\bar{I}_1, \zeta)\, F_c(\bar{I}_1, \bar{\zeta}, \bar{X}, \bar{\kappa}) = \sqrt{J_2} - F_f(\bar{p}^{\text{eff}})\, F_c(\bar{p}^{\text{eff}}, \bar{X}, \bar{\kappa}) \tag{6.42}$$

where

$$F_f(\bar{p}^{\text{eff}}) = a_1 - a_3 \exp[-3a_2\bar{p}^{\text{eff}})] + 3a_4\bar{p}^{\text{eff}} \tag{6.43}$$

and

$$F_c(\bar{p}^{\text{eff}}, \bar{X}, \bar{\kappa}) = \begin{cases} 1 & \text{for} \quad 3\bar{p}^{\text{eff}} \le \bar{\kappa} \\ \sqrt{1 - \left(\dfrac{3\bar{p}^{\text{eff}} - \bar{\kappa}}{\bar{X} - \bar{\kappa}}\right)^2} & \text{for} \quad 3\bar{p}^{\text{eff}} > \bar{\kappa}\,. \end{cases} \tag{6.44}$$

Non-associativity is modeled using a parameter β that modifies $\sqrt{J_2}$.

Summary 6.5.4 ***Hydrostatic strength model***

Drained soil:

$$\bar{X}_d(\bar{\varepsilon}_v^p) - p_0 = p_1 \left[\frac{1 - \exp(-p_3)}{1 - \exp(-p_3 + \bar{\varepsilon}_v^p)} - 1\right]^{1/p_2} \quad , \quad p_3 = -\ln(1 - \phi_0)\,.$$

Partially saturated soil:

$$\bar{X}(\bar{\varepsilon}_v^p) = 3K(\bar{I}_1, \bar{\varepsilon}_v^p, \phi, S_w)\, \bar{\varepsilon}_v^{e,\text{yield}}(\bar{\varepsilon}_v^p)$$

where

$$\varepsilon_v^{e,\text{yield}}(\bar{\varepsilon}_v^p) = \frac{\bar{X}_d(\bar{\varepsilon}_v^p)}{3\,K_d\left(\dfrac{\bar{X}_d(\bar{\varepsilon}_v^p)}{6}, \bar{\varepsilon}_v^p\right)}$$

Summary 6.5.5 ***Pore pressure model***

Solve $g(\bar{\zeta}, \bar{\varepsilon}_v^p) = 0$ for $\bar{\zeta}$.

$$g(\bar{\zeta}, \bar{\varepsilon}_v^p) = -\exp(-\bar{\varepsilon}_v^p) + \phi_0 (1 - S_0) \exp\left[-\frac{1}{\gamma} \ln\left(\frac{\bar{\zeta}}{\bar{p}_r} + 1\right)\right] + \phi_0 S_0 \exp\left(-\frac{\bar{\zeta} - \bar{p}_0}{K_w}\right) + (1 - \phi_0) \exp\left(-\frac{\bar{\zeta}}{K_s}\right).$$

Alternatively, integrate

$$\bar{\zeta} = \int \frac{d\bar{\zeta}}{d\bar{\varepsilon}_v^p} d\bar{\varepsilon}_v^p .$$

where

$$\frac{d\bar{\zeta}}{d\bar{\varepsilon}_v^p} = \frac{\exp(-\bar{\varepsilon}_v^p)}{\mathcal{B}},$$

and

$$\mathcal{B} := \left[\frac{\phi_0 (1 - S_0)}{\gamma(\bar{p}_r + \bar{\zeta})}\right] \exp\left[-\frac{1}{\gamma} \ln\left(\frac{\bar{\zeta}}{\bar{p}_r} + 1\right)\right] + \frac{\phi_0 S_0}{K_w} \exp\left(\frac{\bar{p}_0 - \bar{\zeta}}{K_w}\right) + \frac{1 - \phi_0}{K_s} \exp\left(-\frac{\bar{\zeta}}{K_s}\right).$$

Summary 6.5.6 ***Saturation and porosity evolution***

Saturation:

$$S_w(\varepsilon_v) = \frac{\mathcal{C}(\varepsilon_v)}{1 + \mathcal{C}(\varepsilon_v)}, \quad \mathcal{C}(\varepsilon_v) := \left(\frac{S_0}{1 - S_0}\right) \exp(\varepsilon_v^w) \exp(-\varepsilon_v^a).$$

where ϕ_0, S_0 are the initial porosity and saturation, and

$$\varepsilon_v^w(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v) - \bar{p}_0}{K_w}, \quad \varepsilon_v^a(\varepsilon_v) = -\frac{1}{\gamma} \ln\left[1 + \frac{\bar{p}(\varepsilon_v)}{\bar{p}_r}\right], \quad \varepsilon_v^s(\varepsilon_v) = -\frac{\bar{p}(\varepsilon_v)}{K_s}.$$

Porosity:

$$\phi(\varepsilon_v) = \phi_0 \left(\frac{1 - S_0}{1 - S_w(\varepsilon_v)}\right) \left[\frac{\exp(\varepsilon_v^a)}{\exp(\varepsilon_v)}\right]. \tag{6.45}$$

Note that

$$\exp(\varepsilon_v) = (1 - S_0)\phi_0 \exp(\varepsilon_v^a) + S_0 \phi_0 \exp(\varepsilon_v^w) + (1 - \phi_0) \exp(\varepsilon_v^s)$$

6.6 Computing the stress and internal variables

The partially saturated soil model uses Michael Homel's "consistency bisection" algorithm to find the plastic strain direction and to update the internal state variables. A closest-point return algorithm in transformed stress space is used to project the trial stress state on to the yield surface. Because of the nonlinearities in the material models, it is easier to solve the problem by dividing the strain increment to substeps.

The partially saturated soil model treats the porosity (ϕ) and saturation (S_w) as internal variables in addition to the hydrostatic compressive strength (X), the isotropic backstress (ζ), and the plastic strain ($\boldsymbol{\varepsilon}^{\mathrm{p}}$) which are used by the fully saturated model.

The inputs to the rate-independent stress update algorithm for a single material point are:

- $\boldsymbol{d}^{\mathrm{n}}$: the rate of deformation at time $t = t_n$; defined as $\boldsymbol{d} := \frac{1}{2}(\boldsymbol{l} + \boldsymbol{l}^T)$ where $\boldsymbol{l} = \nabla \mathbf{v}$ and $\mathbf{v}$ is the velocity field.
- Δt : the time step
- $\boldsymbol{\sigma}^{\mathrm{n}}$: the unrotated Cauchy step at time $t = t_n$.
- ϕ^{n} : the porosity at time $t = t_n$.
- S_w^{n} : the saturation at time $t = t_n$.
- X^{n} : the hydrostatic compressive strength at time $t = t_n$.
- ζ^{n} : the trace of the backstress at time $t = t_n$.
- $\boldsymbol{\varepsilon}^{\mathrm{p,n}}$: the plastic strain at time $t = t_n$.

After the return algorithm has been exercised, the outputs from the algorithm are:

- $\boldsymbol{\sigma}^{\mathrm{n+1}}$: the unrotated Cauchy step at time $t = t_{n+1} = t_n + \Delta t$.
- $\phi^{\mathrm{n+1}}$: the porosity at time $t = t_{n+1}$.
- $S_w^{\mathrm{n+1}}$: the saturation at time $t = t_{n+1}$.
- $X^{\mathrm{n+1}}$: the hydrostatic compressive strength at time $t = t_{n+1}$.
- $\zeta^{\mathrm{n+1}}$: the trace of the backstress at time $t = t_{n+1}$.
- $\boldsymbol{\varepsilon}^{\mathrm{p,n+1}}$: the plastic strain at time $t = t_{n+1}$.

The update algorithm uses the standard predictor-corrector approach of hypoelastic-plasticity where a trial predictor stress is computed first and then a corrector return algorithm is used to locate the position of the correct stress on the yield surface. This approach requires that the trial stress ($\boldsymbol{\sigma}^{\mathrm{trial}}$) is computed using the relation

$$\boldsymbol{\sigma}^{\mathrm{trial}} = \boldsymbol{\sigma}^{\mathrm{n}} + \mathbf{C}^{\mathrm{e}} : (\boldsymbol{d}\,\Delta t) \tag{6.46}$$

where $\mathbf{C}^{\mathrm{e}}$ is an elastic modulus that is typically assumed to be constant over the time step Δt. Though this assumption suffices for nonlinear elastic materials if the rate of deformation is small or the timestep is small or both, for large $\boldsymbol{d}\Delta t$ significant errors can enter the calculation. The Vaango implementation assumes that $\mathbf{C}^e$ is the tangent modulus at the beginning of a timestep (or load substep).

Caveat:

The partially saturated soil model has been developed for an explicit dynamics code where tiemsteps are typically very small. Care should be exercised if the application domain requires timesteps to be large.

Remark:

Note that in the Kayenta model (which is the basis for Arenisca), the bulk modulus has a high pressure limit. This limit was used by Michael Homel in Arenisca3 and Arenisca4 to define conservative elastic properties during the stress and internal variable update. However, the bulk modulus model used by the partially saturated version of Arenisca does not have this limit. Therefore the trial stress for the partially saturated model is computed using an alternative approach that assumes that the elastic moduli are those at the beginning of the timestep (or load substep).

After the trial stress is computed, the timestep is subdivided into substeps based on the characteristic dimension of the yield surface relative to the magnitude of the trial stress increment ($\boldsymbol{\sigma}^{\mathrm{trial}} - \boldsymbol{\sigma}^n$). The substep size is then recomputed by comparing the elastic properties at $\boldsymbol{\sigma}^{\mathrm{trial}}$ with those at $\boldsymbol{\sigma}^n$ to make sure that the nonlinear elastic solution is accurate.

The pseudocode for the algorithm is given below.

Algorithm 1 The stress and internal variable update algorithm

procedure UPDATESTRESSANDINTERNALVARS($\boldsymbol{d}^n$, Δt, $\boldsymbol{\sigma}^n$, ϕ^n, S_w^n, X^n, ζ^n, $\boldsymbol{\varepsilon}^{p,n}$)
  $K^n, G^n \leftarrow$ COMPUTEELASTICMODULI($\boldsymbol{\sigma}^n$, $\boldsymbol{\varepsilon}^{p,n}$, ϕ^n, S_w^n) ▷*Compute tangent bulk and shear modulus*
  $\boldsymbol{\sigma}^{trial} \leftarrow$ COMPUTETRIALSTRESS($\boldsymbol{\sigma}^n$, K^n, G^n, $\boldsymbol{d}^n$, Δt) ▷*Compute trial stress*
  $n_{sub} \leftarrow$ COMPUTESTEPDIVISIONS($\boldsymbol{\sigma}^n$, $\boldsymbol{\varepsilon}^{p,n}$, ϕ^n, S_w^n, $\boldsymbol{\sigma}^{trial}$) ▷*Compute number of substeps*
  $\delta t \leftarrow \dfrac{\Delta t}{n_{sub}}$ ▷*Substep timestep*
  $\boldsymbol{\sigma}^{old} \leftarrow \boldsymbol{\sigma}^n$, $\boldsymbol{\varepsilon}^{p,old} \leftarrow \boldsymbol{\varepsilon}^{p,n}$, $\phi^{old} \leftarrow \phi^n$, $S_w^{old} \leftarrow S_w^n$, $X^{old} \leftarrow X^n$, $\zeta^{old} \leftarrow \zeta^n$
  $\chi \leftarrow 1$, $t_{local} \leftarrow 0.0$ ▷*Initialize substep multiplier and accumulated time increment*
  isSuccess $\leftarrow$ FALSE
  repeat
    isSuccess, $\boldsymbol{\sigma}^{new}$, $\boldsymbol{\varepsilon}^{p,new}$, ϕ^{new}, S_w^{new}, X^{new}, $\zeta^{new} \leftarrow$ COMPUTESUBSTEP($\boldsymbol{\sigma}^{old}$, $\boldsymbol{\varepsilon}^{p,old}$, ϕ^{old}, S_w^{old}, X^{old}, ζ^{old}, $\boldsymbol{d}^n$, δt) ▷*Compute updated stress and internal variable for the current substep*
    if isSuccess = TRUE **then**
      $t_{local} \leftarrow t_{local} + \delta t$
      $\boldsymbol{\sigma}^{old} \leftarrow \boldsymbol{\sigma}^{new}$, $\boldsymbol{\varepsilon}^{p,old} \leftarrow \boldsymbol{\varepsilon}^{p,new}$, $\phi^{old} \leftarrow \phi^{new}$, $S_w^{old} \leftarrow S_w^{new}$ $X^{old} \leftarrow X^{new}$, $\zeta^{old} \leftarrow \zeta^{new}$
    else
      $\chi \leftarrow 2\chi$
      $\delta t \leftarrow \delta t/2$ ▷*Halve the timestep*
      if $\chi >$ CHI_MAX **then**
        return IsSuccess, $\boldsymbol{\sigma}^n$, ϕ^n, S_w^n, X^n, ζ^n, $\boldsymbol{\varepsilon}^{p,n}$ ▷*Algorithm has failed to converge*
      end if
    end if
  until $t_{local} \geq \Delta t$
  return IsSuccess, $\boldsymbol{\sigma}^{new}$, ϕ^{new}, S_w^{new}, X^{new}, ζ^{new}, $\boldsymbol{\varepsilon}^{p,new}$ ▷*Algorithm has converged*
end procedure

Algorithm 2 Computing the elastic moduli

procedure COMPUTEELASTICMODULI($\boldsymbol{\sigma}^n$, $\boldsymbol{\varepsilon}^{p,n}$, ϕ^n, S_w^n)
  $K \leftarrow 0$, $G \leftarrow 0$
  $\bar{I}_1 \leftarrow -\mathrm{tr}(\boldsymbol{\sigma}^n)$, $\bar{\varepsilon}_v^p \leftarrow -\mathrm{tr}(\boldsymbol{\varepsilon}^{p,n})$
  if $S_w^n > 0$ **then**
    $K, G \leftarrow$ COMPUTEPARTIALSATURATEDMODULI($\bar{I}_1$, $\bar{\varepsilon}_v^p$, ϕ^n, S_w^n)
  else
    $K, G \leftarrow$ COMPUTEDRAINEDMODULI($\bar{I}_1$, $\bar{\varepsilon}_v^p$)
  end if
  return K, G
end procedure

Algorithm 3 Computing the partially saturated elastic moduli

Require: K_{so}, n_s, $\bar{p}_{so}$, K_{wo}, n_w, $\bar{p}_{wo}$, γ, $\bar{p}_r$

procedure COMPUTEPARTIALSATURATEDMODULI($\bar{I}_1$, $\bar{\varepsilon}_v^p$, ϕ^n, S_w^n)
  if $\bar{I}_1 > 0$ **then**
    $\bar{p} \leftarrow \bar{I}_1/3$
    $K_s \leftarrow K_{so} + n_s(\bar{p} - \bar{p}_{so})$
    $K_w \leftarrow K_{wo} + n_w(\bar{p} - \bar{p}_{wo})$
    $K_a \leftarrow \gamma(\bar{p} + \bar{p}_r)$
    $K_d, G \leftarrow$ COMPUTEDRAINEDMODULI($\bar{I}_1$, $\bar{\varepsilon}_v^p$)
    $K_f \leftarrow 1.0/\left[S_w^n/K_w + (1.0 - S_w^n)/K_a\right]$ ▷*Bulk modulus of air + water mixture*
    numer $\leftarrow (1.0 - K_d/K_s)^2$

denom $\leftarrow (1.0/K_s)\,(1.0 - K_d/K_s) + \phi^{\mathrm{n}}\,(1.0/K_f - 1.0/K_s)$
$K \leftarrow K_d + \mathrm{numer}/\mathrm{denom}$ ▷*Bulk modulus of partially saturated material (Biot-Grassman model)*
else
$K, G \leftarrow$ computeDrainedModuli$(\bar{I}_1, \bar{\varepsilon}_v^{\mathrm{p}})$
end if
return K, G
end procedure

Algorithm 4 Computing the drained elastic moduli

Require: $K_{so}, n_s, \bar{p}_{so}, b_0, b_1, b_2, b_3, b_4, G_0, \nu_1, \nu_2$
procedure computeDrainedModuli$(\bar{I}_1, \bar{\varepsilon}_v^{\mathrm{p}})$
if $\bar{I}_1 > 0$ **then**
$\bar{p} \leftarrow \bar{I}_1/3$
$K_s \leftarrow K_{so} + n_s(\bar{p} - \bar{p}_{so})$
$K_s^{\mathrm{ratio}} \leftarrow K_s/(1.0 - n_s * \bar{p}/K_s)$
$\varepsilon_v^{\mathrm{e}} \leftarrow \mathrm{pow}((b_3 * \bar{p})/(b_1 K_s - b_2 \bar{p}), (1.0/b_4))$;
$y \leftarrow \mathrm{pow}(\varepsilon_v^{\mathrm{e}}, b_4)$
$z \leftarrow b_2 y + b_3$
$K \leftarrow K_s^{\mathrm{ratio}}[b_0 + (1/\varepsilon_v^{\mathrm{e}}) b_1 b_3 b_4 y/z^2]$; ▷ *Compute compressive bulk modulus*
$\nu = \nu_1 + \nu_2 \exp(-K/K_s)$
$G \leftarrow G_0$
if $\nu > 0$ **then**
$G \leftarrow 1.5K\,(1.0 - 2.0\nu)/(1.0 + \nu)$ ▷*Update the shear modulus (if $nu_1, \nu_2 > 0$)*
end if
else
$K \leftarrow b_0 K_{so}$ ▷*Tensile bulk modulus = Bulk modulus at $p = 0$*
$G \leftarrow G_0$ ▷*Tensile shear modulus*
end if
return K, G
end procedure

Algorithm 5 Computing the trial stress

procedure computeTrialStress$(\boldsymbol{\sigma}^{\mathrm{n}}, K^n, G^n, \boldsymbol{d}^{\mathrm{n}}, \Delta t)$
end procedure

Algorithm 6 Computing the initial number of substeps

procedure computeStepDivisions$(\boldsymbol{\sigma}^{\mathrm{n}}, \boldsymbol{\varepsilon}^{\mathrm{p,n}}, \phi^{\mathrm{n}}, S_w^{\mathrm{n}}, \boldsymbol{\sigma}^{\mathrm{trial}})$
end procedure

Algorithm 7 Computing the stress and internal variable update for a substep

procedure computeSubstep$(\boldsymbol{\sigma}^{\mathrm{old}}, \boldsymbol{\varepsilon}^{\mathrm{p,old}}, \phi^{\mathrm{old}}, S_w^{\mathrm{old}}, X^{\mathrm{old}}, \zeta^{\mathrm{old}}, \boldsymbol{d}^{\mathrm{n}}, \delta t)$
$K^{\mathrm{old}}, G^{\mathrm{old}} \leftarrow$ computeElasticModuli$(\boldsymbol{\sigma}^{\mathrm{old}}, \boldsymbol{\varepsilon}^{\mathrm{p,old}}, \phi^{\mathrm{old}}, S_w^{\mathrm{old}})$ ▷*Compute tangent bulk and shear modulus*
$\delta\boldsymbol{\varepsilon} \leftarrow \boldsymbol{d}^{\mathrm{n}} \delta t$ ▷*Compute strain increment*
$\boldsymbol{\sigma}^{\mathrm{trial}} \leftarrow$ computeTrialStress$(\boldsymbol{\sigma}^{\mathrm{old}}, K^{\mathrm{old}}, G^{\mathrm{old}}, \boldsymbol{d}^{\mathrm{n}}, \Delta t)$ ▷*Compute trial stress*
$I_1^{\mathrm{trial}}, \sqrt{J_2^{\mathrm{trial}}} \leftarrow$ stressInvariants$(\boldsymbol{\sigma}^{\mathrm{trial}})$ ▷*Compute invariants of the trial stress*
isElastic $\leftarrow$ evalYieldCondition$(I_1^{\mathrm{trial}}, \sqrt{J_2^{\mathrm{trial}}}, X^{\mathrm{old}}, \zeta^{\mathrm{old}}, K^{\mathrm{old}}, G^{\mathrm{old}}, \beta)$

if isElastic = TRUE **then**
  $\boldsymbol{\sigma}^{\text{new}} \leftarrow \boldsymbol{\sigma}^{\text{trial}}$, $\boldsymbol{\varepsilon}^{\text{p,new}} \leftarrow \boldsymbol{\varepsilon}^{\text{p,old}}$, $\phi^{\text{new}} \leftarrow \phi^{\text{old}}$, $S_w^{\text{new}} \leftarrow S_w^{\text{old}}$, $X^{\text{new}} \leftarrow X^{\text{old}}$, $\zeta^{\text{new}} \leftarrow \zeta^{\text{old}}$
  isSuccess = TRUE
  return isSuccess, $\boldsymbol{\sigma}^{\text{new}}$, $\boldsymbol{\varepsilon}^{\text{p,new}}$ ϕ^{new}, S_w^{new}, X^{new}, ζ^{new}
end if
$\boldsymbol{\sigma}^{\text{o}}$, $\delta\boldsymbol{\varepsilon}^{\text{p,o}} \leftarrow$ nonHardeningReturn($\boldsymbol{\sigma}^{\text{old}}$, $\boldsymbol{\sigma}^{\text{trial}}$, $\delta\boldsymbol{\varepsilon}$, X^{old}, ζ^{old}, K^{old}, G^{old}, β, I_1^{peak}) ▷*Compute return to updated yield surface (no hardening)*
isSuccess, $\boldsymbol{\sigma}^{\text{new}}$, $\boldsymbol{\varepsilon}^{\text{p,new}}$, X^{new}, ζ^{new}, K^{mid}, $G^{\text{mid}} \leftarrow$ consistencyBisection($\boldsymbol{\varepsilon}^{\text{p,old}}$, $\delta\boldsymbol{\varepsilon}^{\text{p,o}}$, ζ^{old}, $\boldsymbol{\sigma}^{\text{o}}$, $\boldsymbol{\sigma}^{\text{trial}}$, K^{old}, G^{old}, β, I_1^{peak})
if iSuccess = FALSE **then**
  return isSuccess, $\boldsymbol{\sigma}^{\text{old}}$, $\boldsymbol{\varepsilon}^{\text{p,old}}$, ϕ^{old}, S_w^{old}, X^{old}, ζ^{old}
end if
return isSuccess, $\boldsymbol{\sigma}^{\text{new}}$, $\boldsymbol{\varepsilon}^{\text{p,new}}$, ϕ^{new}, S_w^{new}, X^{new}, ζ^{new}
end procedure

6.7 The consistency bisection algorithm

6.7.1 Fixed (nonhardening) yield surface

Let the stress at the beginning of the load step be $\boldsymbol{\sigma}^{\text{old}}$ and let the trial stress be $\boldsymbol{\sigma}^{\text{trial}}$. Assume the yield surface is fixed and let the correct projection of the trial stress on to the fixed yield surface be $\boldsymbol{\sigma}^{\text{new,o}}$.

The increment of stress for the load step ($\Delta\boldsymbol{\sigma}^{\text{o}}$) is related to the elastic strain increment ($\Delta\boldsymbol{\varepsilon}^{\text{e,o}}$)by

$$\Delta\boldsymbol{\sigma}^{\text{o}} = \boldsymbol{\sigma}^{\text{new,o}} - \boldsymbol{\sigma}^{\text{old}} = \mathbf{C} : \Delta\boldsymbol{\varepsilon}^{\text{e,o}} \tag{6.47}$$

where $\mathbf{C}$ is a constant elastic modulus tensor. The elastic modulus tensor can be assumed to be an average value of the nonlinear tangent modulus for the load step.

If we know $\mathbf{C}$, we can compute the elastic strain increment using

$$\Delta\boldsymbol{\varepsilon}^{\text{e,o}} = \mathbf{C}^{-1} : \Delta\boldsymbol{\sigma}^{\text{o}} \,. \tag{6.48}$$

For a strain driven update algorithm, the total strain increment $\Delta\boldsymbol{\varepsilon}$ is known. Assuming that the total strain increment can be additively decomposed into an elastic and a plastic part, we can find the plastic strain increment ($\Delta\boldsymbol{\varepsilon}^{\text{p,o}}$) using

$$\Delta\boldsymbol{\varepsilon}^{\text{p,o}} = \Delta\boldsymbol{\varepsilon} - \Delta\boldsymbol{\varepsilon}^{\text{e,o}} \,. \tag{6.49}$$

6.7.2 Hardening yield surface

Now, if we allow the yield surface to harden, the distance between the trial stress point and its projection on to the yield surface decreases compared to that for a fixed yield surface. If $\Delta\boldsymbol{\varepsilon}^{\text{p}}$ is the plastic strain increment for a hardening yield surface, we have

$$\Delta\boldsymbol{\varepsilon}^{\text{p}} > \Delta\boldsymbol{\varepsilon}^{\text{p,o}} \tag{6.50}$$

where the inequality can be evaluated using an appropriate Euclidean norm. Note that this distance is proportional to the consistency parameter $\dot{\lambda}$.

Fully saturated model

In the fully saturated version of the Arenisca model, the internal variables are the hydrostatic compressive strength (X) and the scalar isotropic backstress (ζ). These depend only on the **volumetric** plastic strain increment

$$\Delta\varepsilon_v^{\text{p}} = \text{tr}(\Delta\boldsymbol{\varepsilon}^{\text{p}}) \,. \tag{6.51}$$

Because

$$\Delta\varepsilon_v^{\mathrm{p}} > \Delta\varepsilon_v^{\mathrm{p,o}} \tag{6.52}$$

we can define a parameter, $\eta \in (0,1)$, such that

$$\eta := \frac{\Delta\varepsilon_v^{\mathrm{p}}}{\Delta\varepsilon_v^{\mathrm{p,o}}}. \tag{6.53}$$

Because the solution is bounded by the fixed yield surface, a bisection algorithm can be used to find the parameter η.

Partially saturated model

TODO

6.7.3 Bisection algorithm: Fully saturated

Algorithm 8 The consistency bisection algorithm for fully saturated materials

procedure CONSISTENCYBISECTION($\boldsymbol{\varepsilon}^{\mathrm{p,old}}$, $\delta\boldsymbol{\varepsilon}^{\mathrm{p,o}}$, ζ^{old}, $\boldsymbol{\sigma}^{\mathrm{o}}$, $\boldsymbol{\sigma}^{\mathrm{trial}}$, K^{old}, G^{old}, β, I_1^{peak})
  $\boldsymbol{\sigma}^{\mathrm{new}} \leftarrow \boldsymbol{\sigma}^{\mathrm{o}}$, $\delta\boldsymbol{\varepsilon}^{\mathrm{p}} \leftarrow \delta\boldsymbol{\varepsilon}^{\mathrm{p,o}}$
  $\varepsilon_v^{\mathrm{p,old}} \leftarrow \mathrm{tr}(\boldsymbol{\varepsilon}^{\mathrm{p,old}})$, $\delta\varepsilon_v^{\mathrm{p,old}} \leftarrow \mathrm{tr}(\delta\boldsymbol{\varepsilon}^{\mathrm{p,old}})$
  $i \leftarrow 1$
  $\eta^{\mathrm{in}} \leftarrow 0$, $\eta^{\mathrm{out}} \leftarrow 1$
  repeat
    $j \leftarrow 1$
    isElastic $\leftarrow$ TRUE
    while isElastic = TRUE **do**
      $\eta^{\mathrm{mid}} \leftarrow \frac{1}{2}(\eta^{\mathrm{out}} + \eta^{\mathrm{in}})$
      $X^{\mathrm{new}} \leftarrow$ COMPUTEHYDROSTATICSTRENGTH($\varepsilon_v^{\mathrm{p,old}} + \eta^{\mathrm{mid}}\,\delta\varepsilon_v^{\mathrm{p,o}}$) ▷*Update the hydrostatic compressive strength*
      $\dfrac{\partial\zeta}{\partial\varepsilon_v^{\mathrm{p}}} \leftarrow$ COMPUTEDERIVATIVEOFBACKSTRESS(Arguments?)
      $\zeta^{\mathrm{new}} \leftarrow \zeta^{\mathrm{old}} + \left(\dfrac{\partial\zeta}{\partial\varepsilon_v^{\mathrm{p}}}\right) \times (\eta^{\mathrm{mid}}\,\delta\varepsilon_v^{\mathrm{p,o}})$ ▷*Update the isotropic backstress*
      $I_1^{\mathrm{trial}}, \sqrt{J_2^{\mathrm{trial}}} \leftarrow$ STRESSINVARIANTS($\boldsymbol{\sigma}^{\mathrm{trial}}$) ▷*Compute invariants of the trial stress*
      isElastic $\leftarrow$ EVALYIELDCONDITION(I_1^{trial}, $\sqrt{J_2^{\mathrm{trial}}}$, X^{new}, ζ^{new}, K^{old}, G^{old}, β)
      $\eta^{\mathrm{out}} \leftarrow \eta^{\mathrm{mid}}$ ▷*Too much plastic strain*
      $j \leftarrow j + 1$
      if $j \geq j^{\max}$ **then**
        isSuccess $\leftarrow$ FALSE
        return isSuccess
      end if
    end while
    $\boldsymbol{\sigma}^{\mathrm{mid}} \leftarrow \frac{1}{2}(\boldsymbol{\sigma}^{\mathrm{old}} + \boldsymbol{\sigma}^{\mathrm{new}})$
    $\boldsymbol{\varepsilon}^{\mathrm{p,mid}} \leftarrow \boldsymbol{\varepsilon}^{\mathrm{p,old}} + \frac{1}{2}\eta^{\mathrm{mid}}\,\delta\boldsymbol{\varepsilon}^{\mathrm{p,o}}$
    $K^{\mathrm{mid}}, G^{\mathrm{mid}} \leftarrow$ COMPUTEELASTICMODULI($\boldsymbol{\sigma}^{\mathrm{mid}}$, $\boldsymbol{\varepsilon}^{\mathrm{p,mid}}$)
    $\boldsymbol{\sigma}^{\mathrm{new}}, \delta\boldsymbol{\varepsilon}^{\mathrm{p,new}} \leftarrow$ NONHARDENINGRETURN($\boldsymbol{\sigma}^{\mathrm{old}}$, $\boldsymbol{\sigma}^{\mathrm{trial}}$, $\delta\boldsymbol{\varepsilon}^{\mathrm{new}}$, X^{new}, ζ^{new}, K^{mid}, G^{mid}, β, I_1^{peak}) ▷*Compute return to updated yield surface (no hardening)*
    if $\mathrm{sign}(\mathrm{tr}(\boldsymbol{\sigma}^{\mathrm{trial}} - \boldsymbol{\sigma}^{\mathrm{new}})) \neq \mathrm{sign}(\mathrm{tr}(\boldsymbol{\sigma}^{\mathrm{trial}} - \boldsymbol{\sigma}^{\mathrm{o}}))$ **or** $\|\delta\boldsymbol{\varepsilon}^{\mathrm{p,new}}\|_2 > \eta^{\mathrm{mid}}\,\|\delta\boldsymbol{\varepsilon}^{\mathrm{p,o}}\|_2$ **then**
      $\eta^{\mathrm{out}} \leftarrow \eta^{\mathrm{mid}}$ ▷*Too much plastic strain*
    else
      if $\|\delta\boldsymbol{\varepsilon}^{\mathrm{p,new}}\|_2 < \eta^{\mathrm{mid}}\,\|\delta\boldsymbol{\varepsilon}^{\mathrm{p,o}}\|_2$ **then**

31: $\eta^{\text{in}} \leftarrow \eta^{\text{mid}}$ ▷*Too little plastic strain*
32: **end if**
33: **end if**
34: $i \leftarrow i + 1$
35: **if** $i \geq i^{\max}$ **then**
36: isSuccess ← FALSE
37: **return** isSuccess
38: **end if**
39: **until** abs($\|\delta\boldsymbol{\varepsilon}^{\text{p,new}}\|_2 - \eta^{\text{mid}} \|\delta\boldsymbol{\varepsilon}^{\text{p,o}}\|_2$) < TOLERANCE
40: $\boldsymbol{\varepsilon}^{\text{p,new}} = \boldsymbol{\varepsilon}^{\text{p,old}} + \delta\boldsymbol{\varepsilon}^{\text{p,new}}$ ▷*Update the plastic strain*
41: $X^{\text{new}} \leftarrow$ computeHydrostaticStrength(tr($\boldsymbol{\varepsilon}^{\text{p,new}}$)) ▷*Update the hydrostatic compressive strength*
42: $\frac{\partial\zeta}{\partial\varepsilon_v^{\text{p}}} \leftarrow$ computeDerivativeOfBackstress(Arguments?)
43: $\zeta^{\text{new}} \leftarrow \zeta^{\text{old}} + \left(\frac{\partial\zeta}{\partial\varepsilon_v^{\text{p}}}\right) \times (\text{tr}(\delta\boldsymbol{\varepsilon}^{\text{p,new}}))$ ▷*Update the isotropic backstress*
44: isSuccess ← TRUE
45: **return** isSuccess, $\boldsymbol{\sigma}^{\text{new}}$, $\boldsymbol{\varepsilon}^{\text{p,new}}$, X^{new}, ζ^{new}, K^{mid}, G^{mid}
46: **end procedure**

6.8 The nonhardening return algorithm

Let the plastic flow direction be $\boldsymbol{M}$. Then

$$\dot{\boldsymbol{\varepsilon}^p} = \dot{\lambda}\boldsymbol{M}\,. \tag{6.54}$$

The nonhardening return algorithm uses a transformed space where the computation is carried out in special Lode coordinates (z', r') where

$$z' = z - \frac{\zeta}{\sqrt{3}}\,,\quad z := \frac{I_1}{\sqrt{3}} \quad \text{and} \quad r' = \sqrt{\frac{3K}{2G}}\,r\,,\quad r := \sqrt{2J_2}\,. \tag{6.55}$$

If the flow rule is non-associative, the yield surface parameter $\beta \neq 1$. In that case,

$$r' \leftarrow \beta r'\,. \tag{6.56}$$

The quantities needed by the non-hardening return algorithm are:

Require: as input

- $\boldsymbol{\sigma}^{\text{trial}}$ ▷*Trial stress*
- $\boldsymbol{\sigma}^{\text{old}}$ ▷*Stress at the start of the substep*
- $\delta\boldsymbol{\varepsilon}^{\text{new}}$ ▷*Increment of total strain*
- X^{old} ▷*Hydrostatic compressive strength*
- ζ^{old} ▷*Isotropic backstress (trace)*
- K^{old} ▷*Tangent bulk modulus*
- G^{old} ▷*Tangent shear modulus*
- I_1^{peak} ▷*The location of the yield surface vertex*
- β ▷*The yield surface non-associativity parameter*

The nonhardening return algorithm pseudocode is listed below:

Algorithm 9 Non-hardening return algorithm

1: **procedure** nonHardeningReturn($\boldsymbol{\sigma}^{\text{old}}$, $\boldsymbol{\sigma}^{\text{trial}}$, $\delta\boldsymbol{\varepsilon}^{\text{new}}$, X^{old}, ζ^{old}, K^{old}, G^{old}, β, I_1^{peak})

$I_1^{\text{trial}}, J_2^{\text{trial}} \leftarrow$ STRESSINVARIANTS($\boldsymbol{\sigma}^{\text{trial}}$) ▷*Compute invariants of the trial stress*

$r^{\text{trial}} \leftarrow \beta\sqrt{2J_2^{\text{trial}}}, z^{\text{trial}} \leftarrow \dfrac{I_1^{\text{trial}}}{\sqrt{3}}$ ▷*Compute Lode coordinates of the trial stress*

$(r')^{\text{trial}} \leftarrow r^{\text{trial}}\sqrt{\dfrac{3K^{\text{old}}}{2G^{\text{old}}}}$ ▷*Transform the trial r coordinate*

$I_1^{\text{o}} \leftarrow \zeta^{\text{old}} + \frac{1}{2}(X^{\text{old}} + I_1^{\text{peak}}), J_2^{\text{o}} \leftarrow 0$ ▷*Compute interior point*

$r^{\text{o}} \leftarrow \beta\sqrt{2J_2^{\text{o}}}, z^{\text{o}} \leftarrow \dfrac{I_1^{\text{o}}}{\sqrt{3}}$ ▷*Compute Lode coordinates of the interior point*

$(r')^{\text{o}} \leftarrow r^{\text{o}}\sqrt{\dfrac{3K^{\text{old}}}{2G^{\text{old}}}}$ ▷*Transform the interior point r coordinate*

$\theta \leftarrow 0$

repeat

$z^{\text{new}}, (r')^{\text{new}} \leftarrow$ APPLYBISECTIONALGORITHM($z^{\text{o}}, (r')^{\text{o}}, z^{\text{trial}}, (r')^{\text{trial}}, X^{\text{old}}, \zeta^{\text{old}}, K^{\text{old}}, G^{\text{old}}, \beta$) ▷*Find intersection point on the non-hardening yield surface*

$\theta, z^{\text{rot}}, (r')^{\text{rot}} \leftarrow$ FINDNEWINTERNALPOINT(z^{trial},$(r')^{\text{trial}}, z^{\text{new}}, (r')^{\text{new}}, \theta, X^{\text{old}}, \zeta^{\text{old}}, K^{\text{old}}, G^{\text{old}}, \beta$) ▷*Apply rotation algorithm to find new internal point*

$(r')^{\text{o}} \leftarrow (r')^{\text{rot}}, z^{\text{o}} \leftarrow z^{\text{rot}}$

until $\theta \leq$ TOLERANCE

$I_1^{\text{new}} = \sqrt{3}\, z^{\text{new}}, \sqrt{J_2^{\text{new}}} = \dfrac{2G^{\text{old}}}{3K^{\text{old}}} \dfrac{(r')^{\text{new}}}{\sqrt{2}\beta}$ ▷*Compute updated stress invariants*

$\mathbf{s}^{\text{trial}} \leftarrow \boldsymbol{\sigma}^{\text{trial}} - \frac{1}{3} I_1^{\text{trial}} \boldsymbol{I}$ ▷*Compute deviatoric trial stress*

$\boldsymbol{\sigma}^{\text{new}} = \frac{1}{3} I_1^{\text{new}} \boldsymbol{I} + \dfrac{\sqrt{J_2^{\text{new}}}}{\sqrt{J_2^{\text{trial}}}} \mathbf{s}^{\text{trial}}$ ▷*Compute updated stress*

$\delta\boldsymbol{\varepsilon}^{\text{p,new}} = \delta\boldsymbol{\varepsilon} - \mathbf{C}^{-1} : (\boldsymbol{\sigma}^{\text{new}} - \boldsymbol{\sigma}^{\text{old}})$ ▷*Compute plastic strain increment*

return Outputs:

- $\boldsymbol{\sigma}^{\text{new}}$ ▷*Updated stress tensor*
- $\delta\boldsymbol{\varepsilon}^{\text{p,new}}$ ▷*Increment in plastic strain*

end procedure

Algorithm 10 Apply bisection algorithm to find point on yield surface.

procedure APPLYBISECTIONALGORITHM($z^{\text{o}}, (r')^{\text{o}}, z^{\text{trial}}, (r')^{\text{trial}}, X^{\text{old}}, \zeta^{\text{old}}, K^{\text{old}}, G^{\text{old}}, \beta$)

$\eta^{\text{in}} \leftarrow 0, \eta^{\text{out}} \leftarrow 1$

while $\eta^{\text{out}} - \eta^{\text{in}} \geq$ TOL **do**

$\eta^{\text{mid}} = \frac{1}{2}(\eta^{\text{in}} + \eta^{\text{out}})$

$\begin{bmatrix} z^{\text{mid}} \\ (r')^{\text{mid}} \end{bmatrix} \leftarrow \eta^{\text{mid}} \begin{bmatrix} z^{\text{trial}} - z^{\text{o}} \\ (r')^{\text{trial}} - (r')^{\text{o}} \end{bmatrix} + \begin{bmatrix} z^{\text{o}} \\ (r')^{\text{o}} \end{bmatrix}$

isElastic $\leftarrow$ EVALYIELDCONDITION($z^{\text{mid}}, (r')^{\text{mid}}, X^{\text{old}}, \zeta^{\text{old}}, K^{\text{old}}, G^{\text{old}}, \beta$)

if isElastic = TRUE **then**

$\eta^{\text{in}} \leftarrow \eta^{\text{mid}}$

else

$\eta^{\text{out}} \leftarrow \eta^{\text{mid}}$

end if

end while

$z^{\text{new}} \leftarrow z^{\text{mid}}, (r')^{\text{new}} \leftarrow (r')^{\text{mid}}$

return $z^{\text{new}}, (r')^{\text{new}}$

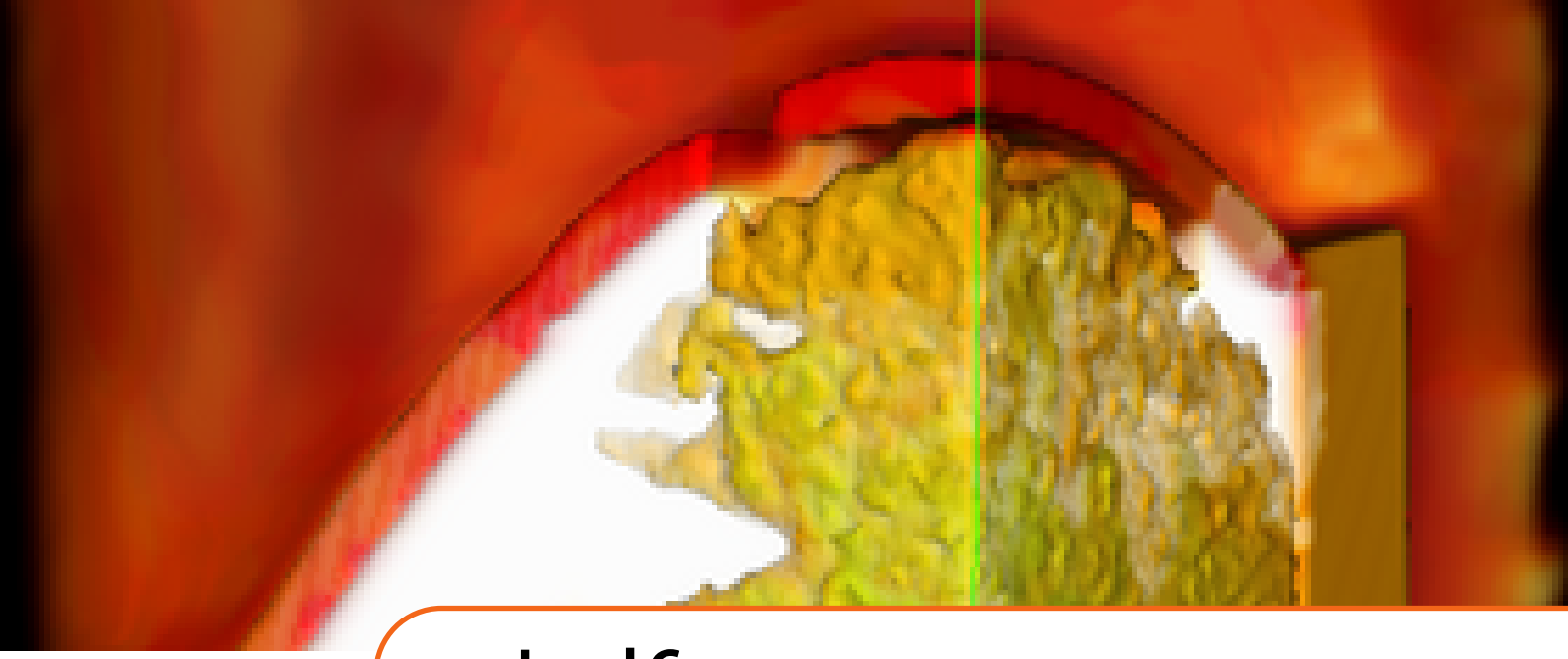
end procedure

Algorithm 11 Rotation around trial state to find internal point inside yield surface

procedure FINDNEWINTERNALPOINT(z^{trial}, $(r')^{\text{trial}}$, z^{new}, $(r')^{\text{new}}$, θ, X^{old}, ζ^{old}, K^{old}, G^{old}, β)
  $n \leftarrow 0$
  repeat
    $n \leftarrow n + 1$
    $\theta \leftarrow (-1)^n \times \frac{\pi}{2} \times \left(\frac{1}{2}\right)^{\frac{\text{floor}(n)}{2}}$
    $[\mathsf{Q}] \leftarrow \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$
    $\begin{bmatrix} z^{\text{rot}} \\ (r')^{\text{rot}} \end{bmatrix} \leftarrow [\mathsf{Q}] \cdot \begin{bmatrix} z^{\text{new}} - z^{\text{trial}} \\ (r')^{\text{new}} - (r')^{\text{trial}} \end{bmatrix} + \begin{bmatrix} z^{\text{trial}} \\ (r')^{\text{trial}} \end{bmatrix}$
    isElastic $\leftarrow$ EVALYIELDCONDITION(z^{rot}, $(r')^{\text{rot}}$, X^{old}, ζ^{old}, K^{old}, G^{old}, β)
  until isElastic = FALSE
  return θ, z^{rot}, $(r')^{\text{rot}}$
end procedure

Algorithm 12 Evaluate the yield condition

procedure EVALYIELDCONDITION(z^{new}, $(r')^{\text{new}}$, X^{old}, ζ^{old}, K^{old}, G^{old}, β)
  $I_1^{\text{new}} \leftarrow \sqrt{3}\, z^{\text{new}}$, $\sqrt{J_2^{\text{new}}} \leftarrow \frac{2G^{\text{old}}}{3K^{\text{old}}} \times \frac{1}{\sqrt{2}\,\beta} \times (r')^{\text{new}}$ ▷*Transform back into stress space*
  isElastic $\leftarrow$ EVALYIELDCONDITION(I_1^{new}, $\sqrt{J_2^{\text{new}}}$, X^{old}, ζ^{old}, K^{old}, G^{old}, β)
  return isElastic
end procedure



7 — Load Curves

It is often more convenient to apply a specified load at the MPM particles. The load may be a function of time. Such a load versus time curve is called a **load curve**.

In Vaango, the load curve infrastructure is available for general use (and not only for particles). However, it has been implemented only for a special case of pressure loading.

We invoke the load curve in the <MPM> section of the input file using

```
<use_load_curves> true </use_load_curves>i
```

The default value is <use_load_curves> false </use_load_curves>.

In Vaango, a load curve infrastructure is implemented in the file .../MPM/PhysicalBC/LoadCurve.h. This file is essentially a templated structure that has the following private data

```
// Load curve information
std::vector<double> d_time;
std::vector<T> d_load;
int d_id;
```

The variable d_id is the load curve ID, d_time is the time, and d_load is the load. Note that the load can have any form - scalar, vector, matrix, etc.

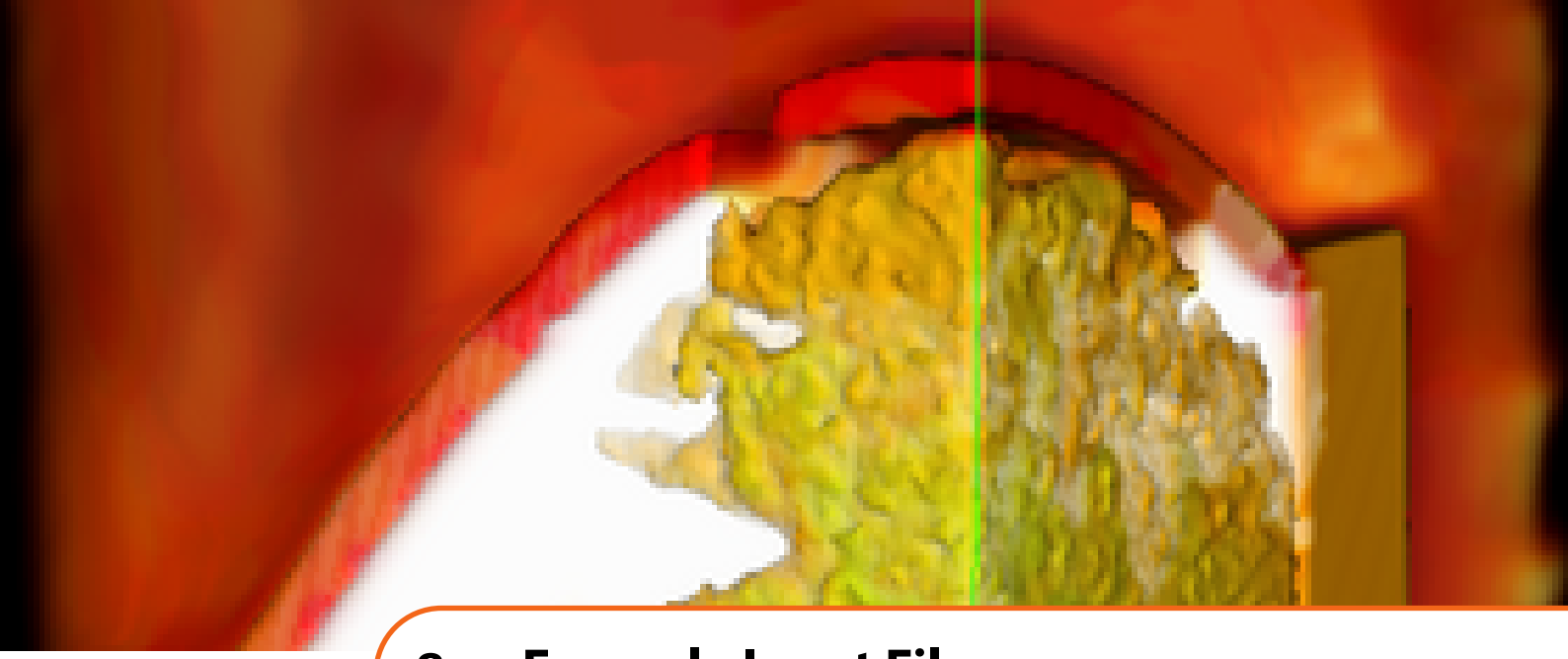
In our current implementation, the actual specification of the load curve information is in the <PhysicalBC> section of the input file. The implementation is limited in that it applies only to pressure boundary conditions for some special geometries (the implementation is in .../MPM/PhysicalBC/PressureBC.cc). However, the load curve template can be used in other, more general, contexts.

A sample input file specification of a pressure load curve is shown below. In this case, a pressure is applied to the inside and outside of a cylinder. The pressure is ramped up from 0 to 1 GPa on the inside and from 0 to 0.1 MPa on the outside over a time of 10 microsecs.

```
<PhysicalBC>
  <MPM>
    <pressure>
      <geom_object>
        <cylinder label = "inner cylinder">
          <bottom>          [0.0,0.0,0.0]   </bottom>
          <top>             [0.0,0.0,.02]   </top>
          <radius>          0.5             </radius>
        </cylinder>
```

```
        </geom_object>
        <load_curve>
          <id>1</id>
          <time_point>
            <time> 0 </time>
            <load> 0 </load>
          </time_point>
          <time_point>
            <time> 1.0e-5 </time>
            <load> 1.0e9 </load>
          </time_point>
        </load_curve>
      </pressure>
      <pressure>
        <geom_object>
          <cylinder label = "outer cylinder">
            <bottom>           [0.0,0.0,0.0]   </bottom>
            <top>              [0.0,0.0,.02]   </top>
            <radius>           1.0             </radius>
          </cylinder>
        </geom_object>
        <load_curve>
          <id>2</id>
          <time_point>
            <time> 0 </time>
            <load> 0 </load>
          </time_point>
          <time_point>
            <time> 1.0e-5 </time>
            <load> 101325.0 </load>
          </time_point>
        </load_curve>
      </pressure>
    </MPM>
  </PhysicalBC>
```

The complete input file can be found in `Vaango/StandAlone/inputs/MPM/thickCylinderMPM.ups`.



8 — Example Input Files

8.1 Hypoelastic-plastic model

An example of the portion of an input file that specifies a copper body with a hypoelastic stress update, Johnson-Cook plasticity model, Johnson-Cook Damage Model and Mie-Gruneisen Equation of State is shown below.

```
<material>

  <include href="inputs/MPM/MaterialData/MaterialConstAnnCopper.xml"/>
  <constitutive_model type="hypoelastic_plastic">
    <tolerance>5.0e-10</tolerance>
    <include href="inputs/MPM/MaterialData/IsotropicElasticAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/JohnsonCookPlasticAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/JohnsonCookDamageAnnCopper.xml"/>
    <include href="inputs/MPM/MaterialData/MieGruneisenEOSAnnCopper.xml"/>
  </constitutive_model>

  <burn type = "null" />
  <velocity_field>1</velocity_field>

  <geom_object>
    <cylinder label = "Cylinder">
      <bottom>[0.0,0.0,0.0]</bottom>
      <top>[0.0,2.54e-2,0.0]</top>
      <radius>0.762e-2</radius>
    </cylinder>
    <res>[3,3,3]</res>
    <velocity>[0.0,-208.0,0.0]</velocity>
    <temperature>294</temperature>
  </geom_object>

</material>
```

The general material constants for copper are in the file `MaterialConstAnnCopper.xml`. The contents are shown below

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <density>8930.0</density>
  <toughness>10.e6</toughness>
  <thermal_conductivity>1.0</thermal_conductivity>
```

```
    <specific_heat>383</specific_heat>
    <room_temp>294.0</room_temp>
    <melt_temp>1356.0</melt_temp>
  </Uintah_Include>
```

The elastic properties are in the file `IsotropicElasticAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <shear_modulus>45.45e9</shear_modulus>
  <bulk_modulus>136.35e9</bulk_modulus>
</Uintah_Include>
```

The constants for the Johnson-Cook plasticity model are in the file `JohnsonCookPlasticAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <plasticity_model type="johnson_cook">
    <A>89.6e6</A>
    <B>292.0e6</B>
    <C>0.025</C>
    <n>0.31</n>
    <m>1.09</m>
  </plasticity_model>
</Uintah_Include>
```

The constants for the Johnson-Cook damage model are in the file `JohnsonCookDamageAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <damage_model type="johnson_cook">
    <D1>0.54</D1>
    <D2>4.89</D2>
    <D3>-3.03</D3>
    <D4>0.014</D4>
    <D5>1.12</D5>
  </damage_model>
</Uintah_Include>
```

The constants for the Mie-Gruneisen model (as implemented in the Uintah-Vaango Computational Framework) are in the file `MieGruneisenEOSAnnCopper.xml`. The contents of this file are shown below.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_Include>
  <equation_of_state type="mie_gruneisen">
    <C_0>3940</C_0>
    <Gamma_0>2.02</Gamma_0>
    <S_alpha>1.489</S_alpha>
  </equation_of_state>
</Uintah_Include>
```

As can be seen from the input file, any other plasticity model, damage model and equation of state can be used to replace the Johnson-Cook and Mie-Gruneisen models without any extra effort (provided the models have been implemented and the data exist).

The material data can easily be taken from a material database or specified for a new material in an input file kept at a centralized location. At this stage material data for a range of materials is kept in the directory `.../Vaango/StandAlone/inputs/MPM/MaterialData`.

8.2 Elastic-plastic model

The <constitutive_model type="elastic_plastic"> model is more stable (and also more general) than the <constitutive_model type="hypoelastic_plastic"> model. A sample input file for this model is shown below.

```
<MPM>
  <do_grid_reset> false </do_grid_reset>
  <time_integrator>explicit</time_integrator>
  <boundary_traction_faces>[zminus,zplus]</boundary_traction_faces>
  <dynamic>true</dynamic>
  <solver>simple</solver>
  <convergence_criteria_disp>1.e-10</convergence_criteria_disp>
  <convergence_criteria_energy>4.e-10</convergence_criteria_energy>
  <DoImplicitHeatConduction>true</DoImplicitHeatConduction>
  <interpolator>linear</interpolator>
  <minimum_particle_mass> 1.0e-8</minimum_particle_mass>
  <maximum_particle_velocity> 1.0e8</maximum_particle_velocity>
  <artificial_damping_coeff> 0.0 </artificial_damping_coeff>
  <artificial_viscosity> true </artificial_viscosity>
  <accumulate_strain_energy> true </accumulate_strain_energy>
  <use_load_curves> false </use_load_curves>
  <turn_on_adiabatic_heating>   false    </turn_on_adiabatic_heating>
  <do_contact_friction_heating> false    </do_contact_friction_heating>
  <create_new_particles>        false    </create_new_particles>
  <erosion algorithm = "none"/>
</MPM>

<MaterialProperties>
  <MPM>
    <material name = "OFHCCu">
      <density>              8930.0 </density>
      <thermal_conductivity> 386.0  </thermal_conductivity>
      <specific_heat>        414.0  </specific_heat>
      <room_temp>            294.0  </room_temp>
      <melt_temp>            1356.0 </melt_temp>
      <constitutive_model type="elastic_plastic">
        <isothermal>                    false   </isothermal>
        <tolerance>                     1.0e-12 </tolerance>
        <do_melting>                    false   </do_melting>
        <evolve_porosity>               false   </evolve_porosity>
        <evolve_damage>                 false   </evolve_damage>
        <check_TEPLA_failure_criterion> false   </
            check_TEPLA_failure_criterion>
        <check_max_stress_failure>      false   </check_max_stress_failure>
        <initial_material_temperature>  696.0   </
            initial_material_temperature>

        <shear_modulus>           46.0e9  </shear_modulus>
        <bulk_modulus>            129.0e9 </bulk_modulus>
        <coeff_thermal_expansion> 1.76e-5 </coeff_thermal_expansion>
        <taylor_quinney_coeff>    0.9     </taylor_quinney_coeff>
        <critical_stress>         129.0e9 </critical_stress>

        <equation_of_state type = "mie_gruneisen">
          <C_0>     3940  </C_0>
          <Gamma_0> 2.02  </Gamma_0>
          <S_alpha> 1.489 </S_alpha>
        </equation_of_state>

        <plasticity_model type="mts_model">
          <sigma_a>40.0e6</sigma_a>
          <mu_0>47.7e9</mu_0>
```

```
            <D>3.0e9</D>
            <T_0>180</T_0>
            <koverbcubed>0.823e6</koverbcubed>
            <g_0i>0.0</g_0i>
            <g_0e>1.6</g_0e>
            <edot_0i>0.0</edot_0i>
            <edot_0e>1.0e7</edot_0e>
            <p_i>0.0</p_i>
            <q_i>0.0</q_i>
            <p_e>0.666667</p_e>
            <q_e>1.0</q_e>
            <sigma_i>0.0</sigma_i>
            <a_0>2390.0e6</a_0>
            <a_1>12.0e6</a_1>
            <a_2>1.696e6</a_2>
            <a_3>0.0</a_3>
            <theta_IV>0.0</theta_IV>
            <alpha>2</alpha>
            <edot_es0>1.0e7</edot_es0>
            <g_0es>0.2625</g_0es>
            <sigma_es0>770.0e6</sigma_es0>
          </plasticity_model>

          <shear_modulus_model type="mts_shear">
            <mu_0>47.7e9</mu_0>
            <D>3.0e9</D>
            <T_0>180</T_0>
          </shear_modulus_model>

          <melting_temp_model type = "constant_Tm">
          </melting_temp_model>

          <yield_condition type = "vonMises">
          </yield_condition>

          <stability_check type = "none">
          </stability_check>

          <damage_model type = "hancock_mackenzie">
            <D0> 0.0001 </D0>
            <Dc> 0.7    </Dc>
          </damage_model>

          <compute_specfic_heat> false </compute_specfic_heat>
          <specific_heat_model type="constant_Cp">
          </specific_heat_model>

        </constitutive_model>
        <geom_object>
          <box label = "box">
            <min>[0.0,    0.0,    0.0]</min>
            <max>[1.0e-2, 1.0e-2, 1.0e-2]</max>
          </box>
          <res>[1,1,1]</res>
          <velocity>[0.0, 0.0, 0.0]</velocity>
          <temperature>696</temperature>
        </geom_object>
      </material>

    </MPM>
  </MaterialProperties>
```

8.2.1 An exploding ring experiment

The follwing shows the complete input file for an expanding ring test.

```
<?xml version='1.0' encoding='ISO-8859-1' ?>
<Uintah_specification>
<!--Please use a consistent set of units, (mks, cgs,...)-->
    <!-- First crack at the tuna can problem -->

   <Meta>
       <title>Pressurization of a container via burning w/o fracture</title>
   </Meta>&gt;
   <SimulationComponent>
     <type> mpmice </type>
   </SimulationComponent>
    <!--______________________________________________________________________-->
    <!--   T  I  M  E     V  A  R  I  A  B  L  E  S                            -->
    <!--______________________________________________________________________-->
   <Time>
       <max_Timesteps>   99999          </max_Timesteps>>
       <maxTime>             2.00e-2    </maxTime>
       <initTime>            0.0        </initTime>
       <delt_min>            1.0e-12    </delt_min>
       <delt_max>            1.0        </delt_max>
       <delt_init>           2.1e-8     </delt_init>
       <timestep_multiplier> 0.5        </timestep_multiplier>
   </Time>
    <!--______________________________________________________________________-->
    <!--   G  R  I  D     V  A  R  I  A  B  L  E  S                            -->
    <!--______________________________________________________________________-->
    <Grid>
    <BoundaryConditions>
      <Face side = "x-">
        <BCType id = "all" label = "Symmetric" var = "symmetry">
        </BCType>
      </Face>
      <Face side = "x+">
        <BCType id = "0" label = "Pressure" var = "Neumann">
                            <value>  0.0 </value>
        </BCType>
        <BCType id = "all" label = "Velocity" var = "Dirichlet">
                            <value> [0.,0.,0.] </value>
        </BCType>
        <BCType id = "all" label = "Temperature" var = "Neumann">
                            <value> 0.0  </value>
        </BCType>
        <BCType id = "all" label = "Density" var = "Neumann">
                            <value> 0.0  </value>
        </BCType>
      </Face>
      <Face side = "y-">
        <BCType id = "all" label = "Symmetric" var = "symmetry">
        </BCType>
      </Face>
      <Face side = "y+">
        <BCType id = "0" label = "Pressure" var = "Neumann">
                            <value> 0.0   </value>
        </BCType>
        <BCType id = "all" label = "Velocity" var = "Dirichlet">
                            <value> [0.,0.,0.] </value>
        </BCType>
        <BCType id = "all" label = "Temperature" var = "Neumann">
                            <value> 0.0  </value>
```

```
      </BCType>
      <BCType id = "all" label = "Density" var = "Neumann">
                          <value> 0.0  </value>
      </BCType>
    </Face>
    <Face side = "z-">
      <BCType id = "all" label = "Symmetric" var = "symmetry">
      </BCType>
    </Face>
    <Face side = "z+">
      <BCType id = "all" label = "Symmetric" var = "symmetry">
      </BCType>
    </Face>
  </BoundaryConditions>
     <Level>
         <Box label = "1">
            <lower>        [ -0.08636, -0.08636, -0.0016933] </lower>
            <upper>        [ 0.08636, 0.08636, 0.0016933]    </upper>
            <extraCells>   [1,1,1]    </extraCells>
            <patches>      [2,2,1]    </patches>
            <resolution>   [102, 102, 1]                 </resolution>
         </Box>
     </Level>
  </Grid>

  <!--__________________________________________________________________--> 
  <!--   O U P U T    V A R I A B L E S                                    --> 
  <!--__________________________________________________________________--> 
<DataArchiver>
    <filebase>explodeRFull.uda</filebase>
    <outputTimestepInterval> 20 </outputTimestepInterval>
    <save label = "rho_CC"/>
    <save label = "press_CC"/>
    <save label = "temp_CC"/>
    <save label = "vol_frac_CC"/>
    <save label = "vel_CC"/>
    <save label = "g.mass"/>
    <save label = "p.x"/>
    <save label = "p.mass"/>
    <save label = "p.temperature"/>
    <save label = "p.porosity"/>
    <save label = "p.particleID"/>
    <save label = "p.velocity"/>
    <save label = "p.stress"/>
    <save label = "p.damage" material = "0"/>
    <save label = "p.plasticStrain" material = "0"/>
    <save label = "p.strainRate" material = "0"/>
    <save label = "g.stressFS"/>
    <save label = "delP_Dilatate"/>
    <save label = "delP_MassX"/>
    <save label = "p.localized"/>
    <checkpoint cycle = "2" timestepInterval = "20"/>
</DataArchiver>

<Debug>
</Debug>
  <!--__________________________________________________________________--> 
  <!--    I C E    P A R A M E T E R S                                   --> 
  <!--__________________________________________________________________--> 
  <CFD>
     <cfl>0.5</cfl>
     <CanAddICEMaterial>true</CanAddICEMaterial>
     <ICE>
```

```
    <advection type = "SecondOrder"/>
    <ClampSpecificVolume>true</ClampSpecificVolume>
  </ICE>
</CFD>

<!--__________________________________________________________________-->
<!--     P H Y S I C A L     C O N S T A N T S                        -->
<!--__________________________________________________________________-->
<PhysicalConstants>
   <gravity>            [0,0,0]   </gravity>
   <reference_pressure> 101325.0  </reference_pressure>
</PhysicalConstants>

<MPM>
  <time_integrator>                explicit   </time_integrator>
  <nodes8or27>                     27         </nodes8or27>
  <minimum_particle_mass>          3.e-12     </minimum_particle_mass>
  <maximum_particle_velocity>      1.e3       </maximum_particle_velocity>
  <artificial_damping_coeff>       0.0        </artificial_damping_coeff>
  <artificial_viscosity>           true       </artificial_viscosity>
  <artificial_viscosity_coeff1>    0.07       </artificial_viscosity_coeff1
     >
  <artificial_viscosity_coeff2>    1.6        </artificial_viscosity_coeff2
     >
  <turn_on_adiabatic_heating>      false      </turn_on_adiabatic_heating>
  <accumulate_strain_energy>       false      </accumulate_strain_energy>
  <use_load_curves>                false      </use_load_curves>
  <create_new_particles>           false      </create_new_particles>
  <manual_new_material>            false      </manual_new_material>
  <DoThermalExpansion>             false      </DoThermalExpansion>
  <testForNegTemps_mpm>            false      </testForNegTemps_mpm>
  <erosion algorithm = "ZeroStress"/>
</MPM>

<!--__________________________________________________________________-->
<!--    MATERIAL PROPERTIES INITIAL CONDITIONS                        -->
<!--__________________________________________________________________-->
<MaterialProperties>
   <MPM>
     <material name = "Steel Ring">
       <include href="inputs/MPM/MaterialData/MatConst4340St.xml"/>
       <constitutive_model type="elastic_plastic">
         <isothermal>                    false </isothermal>
         <tolerance>                  1.0e-10  </tolerance>
         <evolve_porosity>               true  </evolve_porosity>
         <evolve_damage>                 true  </evolve_damage>
         <compute_specific_heat>         true  </compute_specific_heat>
         <do_melting>                    true  </do_melting>
         <useModifiedEOS>                true  </useModifiedEOS>
         <check_TEPLA_failure_criterion> true  </
             check_TEPLA_failure_criterion>
         <initial_material_temperature>  600.0 </
             initial_material_temperature>
         <taylor_quinney_coeff>          0.9   </taylor_quinney_coeff>
         <check_max_stress_failure>      false </check_max_stress_failure>
         <critical_stress>              12.0e9 </critical_stress>

         <!-- Warning: you must copy link this input file into your -->
         <!-- sus directory or these paths won't work.              -->

         <include href="inputs/MPM/MaterialData/IsoElastic4340St.xml"/>
         <include href="inputs/MPM/MaterialData/MieGrunEOS4340St.xml"/>
         <include href="inputs/MPM/MaterialData/ConstantShear.xml"/>
```

```
      <include href="inputs/MPM/MaterialData/ConstantTm.xml"/>
      <include href="inputs/MPM/MaterialData/JCPlastic4340St.xml"/>
      <include href="inputs/MPM/MaterialData/VonMisesYield.xml"/>
      <include href="inputs/MPM/MaterialData/DruckerBeckerStabilityCheck
          .xml"/>
      <include href="inputs/MPM/MaterialData/JCDamage4340St.xml"/>
      <specific_heat_model type="steel_Cp"> </specific_heat_model>

      <initial_mean_porosity>          0.005 </initial_mean_porosity>
      <initial_std_porosity>           0.001 </initial_std_porosity>
      <critical_porosity>              0.3   </critical_porosity>
      <frac_nucleation>                0.1   </frac_nucleation>
      <meanstrain_nucleation>          0.3   </meanstrain_nucleation>
      <stddevstrain_nucleation>        0.1   </stddevstrain_nucleation>
      <initial_porosity_distrib>       gauss </initial_porosity_distrib>

      <initial_mean_scalar_damage>     0.005  </
          initial_mean_scalar_damage>
      <initial_std_scalar_damage>      0.001 </initial_std_scalar_damage>
      <critical_scalar_damage>         1.0   </critical_scalar_damage>
      <initial_scalar_damage_distrib> gauss </
          initial_scalar_damage_distrib>
    </constitutive_model>

        <geom_object>
           <difference>
            <cylinder label = "outer cylinder">
              <bottom>           [0.0,0.0,-.05715]   </bottom>
              <top>              [0.0,0.0, .05715]   </top>
              <radius>           0.05715            </radius>
           </cylinder>
           <cylinder label = "inner cylinder">
              <bottom>           [0.0,0.0,-.0508]    </bottom>
              <top>              [0.0,0.0, .0508]    </top>
              <radius>           0.0508              </radius>
           </cylinder>
           </difference>
          <res>                 [2,2,2]          </res>
          <velocity>            [0.0,0.0,0.0]    </velocity>
          <temperature>         600              </temperature>
        </geom_object>
</material>
<material name = "reactant">
    <include href="inputs/MPM/MaterialData/MatConstPBX9501.xml"/>
    <constitutive_model type = "visco_scram">
      <include href="inputs/MPM/MaterialData/ViscoSCRAMPBX9501.xml"/>
      <include href="inputs/MPM/MaterialData/TimeTempPBX9501.xml"/>
      <randomize_parameters>          false </randomize_parameters>
      <use_time_temperature_equation> true  </
          use_time_temperature_equation>
      <useObjectiveRate>              true  </useObjectiveRate>
      <useModifiedEOS>                true  </useModifiedEOS>
    </constitutive_model>
       <geom_object>
          <difference>
            <cylinder label = "inner cylinder"> </cylinder>
            <cylinder label = "inner hole">
              <bottom>           [0.0,0.0,-.0508]    </bottom>
              <top>              [0.0,0.0, .0508]    </top>
              <radius>           0.01               </radius>
            </cylinder>
          </difference>
          <res>                 [2,2,2]          </res>
```

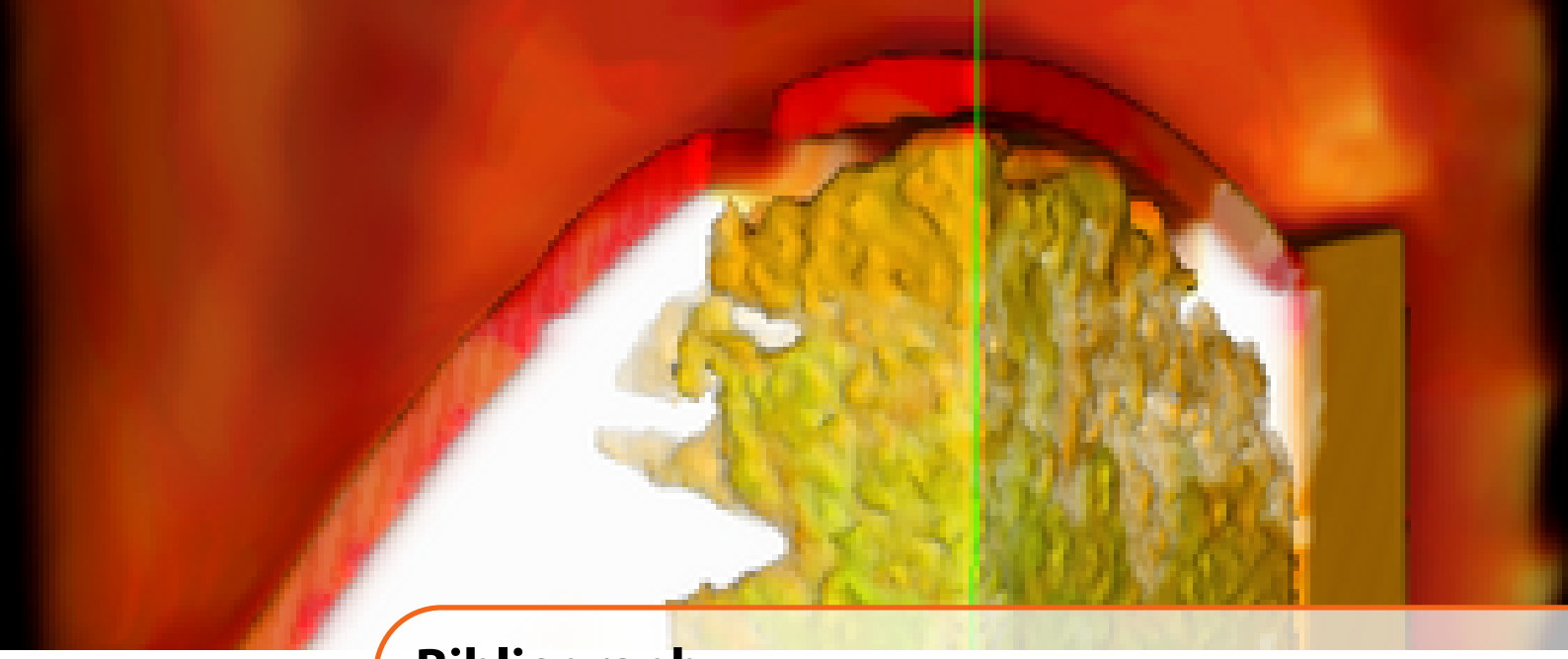
```
            <velocity>            [0.0,0.0,0.0]   </velocity>
            <temperature>         440.0           </temperature>
          </geom_object>
      </material>

        <contact>
          <type>approach</type>
          <materials>              [0,1]         </materials>
          <mu> 0.0 </mu>
        </contact>
        <thermal_contact>
        </thermal_contact>
    </MPM>

     <ICE>
       <material>
         <EOS type = "ideal_gas">
         </EOS>
         <dynamic_viscosity>          0.0            </dynamic_viscosity>
         <thermal_conductivity>       0.0            </thermal_conductivity>
         <specific_heat>              716.0          </specific_heat>
         <gamma>                      1.4            </gamma>
         <geom_object>
           <difference>
                <box>
                  <min>           [-0.254,-0.254,-0.254] </min>
                  <max>           [ 0.254, 0.254, 0.254] </max>
                </box>
               <cylinder label = "outer cylinder"> </cylinder>
             </difference>
           <cylinder label="inner hole"> </cylinder>
           <res>                        [2,2,2]        </res>
           <velocity>           [0.0,0.0,0.0]       </velocity>
           <!--
           <temperature>        300.0               </temperature>
           <density>    1.1792946927374306000e+00   </density>
           -->
           <temperature>        400.0               </temperature>
           <density>            0.884471019553073   </density>
           <pressure>           101325.0             </pressure>
         </geom_object>
       </material>
    </ICE>

    <exchange_properties>
       <exchange_coefficients>
            <momentum>  [0, 1e15, 1e15]     </momentum>
            <heat>      [0, 1e10, 1e10]     </heat>
      </exchange_coefficients>
    </exchange_properties>
  </MaterialProperties>

  <AddMaterialProperties>
    <ICE>
       <material name = "product">
         <EOS type = "ideal_gas">
         </EOS>
         <dynamic_viscosity>          0.0            </dynamic_viscosity>
         <thermal_conductivity>       0.0            </thermal_conductivity>
         <specific_heat>              716.0          </specific_heat>
         <gamma>                      1.4            </gamma>
         <geom_object>
                <box>
```

```
                    <min>           [ 1.0, 1.0, 1.0] </min>
                    <max>           [ 2.0, 2.0, 2.0] </max>
                  </box>
              <res>                       [2,2,2]        </res>
              <velocity>             [0.0,0.0,0.0]       </velocity>
              <temperature>          300.0               </temperature>
              <density>     1.17929469273743060000e+00   </density>
              <pressure>             101325.0             </pressure>
            </geom_object>
          </material>
      </ICE>

      <exchange_properties>
         <exchange_coefficients>
              <momentum>  [0, 1e15, 1e15, 1e15, 1e15, 1e15]     </momentum>
              <heat>      [0, 1e10, 1e10, 1e10, 1e10, 1e10]     </heat>
              <!--
              <heat>      [0, 1, 1, 1, 1, 1]     </heat>
              -->
        </exchange_coefficients>
      </exchange_properties>
    </AddMaterialProperties>


    <Models>
      <Model type="Simple_Burn">
        <Active>       false        </Active>
        <fromMaterial> reactant     </fromMaterial>
        <toMaterial>   product      </toMaterial>
        <ThresholdTemp>       450.0 </ThresholdTemp>
        <ThresholdPressure> 50000.0 </ThresholdPressure>
        <Enthalpy>        2000000.0 </Enthalpy>
        <BurnCoeff>            75.3 </BurnCoeff>
        <refPressure>      101325.0 </refPressure>
      </Model>
    </Models>


</Uintah_specification>
```

The PBS script used to run this test is

```
#
# ASK PBS TO SEND YOU AN EMAIL ON CERTAIN EVENTS: (a)bort (b)egin (e)nd (n)ever
#
# (User May Change)

#PBS -m abe

#
# SET THE NAME OF THE JOB:
#
# (User May Change)

#PBS -N ExplodeRing

#
# SET THE QUEUE IN WHICH TO RUN THE JOB.
#      (Note, there is currently only one queue, so you should never change
    this field.)

#PBS -q defaultq
```

```
#
# SET THE RESOURCES (# NODES, TIME) REQESTED FROM THE BATCH SCHEDULER:
#   - select: <# nodes>,ncpus=2,walltime=<time>
#     - walltime: walltime before PBS kills our job.
#                 [[hours:]minutes:]seconds[.milliseconds]
#                 Examples:
#                   walltime=60      (60 seconds)
#                   walltime=10:00   (10 minutes)
#                   walltime=5:00:00 (5 hours)
#
# (User May Change)

#PBS -l select=2:ncpus=2,walltime=24:00

#
# START UP LAM

cd $PBS_O_WORKDIR
lamboot

# [place your command here] >& ${PBS_O_WORKDIR}/output.${PBS_JOBID}
mpirun -np 4 ../sus_opt explodeRFull.ups >& output.${PBS_JOBID}

#
# REMEMBER, IF YOU ARE RUNNING TWO SERIAL JOBS, YOU NEED A:
# wait

#
# STOP LAM

lamhalt -v
exit
```



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