Appendix A

Algorithm of SNAC

A.1 Governing equations

The software package SNAC solves the momentum and the heat energy balance equations in the following differential form:

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i = \rho \frac{Dv_i}{Dt}, \tag{A.1}$$

$$\frac{\partial q_i}{\partial x_i} + r = \rho C_p \frac{DT}{Dt}. \tag{A.2}$$

In the momentum balance equation, ρ is the mass density, v_i is velocity, σ_{ij} is the Cauchy stress tensor, and g_i is the gravitational acceleration. T is temperature, C_p is the specific heat at constant pressure, q_i is the heat flux vector, and r is the volumetric heat source. D/Dt represents the material time derivative. In this study, no heat sources are considered, including shear heating. Viscosity is temperature- and/or stress-dependent. The elastic component of stress has an extra contribution from thermal stress.

A.2 Spatial discretization

A 3-D domain is discretized into hexahedral elements, each of which is filled with two sets of 5 tetrahedra (Fig. A.1a). In this mesh hierarchy, called the mixed discretization (Marti and Cundall, 1982), hexahedral elements are used only as an averaging

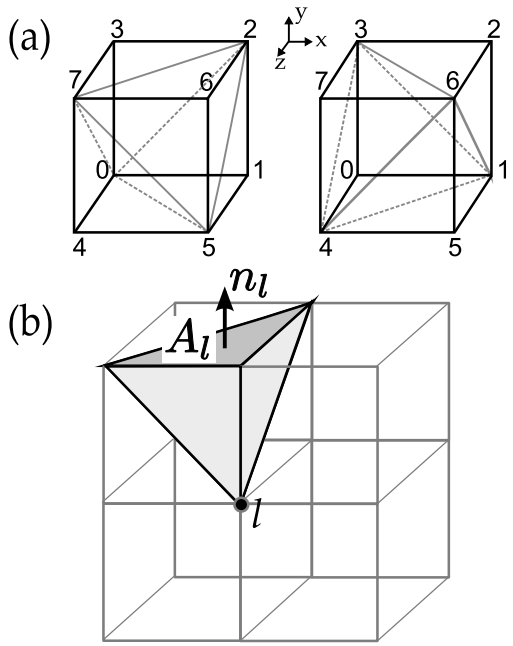

Figure A.1: (a) Two configurations of five tetrahedra in a hexahedral element used in the mixed discretization. Numbers next to apexes indicate the local node numbering. (b) Conventions for the notation. A_l and n_l denote the face and the unit normal vector, respectively, associated with a local node l.

unit for volumetric strain. The averaging is enforced at all times, for incompressible viscoelastic or plastic constitutive laws. The use of two equivalent sets of tetrahedra is required to ensure a symmetric response. For a given loading, responses of one set of tetrahedra can be different from those of the other set because of the differently orientated faces of tetrahedra in each set (e.g., Zienkiewicz et al., 1995).

The approximation of partial derivatives with respect to spatial variables follows the integral definitions (e.g., Wilkins, 1964):

$$\int_{\Omega} f_{,i} dV = \int_{\partial\Omega} f n_i d\Gamma, \tag{A.3}$$

where Ω represent a tetrahedron as an integration domain, $\partial\Omega$ is the boundary surfaces of the tetrahedron, $f_{,i}$ is the partial derivative of a variable f with respect to i-th spatial coordinate, n_i is the i-th component of the unit normal vector of the surface.

If the partial derivative is constant within a tetrahedron, it is evaluated as

$$f_{,i} = \frac{1}{V}\int_{\partial\Omega} f n_i d\Gamma, \tag{A.4}$$

where V is the volume of the tetrahedron. By further substituting an algebraic expression for the surface integral, reordering terms, and using $\int_{\partial\Omega} n_i d\Gamma = 0$ (when $f = 1$ in (A.4)),

$$\begin{aligned} f_{,i} &= \frac{1}{V}\sum_{l=1}^{4} \bar{f}^l n_i^l A^l = \frac{1}{V}\sum_{l=1}^{4}\frac{1}{3}\sum_{m=1,\neq l}^{4} f^m n_i^l A^l \\ &= \frac{1}{3V}\sum_{m=1}^{4} f^m \sum_{l=1,\neq m}^{4} n_i^l A^l \\ &= -\frac{1}{3V}\sum_{m=1}^{4} f^m n_i^m A^m, \end{aligned} \tag{A.5}$$

where l is the local node index varying from 1 to 4, A^l and n^l are the area and the unit normal vector of the triangular surface not having the node l as one of its apexes (Fig. A.1b). Hereafter, we call such a face a *corresponding* face to node l. $\bar{f}^l$ is the averaged f on the surface l.

A.3 Nodal assemblage

We can convert the differential equation for momentum balance (A.1) (the following description is applied to the heat equation in the same fashion) to a principle of minimum work rate as in the standard finite element formulation:

$$\int_\Omega \delta v_i \rho \frac{Dv_i}{Dt} dV = \int_\Omega \delta v_i \rho g_i dV + \int_\Omega \delta\xi_{ij}\sigma_{ij} dV, \tag{A.6}$$

where ξ_{ij} are components of the strain rate tensor, δv_i and $\delta\xi_{ij}$ represent variations of velocity and strain rate, and Ω here corresponds to the whole domain. The local contribution to nodes corresponding to each term can be computed by following the standard finite element procedure for linear tetrahedral elements. However, our

method does not need to construct coefficient matrices such as mass and stiffness matrices since it adopts an explicit time discretization. The resultant momentum equation is

$$M^n \frac{Dv_i^n}{Dt} = \frac{1}{3} T_i^{[n]} + \frac{1}{4} \rho^{[n]} g_i V^{[n]}, \tag{A.7}$$

where the superscript n represents values evaluated at the global node n, the superscript $[n]$ means the sum of contributions from all the tetrahedra having the global node n as an apex, T_i is the traction that is defined as $\sigma_{ij} n_j$ and evaluated on a face of one of the contributing tetrahedra. The nodal mass M^n is not the actual inertial mass but an adjusted one to satisfy a local stability criterion discussed in the section A.5. The correspondence between an apex and a face for the traction calculation is determined as in the derivation of the expression, (A.5). Note that the factor of 1/3 in the traction term is inherited from (A.5) and the factor of 1/4 in the body force term implies that the nodal contribution takes one quarter of a tetrahedrons volume-dependent quantity.

While looping over the entire set of nodes, mass and nodal forces are assembled by adding up the contributions from boundary conditions and all the tetrahedra sharing that node as one of their apexes. The structured mesh of SNAC renders the assemblage step conveniently static. The acquired net force (or heat flux) at each node is used to update velocities and node coordinates (or temperature).

A.4 Damping and explicit time marching

We seek static or quasi-static solutions through a dynamic relaxation method. Instead of adding a usual velocity-dependent friction term, we adopt a local non-viscous damping scheme (Cundall, 1987):

$$F_i^{damped} = F_i - \alpha \ \mathrm{sgn}(v_i) |F_i|, \tag{A.8}$$

where F_i is the i-th component of the residual force vector, α is a positive coefficient less than 1, $\mathrm{sgn}(v_i)$ returns the sign of the i-th component of velocity, v_i. Once net

forces are assembled and damped, velocity at that node is updated using a forward Euler method:

$$v(t + \frac{\Delta t}{2}) = v(t - \frac{\Delta t}{2}) + \Delta t \frac{F_i^{damped}}{M} \tag{A.9}$$

$$x(t + \Delta t) = x(t) + \Delta t v(t + \frac{\Delta t}{2}). \tag{A.10}$$

Damping is irrelevant to the update of temperature field, but the same forward Euler method is used.

A.5 Mass scaling for numerical stability

The conventional CourantFriedrichsLewy (CFL) condition imposes a stringent upper limit for the time step size such that dynamic relaxation takes long time to get quasi-static solution over a geological time scale. To overcome this limit, a mass scaling technique is applied. This technique adjusts each nodal mass such that the stability condition for a user-specified time step can be locally satisfied. The stability condition to be satisfied, however, is not the same as in the CFL condition, i.e., $\Delta t \leq (l_{min}/v_p)$, where Δt is the time step, l_{min} is the minimum element size, and v_p is the P wave velocity. Instead, through an analogy of continuum to an infinite mass-spring system, we use a criterion that does not explicitly include length scale and P wave velocity (see Ch. 9 in Bathe, 1996):

$$\Delta t \leq \frac{T}{\pi}, \tag{A.11}$$

where T is the period of system, $2\pi(m/k)^{1/2}$, m is a point mass, and k is the stiffness of the spring attached to the point mass. Now, reducing the infinite series of mass and springs in one dimension to a single mass-spring system, the stiffness of that single system becomes $4k$, leading to an expression for the mass scaling:

$$m \geq k(\Delta t)^2. \tag{A.12}$$

For a given size of Δt, the nodal mass is adjusted according to (A.12) to automatically satisfy the stability critetion, (A.11). The value of k is computed by equating internal

force contribution at a node with ku_i:

$$\begin{aligned} \frac{1}{3}T_i &= -ku_i \Rightarrow \\ \frac{1}{3}(\lambda + 2\mu)(\dot{\epsilon}_{ii}dt)n_i S &= -k(v_i dt) \text{ (no sum)}, \end{aligned} \tag{A.13}$$

where only the volumetric contribution from internal forces is taken into account. By substituting the approximation for the partial derivative (A.5) into the above equation and dividing both sides by $v_i dt$, we obtain

$$k_i^l = \frac{1}{9V}(\lambda + 2\mu)(n_i^l S^l)^2, \tag{A.14}$$

where l is the local index for apexes of a tetrahedron and the surface-related quantities are computed on the corresponding face of the tetrahedron. Finally, a tetrahedron's contribution to the scaled mass is given as

$$m^l = \frac{\lambda + 2\mu}{9V} \max[(n_i^l S^l)^2, i = 1, \ldots, 3]. \tag{A.15}$$

As in the standard FEM, appropriate mappings between local and global indices are required.

A.6 Constitutive update

SNAC uses a general elasto-visco-plastic rheological model to update the Cauchy stress tensor (e.g., Albert et al., 2000). First, the initial guess of stress is acquired by the Maxwell viscoelastic constitutive law (Poliakov et al., 1993). If this initial guess exceeds a given yield stress, it is projected onto the yield surface using a return mapping method (Simo and Hughes, 2004); otherwise, the viscoelastic stress update is retained. This elasto-visco-plastic model can deal with various constitutive laws that are typically used for the Earth's crustal and mantle material as its limiting cases. For example, elastic, viscoelastic and elastoplastic material are realized in the following cases:

1. Elastic material corresponds to the limit of infinite viscosity and yield stress.

2. Viscoelastic material corresponds to the limit of infinite yield strength.

3. Elasoplastic material corresponds to the inifinte viscosity.

Using the viscoplastic rheology is physically more realistic than using one of the limiting cases listed above since all materials have dissipative mechanisms and hence viscosity. This viscosity also provides a length scale for the problem of localization, which in turn enables physically meaningful mesh independent solution when the mesh size is smaller than this length scale.

Since the nodal variables are velocities and whose spatial gradients are deformation rates, we formulate the constitutive update in terms of strain rate. The objective stress rate of choice is the Jaumann or the corotational stress rate ($\Delta\sigma^{\Delta J}$) (Rudnicki and Rice, 1975)

$$\Delta\sigma^{\Delta J} = \frac{\partial(\Delta\sigma)}{\partial t} - W \cdot \Delta\sigma - \Delta\sigma \cdot W^T, \tag{A.16}$$

where $W_{ij} = (1/2)(\partial v_i/\partial x_j$-$\partial v_j/\partial x_i)$ are the components of spin tensor and $\Delta\sigma$ is the increment of stress tensor. Correction to the stresses due to rotation can be given as

$$\sigma^{t+\Delta t} = \sigma^t + \Delta\sigma^{\Delta J}.\Delta t \tag{A.17}$$

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