Chapter 3

Numerical methods

The equations which describe the processes to be modelled (see chapter 2) can only be solved analytically in very simplified cases, and therefore discretization of the equations is required to solve them numerically on computers. Two different methods are used to evaluate the evolution of the different quantities. For the evolution of the temperature and velocity fields, a finite element method (Cuvelier et al., 1986) is applied, based on the SEPRAN package (Segal and Praagman, 2002). The discretization of the finite element equations will be described in more detail in sections 3.1 and 3.2. For the evolution of composition and trace element concentrations, a particle tracer method is used (Hockney and Eastwood, 1988), which will be described in section 3.4.

3.1 Discretization of the energy equation

Discretization of the energy equation (2.4), described in appendix B, results in the following system of equations:

$$M\dot{\vec{T}} + A\vec{T} = \vec{R} \tag{3.1}$$

In this expression, $\vec{T}$ is a vector containing the temperature values at the nodal points of the finite element mesh. M is the mass matrix, in which the heat capacity and part of the effect of adiabatic compression and latent heat consumption and release is included. A is the stiffness matrix, combining the effects of advection, diffusion, adiabatic compression and latent heat. The right hand side vector $\vec{R}$ includes internal heating and heating by viscous dissipation, as well as terms from latent heat effects and adiabatic compression. This set of equations is constructed for a mesh of triangular elements, which are in fact sub-elements of the quadratic triangular elements used for the Stokes equation (see section 3.2) using linear base functions (Van den Berg et al., 1993). In order to stabilize the solution of the discrete heat equation (3.1) in regions where advection dominates diffusion, the classical Streamline Upwind Petrov Galerkin method (see Segal, 1993) is applied.

3.2 Discretization of the Stokes equation

The discretization of the Stokes equation (2.6) results in a system of linear equations:

$$S\vec{U} + L^T\vec{p} = \vec{F} \tag{3.2}$$

where $\vec{U}$ and $\vec{p}$ are vectors of the velocity components in the nodal points and the dynamical pressure in the barycenters of the elements, respectively. This equation is solved using the penalty function method (Cuvelier et al., 1986), using a small but finite perturbation to the continuity equation, which in discretized form becomes (Cuvelier et al., 1986):

$$D\vec{p} = \frac{1}{\varepsilon}L\vec{U} \tag{3.3}$$

with D the pressure mass matrix and ε the penalty function parameter (10^{-6}).

Equation (3.3) is used to eliminate the pressure from (3.2). The resulting discretized Stokes equation is solved on a mesh consisting of triangular quadratic Crouzeix-Raviart elements (Segal and Praagman, 2002).

3.3 Time integration

The combination of energy and Stokes equations is integrated in time using a predictor-corrector time stepping scheme (Van den Berg et al., 1993). In the predictor step, the energy equation is integrated using an Euler implicit scheme:

$$M[\vec{U}^{(n)}]\Delta t^{-1}[\vec{T}^{*(n+1)} - \vec{T}^{(n)}] + A[\vec{U}^{(n)}]\vec{T}^{*(n+1)} = \vec{R}^{(n+1)} \tag{3.4}$$

Using the predicted temperature vector $\vec{T}^{*(n+1)}$, a solution for the Stokes equation for the predictor step $\vec{U}^{*(n+1)}$ is computed:

$$S\vec{U}^{*(n+1)} = \vec{F}[\vec{T}^{*(n+1)}] \tag{3.5}$$

In the corrector step, both the old solution for t^n and the predicted solution for $t^{(n+1)}$ are used in a Crank-Nicolson integration step:

$$M[\vec{U}^{*(n+1)}]\Delta t^{-1}[\vec{T}^{(n+1)} - \vec{T}^{(n)}] + \frac{1}{2}A[\vec{U}^{*(n+1)}]\vec{T}^{(n+1)} + \frac{1}{2}A[\vec{U}^{(n)}]\vec{T}^{(n)} =$$

$$\frac{1}{2}[\vec{R}^{(n+1)} + \vec{R}^{(n)}] \tag{3.6}$$

followed by a corrector step for the Stokes equation:

$$S\vec{U}^{(n+1)} = \vec{F}[\vec{T}^{(n+1)}] \tag{3.7}$$

The non-linearity in the Stokes equation, introduced by the strain rate dependence of the dislocation creep and yield components of the viscosity (see section 2.3), resulting in

the stiffness matrix being dependent on the velocity solution, is solved by Picard iteration until the difference between successive solutions drops below a prescribed threshold of 10^{-2} in a suitable norm (Van den Berg et al., 1993).

The time step Δt is determined by taking the minimum of time steps prescribed by two criteria. The first is the Courant-Friedrichs-Levy criterion (see Van den Berg et al., 1993):

$$\Delta t_{cfl} = \min \left[\frac{h_x}{u_x}, \frac{h_y}{u_y} \right] \tag{3.8}$$

The time step Δt_{cfl} resulting from this criterion is multiplied by a factor f_{cfl}, which has a value of 0.01-0.5. The second criterion for the integration time step is that the normalized difference between the supremum norms of the old and the predicted temperature vector must not exceed a prescribed factor ϵ_T, which has a value of 0.02.

3.4 Particle tracers

The evolution of quantities like composition and trace element concentration is evaluated in a Lagrangian framework, to prevent numerical problems associated with non-physical oscillations and artificial diffusion of these quantities which is inherent to using an advection-diffusion equation in an Eulerian framework (Vreugdenhil, 1993; Segal, 1993). A particle tracer method is applied (Hockney and Eastwood, 1988). A set of particle tracers (generally 300,000-400,000) is homogeneously but randomly distributed over the computational domain. Associated with each tracer, values are defined for different fields like composition and trace element concentration, but also for other quantities used in the computations (effective thermal expansivity α and specific heat c_p, buoyancy, internal heating rate).

All these quantities are in some way a function of quantities which are defined on the particle tracers. The latent heat effect of partial melting, evaluated on the particle tracers, is included in the effective thermal expansivity and effective specific heat (see appendix B). The compositional part of the buoyancy depends on the tracer defined composition, and the basalt to eclogite phase transition, also defined on the tracers, has a buoyancy effect as well. The internal heating rate depends on the trace element concentration, which is also defined and evolved on the particle tracers. The quantities which are a function of the tracer fields are computed on the tracers as well, so that interpolation of the resulting fields from the tracers to the finite elements is postponed to the latest. This results in a higher accuracy being maintained because of the higher spatial resolution of the particle tracer field relative to the finite elements compared to the case where these quantities are computed on the finite elements after interpolation of the required quantities from the tracers to the mesh. This is specifically important for resolving the buoyancy effect of thin strands of material well below the scale of the finite elements, and for accurately accounting for the consumption of latent heat in the vicinity of the solidus.

The values of these quantities are adjusted each time step according to the appropriate equations, see chapter 2, due to partial melting.

The advective part of the change in the Eulerian fields is dealt with by advection of the particle tracers with the convective flow field. A fourth order Runge-Kutta scheme is applied. Interpolation of tracer particle field values to the finite element mesh is done using the Particle-in-Cell (PIC) method (Hockney and Eastwood, 1988). Tracer values are first interpolated to the nodal points of a regular grid, called the helpcell mesh. Helpcell nodal point values are then interpolated to the finite element Gauss point on which the field value is required using a bilinear interpolation from the grid points of the helpcell containing the evaluation point.

3.5 Crustal growth

The helpcell mesh is also used in the computation of melt segregation and production of crust through an inflow boundary condition, see section 2.7. The degree of depletion increment is integrated over columns centered on the helpcell mesh nodal points. For each column, the amount of melt produced is calculated (separately for melting peridotite, which forms basalt, and melting basalt/eclogite, which may form a felsic melt) and, using the time step Δt, transformed into an inflow velocity which is prescribed on the top helpcell nodal point on which the column is centered, see Figure 2.2. In the same manner, the concentration of trace elements in the inflowing crust is calculated, separately for basaltic and felsic material. The inflow velocity on the top boundary which is calculated in this way on the helpcell nodal points is interpolated to the finite element mesh nodal points on the top boundary using quadratic interpolation. When inflow of both felsic and basaltic material is prescribed, inflowing tracers are randomly assigned either a felsic or a basaltic composition, such that the ratio of the two types of inflowing tracers represents the ratio of inflow velocities for the two species.