A community benchmark for subduction zone modeling

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A B S T R A C T

We have developed a suite of benchmarks to facilitate the comparison of numerical models for the dynamics and thermal structure of subduction zones. The benchmark cases are based on a thermodynamical approach in which the slab is prescribed kinematically and the wedge flow is computed dynamically. We propose various cases to investigate the influence of boundary conditions and rheology on wedge flow and resulting thermal structure. A comparison between the codes suggest that accurate modeling of the thermal field requires a good implementation of the velocity discontinuity along the seismogenic zone and high resolution in the thermal boundary layers. A minor modification to the boundary conditions of the wedge flow is also necessary to avoid a pressure singularity that exists in analytical solutions of the cornerflow model.

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1. Introduction

Subduction zones form the location of explosive arc volcanism, large underthrusting earthquakes and deep earthquakes in Benioff zones. The generation of arc volcanism is generally attributed to the release of volatiles from the subducting plate into the hot overlying wedge and subsequent lowering of the peridotite solidus. Direct melting of subducted sediments and pressure-release melting in the wedge can also assist in the formation of magmas. Intermediate-depth seismicity within the slab is generally attributed to dehydration-embrittlement due to the release of water once the subducted oceanic crust and mantle go through key phase changes (Kirby et al., 1996). The up- and down-dip limits of the megathrust seismogenic zone are at least partially controlled by the thermal structure of subduction zones (Hyndman and Wang, 1995). Temperature and pressure form therefore fundamental controls on the processes leading to volcanism and intermediate-depth seismicity (Kerrick and Connolly, 2001). Forward models that use information about the subduction zone geometry, convergence rate, and age of the incoming plate can be useful in constraining the temperature distribution and allow for quantitative tests of hypotheses about the dynamics and structure of subduction zones. It is generally understood that viscous coupling between the subducting slab and overriding mantle causes a downward flow in the wedge which leads to a reduced pressure in the tip of the wedge. This in turn induces flow of the upper portions of the wedge (Fig. 1a). This cornerflow in the wedge advects hot mantle into the region above the slab and below the overriding plate and therefore creates the environment for the ‘subduction factory’. Many thermal subduction zone models, past and present, are based on this cornerflow scenario, although different approaches are used to approximate the flow in the wedge. Semi-analytical model approaches include those that couple separate parts of the subduction zone that can be described analytically (Davies, 1999; England and Wilkins, 2004) or use a simplified parameterization of the thermal effects of the wedge with a finite-difference scheme for the slab (Minear and Toksoz, 1970). In some numerical models for thermal structure an analytical cornerflow model for isoviscous
rheology (Batchelor, 1967; McKenzie, 1969) was used to prescribe the flow in the wedge (e.g. Peacock and Wang, 2001). More recently it has become common to determine the flow in the wedge self-consistently by solving the Stokes equations for viscous flow (e.g. Furukawa, 1993; Van Keken et al., 2002) or to use fully dynamic models of subduction zones (e.g. Billen and Hirth, 2007).

While fully dynamic models are needed to develop an understanding of the dynamics of subduction zones and the self-consistent generation of plate tectonics in mantle convection (Gurnis and Hager, 1988; King and Hager, 1994; King and Ita, 1995; Kincaid and Sacks, 1997; Chen and King, 1998; Zhong et al., 1998; Van Hunen et al., 2002; Billen and Hirth, 2007), models that prescribe the kinematics of the slab are simpler and better suited in some cases. Such models are particularly appropriate for the study of the Earth’s subduction zones where the slab geometry is well described by Benioff zone seismicity and local seismic studies and those where the relative plate motion can be extracted from global tectonic models (e.g. Rondenay et al., 2008). This thermo-mechanical approach should yield a reasonable prediction of the temperatures in the slab, which then can be linked to the morphic processes leading to slab dehydration, arc volcanism and seismogenesis. High accuracy of the thermal models is needed since thermodynamic, field-based and experimental predictions of the relevant metamorphic phase changes predict relatively narrow pressure-temperature ranges for the key phase changes (Schmidt and Poli, 1998; Connolly and Kerrick, 2002; Hacker et al., 2003; Forneris and Holloway, 2004; Abers et al., 2006).

In recent years it has become clear that the temperature-dependence of the rheology of mantle silicates causes strong focusing of the flow in the wedge. This focusing increases the temperature at the top of the slab, results in narrow thermal and rheological boundary layers, and enhances the effects of decompression melting and importance of buoyancy (or secondary convection) in the mantle wedge (Furukawa, 1993; Billen and Gurnis, 2001; Van Keken et al., 2002; Conder et al., 2002; Kelemen et al., 2003; Gerya and Yuen, 2003; Cagnioncle et al., 2007; Morgan et al., 2007). Since the targeted accuracy for use of these models in petrological studies is on the order of tens of degrees there is a strong need for methods that can solve the governing equations accurately. Achieving such accuracy is made more challenging due to the strong boundary layers that develop with realistic mantle rheology.

As a community of modelers that is interested in the thermal structure and dynamics of subduction zones we have developed a benchmark that allows us to compare numerical approaches. The benchmark suite was originally proposed at the 2002 MARGINS workshop on subduction zone modeling (held at the University of Michigan in Ann Arbor, MI). We compile here the contributions from seven different groups with independent codes. The cases are based on a simple 2D Cartesian geometry with a kinematically described slab that dips at 45° below an overriding plate of constant thickness (Fig. 1b). In the first set of models we explore the consequences of an isoviscous wedge, starting with the Batchelor analytical solution (Batchelor, 1967), followed by a numerical solution of the wedge flow. This set of models includes a test of the type of boundary conditions that are imposed at the inflow and outflow boundaries of the wedge (Fig. 1c). In the second set of models we explore the effects of more realistic temperature- and stress-dependent rheology in the mantle wedge.

An artefact of the mathematical simplification we employ a discontinuity in the velocity boundary conditions for the Stokes equations in the wedge tip. This causes an (integrable) singularity in pressure but as discussed below leads to some numerical difficulties when the Stokes flow is solved numerically. In nature the transition from fault contact at the seismogenic zone to the full viscous coupling between slab and mantle wedge is finite and can be approximated by improved and more detailed rheological descriptions and freely evolving slabs (Sobolev and Babeyko, 2005; Gorczyk et al., 2007; Gerya et al., 2008).

The main goal in performing this benchmark is to demonstrate the ability of numerical simulations to give an accurate solution to the problem as posed. It should be noted, however, that the models described here do not account for many factors that would modify the flow field in the wedge. The modification could have impacts on thermal structure that are significantly larger than differences between simulation results from different codes. These factors include the dynamical effects of mineralogical phase changes including the likely serpentization of the wedge corner (Hyndman and Peacock, 2003; Gorczyk et al., 2007), melting and melt transport (Katz et al., 2007; Cagnioncle et al., 2007), and three-dimensional effects (Kneller et al., 2007; Behn et al., 2007).

In the remainder of this paper we will first describe the benchmark cases in detail. This is followed by a description of the contributing codes and a full comparison of the benchmark results. We hope that this comparison will spark a broader comparison with other codes and that this paper will have a similar impact on the community as previous benchmarks for mantle convection modeling (Blankenbach et al., 1989; Travis et al., 1990; Busse et al., 1993; Van Keken et al., 1997).

2. Description of the benchmark cases

The benchmark geometry is the same for all cases and is displayed in Fig. 1b. The domain is arbitrarily chosen to be 660 km
wide × 600 km deep. The origin of the coordinate system $\mathbf{x} = (x, y) = (x_1, x_2)$ is at the top left. The inflow boundaries (at both wedge and trench sides) and top of the model have prescribed temperature. The wedge is assumed to be an incompressible fluid that is driven only by the kinematic forcing of the slab. The wedge is confined by the top of the slab and the base of the rigid overriding plate (located at a depth of 50 km). The boundary conditions for the wedge are no-slip below the overriding plate and constant velocity along the top of the slab. The velocity boundary conditions for the boundaries of the wedge are either provided by the Batchelor cornerflow solution (cases 1a and 1b) or based on free inflow/outflow boundaries. The velocity field is discontinuous between the slab and the overriding plate which effectively mimics the fault representative of the seismogenic zone in subduction zones.

2.1. Governing equations

The flow in the wedge is assumed to be driven exclusively by the kinematic velocity of the slab and we ignore thermal buoyancy in the wedge. This simplifies the governing equations and reflects that the main source of buoyancy in a subduction zone is due to the excess density of the slab. Secondary forms of buoyancy can become important for low viscosity zones in the wedge which may be caused by hydration or melting (Billen and Gurnis, 2001; Cagnioncle et al., 2007). The velocity and pressure in the wedge is found by solving the conservation of mass

$$\nabla \cdot \mathbf{v} = 0 $$

(1)

and the conservation of momentum

$$\nabla \cdot \mathbf{v} - \nabla P = 0 $$

(2)

where $\mathbf{v}$ is velocity, $\tau$ is the deviatoric stress tensor, and $P$ the dynamic pressure. The deviatoric stress tensor is given by

$$\tau = 2\eta \dot{\varepsilon} $$

(3)

where $\eta$ is the effective dynamic viscosity and the components of the strain rate tensor $\dot{\varepsilon}$ are given by

$$\dot{\varepsilon}_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) $$

(4)

All benchmark cases are assumed to be steady-state and we ignore heat production so that the temperature is found from the steady-state heat advection–diffusion equation

$$\rho c_p (\nabla \cdot \mathbf{v}) T = \nabla \cdot (k \nabla T) $$

(5)

where $\rho$ is density, $c_p$ the specific heat, $T$ the temperature, and $k$ the thermal conductivity. The effective shear viscosity $\eta$ follows from (3):

$$\eta = \frac{\tau}{2\dot{\varepsilon}} $$

(6)

where the second invariants of the strain-rate and deviatoric stress tensor are defined by

$$\dot{\varepsilon} = \left[ \frac{1}{2} \sum_{ij} \dot{\varepsilon}_{ij} \dot{\varepsilon}_{ij} \right]^{1/2}, \quad \tau = \left[ \frac{1}{2} \sum_{ij} \tau_{ij} T_{ij} \right]^{(1/2)} $$

(7)

A general simplified equation for the viscosity of olivine deforming by diffusion creep assuming zero activation volume (ignoring effects of hydration and grain-size dependence) is

$$\eta_{\text{diff}}(T) = A_{\text{diff}} \exp \left( \frac{E_{\text{diff}}}{R T} \right) $$

(8)

while the viscosity for deformation by dislocation creep is given by

$$\eta_{\text{disl}}(T, \dot{\varepsilon}) = A_{\text{disl}} \left( \frac{E_{\text{disl}}}{R T} \right)^{(1-n)/n} \dot{\varepsilon} $$

(9)

where $A$ is a pre-factor, $E$ the activation energy, and $n$ is the power-law exponent (e.g. Karato and Wu., 1993). Since the flow is driven by a fixed velocity boundary condition the range of the dynamic viscosity influences the solution, particularly near the return flow in the tip of the wedge. A large dynamic range in viscosity leads to unrealistic high stress and unrealistic deformation in high viscosity regions. This could be avoided by inclusion of physically realistic self-limiting processes, such as a transition to higher stress flow mechanisms or the inclusion of viscous dissipation (e.g. Kneller et al., 2007; Wada et al., 2008). For the ease of the numerical comparison it is simpler and sufficient to truncate the viscosity at a fixed maximum $\eta_{\text{max}}$. For the benchmark cases described below we will use the modified viscosity laws:

$$\eta_{\text{diff, effective}} = \left( \frac{1}{\eta_{\text{diff}}} + \frac{1}{\eta_{\text{max}}} \right)^{-1} $$

(10)

$$\eta_{\text{disl, effective}} = \left( \frac{1}{\eta_{\text{disl}}} + \frac{1}{\eta_{\text{max}}} \right)^{-1} $$

(11)

A full list of symbols with reference values is provided in Table 1.

2.2. Case 1a: analytical cornerflow model

The velocity in the slab is constant and dips at 45° with a dimensional speed of 5 cm/yr. The wedge flow is prescribed by the analytical expression for cornerflow (Batchelor, 1967). This case requires only the solution of the heat advection–diffusion Eq. (5). The top boundary condition is $T = T(y = 0) = 273$ K. At the inflow boundary of the wedge temperature is fixed at $T_0 = 1573$ K and a linear geotherm is used at the left hand boundary of the overriding plate from 0 to 50 km depth. The temperature at the slab inflow boundary is described by an error-function solution for half-space cooling for 50 Myr

$$T(x = 0, y) = T_s + (T_0 - T_s) \text{erf} \left( \frac{y}{2 \sqrt{\kappa T_0}} \right) $$

(12)

where $t_50$ is the age in seconds and $\kappa$ is the thermal diffusivity (Table 1). At the slab and wedge outflow boundaries we prescribe the natural boundary condition (zero curvature) for the heat equation.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Nomenclature and reference values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity</td>
<td>Symbol</td>
</tr>
<tr>
<td>Velocity</td>
<td>$\dot{\varepsilon}$</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>$\eta$</td>
</tr>
<tr>
<td>Stress tensor</td>
<td>$\tau$</td>
</tr>
<tr>
<td>Strain rate tensor</td>
<td>$\dot{\varepsilon}$</td>
</tr>
<tr>
<td>Dynamic pressure</td>
<td>$P$</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$k$</td>
</tr>
<tr>
<td>Heat capacity</td>
<td>$c_p$</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>$\kappa$</td>
</tr>
<tr>
<td>Activation energy (diffusion creep)</td>
<td>$E_{\text{diff}}$</td>
</tr>
<tr>
<td>Activation energy (dislocation creep)</td>
<td>$E_{\text{disl}}$</td>
</tr>
<tr>
<td>Power-law exponent for dislocation creep</td>
<td>$n$</td>
</tr>
<tr>
<td>Pre-exponential constant (diffusion creep)</td>
<td>$A_{\text{diff}}$</td>
</tr>
<tr>
<td>Pre-exponential constant (dislocation creep)</td>
<td>$A_{\text{disl}}$</td>
</tr>
<tr>
<td>Maximum viscosity</td>
<td>$\eta_{\text{max}}$</td>
</tr>
<tr>
<td>Gas constant</td>
<td>$R$</td>
</tr>
</tbody>
</table>

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2.3. Case 1b: dynamical flow in isoviscous wedge I

This case is the same as 1a, except that the solution for the wedge flow is determined by solving Eqs. (1) and (2). We use essential boundary conditions for velocity where the velocity components are prescribed by the Batchelor solution. This allows us to evaluate the quality of the Stokes solution without inducing changes due to modifications of the boundary conditions. One important issue is the discontinuity in the velocity boundary conditions at the wedge tip (located at 50 km depth). The discontinuity causes a well-known pressure singularity that is analytically resolvable, but may cause numerical problems for some numerical algorithms and/or for computational grids that are not sufficiently dense (Van Keken et al., 2002). We will illustrate this in the results section below.

In order to avoid the numerical difficulties we allow the option of changing the boundary condition so that the velocity at the bottom of the wedge increases linearly from \( v = 0 \) at position of the corner point \( x_c = (50, 50) \) to \( v = v_0 \), a short distance down stream from the corner point. Formally, this change is from

\[
\vec{v}(x_s) = \vec{v}_0 \quad \text{for} \quad |x_s| \geq |x_c| \quad (13)
\]

to

\[
\vec{v}(x_s) = \frac{|x_s| - |x_c|}{|x_c - x_s|} \vec{v}_0 \quad \text{for} \quad |x_s| \leq |x_c| \quad (14)
\]

\[
\vec{v}(x_s) = \vec{v}_0 \quad \text{for} \quad |x_s| \geq |x_c| \quad (15)
\]

where \( x_s \) is a coordinate along the slab–wedge interface and \( x_c \) is the position down-slab where full coupling between slab and wedge is achieved. This should be a short distance \( D \) from the corner point so that

\[
\vec{x}_c = \vec{x} + \left( \frac{\sqrt{2D}}{2}, \frac{\sqrt{2D}}{2} \right) \quad (16)
\]

The velocity ramp is on the wedge side only and this short segment should be treated as an extension of the velocity discontinuity from \( x = (0, 0) \) to \((50, 50)\). This transition can be thought of as a healing fault, where the tangential velocity across the slab–wedge interface changes from discontinuous to continuous.

2.4. Case 1c: dynamical flow in isoviscous wedge II

This case is the same as 1b, except that natural boundary conditions for stress at the inflow and outflow boundaries of the wedge are prescribed. This implies that both the normal and tangential components of the total stress \( \sigma - \Pi I \) are zero where \( I \) is the identity tensor.

2.5. Case 2a: dynamical flow with diffusion creep

This case is the same as 1c, except that the viscosity of the wedge is given by Eq. (10). See Table 1 for the rheological parameters.

2.6. Case 2b: dynamical flow with dislocation creep

This case is the same as 1c, except that the viscosity of the wedge is given by Eq. (11). See Table 1 for the rheological parameters.

3. Contributing codes

We identify the contributed results of the benchmarks by a short identifier (such as VT for Virginia Tech) and define those identifiers below in bold. The finite difference methods use uniform meshes with the same grid resolution in \( x \) and \( y \). The finite element methods generally employ grid refinement in the boundary layers. All contributors (except Currie, He and Wang) report values on multiple grids with varying number of nodal points.

Mark Behn (WHOI) uses Comsol 3.2b (http://www.comsol.com) with quadratic triangular elements for the heat equation and P2–P1 elements for the Stokes equations. The UMFPACK (http://www.cise.ufl.edu/research/sparse/umfpack) unsymmetric multifrontal method is used for direct LU factorization. For cases 2a and 2b a damped Newton method is used starting from an initial solution from the constant viscosity calculation. Grid refinement is used in the boundary layers.

Amandine Cagnioncle and Marc Parmentier (Brown) use a mixed finite element and finite volume approach. The heat conservation equation is discretized with a finite volume approximation. Adveective fluxes at volume faces are derived by upwinding with a subsequent correction that minimizes the numerical diffusion that results from pure upwinding (Smolarkiewicz and Margolin, 1998). This method is most easily formulated by splitting the advection and diffusion operators over a time-step. The method is fully explicit and is therefore well suited to multiprocessor applications. As one of a number of ‘flux corrected transport’ formulations, this offers an efficient alternative to particle tracers in problems where small numerical diffusion is required. In cases where comparisons have been made of advection without diffusion, this method appears to work as well as tracer particles (Alley and Parmentier, 1998). Viscous flow solutions are obtained using a standard penalty function formulation on a grid of linear four-node elements with nodes at the centers of finite volume elements in the advection–diffusion formulation. Finite volume face-centered velocities are calculated by linear interpolation of the fine element nodal velocities. The advection operator in the finite volume formulation assumes divergence-free velocity fields; so that any numerically non-zero divergence will appear as a source term. To correct for non-divergence-free staggered velocities, we add a small isotropic velocity field in each finite volume thereby making the staggered, face-centered velocities exactly divergence-free. For well-resolved velocity fields, for example one calculated with the penalty formulation, such effects are small. For the cornerflow solution used here, which has a discontinuity in velocity and a resulting singularity in pressure, the departure from divergence-free conditions can be locally large. The magnitude of the divergence correction can be monitored as an indicator of the resolution of the velocity fields.

Claire Currie, Jiangheng He and Kelin Wang (PGC) use the finite element code PGCTherm. Nine-node isoparametric elements are used for temperature and velocity, with compatible four-node elements for pressure. Galerkin-least squares (Hughes et al., 1989) is used to stabilize the solution of the heat equation for advection dominated flows. The Stokes and heat equations are solved simultaneously and a non-linear iteration is performed using a multi-corrector fixed point algorithm. The mesh used to produce the results in this paper has 11 k elements (46 k nodes). The left-most portion of the wedge of 1 m horizontal width is removed to ease mesh construction. The wedge ‘tip’ in the PGC model is therefore a vertical line of 1 m height. Near this tip a special grid refinement is used that results in very small elements (ranging from \( 4 \times 10^{-4} \) to \( 70 \) m) in the 1 km region near the tip. The maximum element size is 20 km. The mesh is generated with numerous mesh lines radiating from the wedge tip. The PGC group was unable to construct a mesh with low resolution near the wedge tip with reasonable element aspect ratio. For this reason PGC contributed only results obtained on a single mesh with the highest mesh resolution in the tip.

Richard Katz and Marc Spiegelman (LDEO) use a uniform finite volume discretization with staggered velocity components and

Scott King (VT) uses a grid of quadrilateral elements with streamline upwind Petrov–Galerkin (SUPG), which is a form of the Galerkin-least-squares approach (Hughes et al., 1989) for the heat equation. A Q1–P0 quadrilateral element is used for the Stokes equation. A penalty function method is used to eliminate pressure from the discretized set of equations for the Stokes equation which can then be solved by efficient Cholesky factorization (Hughes et al., 1979). Picard iteration is used to speed up convergence to a steady solution. The finest mesh employed contains 360 × 180 elements with 1 km grid spacing near the tip of the wedge. The finite element approach used here forms also the basis for the free convection code ConMan (King et al., 1990).

Shu-Chuan Lin (NTU) employs a finite volume discretization with a cell-centered collocated grid using a primitive variable formulation. The energy equation is solved with a power-law scheme which is a combination of a central-difference scheme and an upwind scheme with variable weighting (dependent on the local Peclet number). The Stokes equations are solved with SIMPLE (Patankar, 1980).

Peter van Keken (UM) uses a finite element approach based on the Sepran software (Cuvelier et al., 1986) (http://www.mcs.anl.gov/petsc). Linear triangles with SUPG (using the double asymptotic approach) are used for the heat equation. The Stokes equations are either solved with a penalty function method on P2–P1 triangular elements or with the integrated method using linear Taylor–Hood elements that directly solves for velocity and pressure after renumbering of the unknowns in the discretized set of equations. These methods yield similar accuracy for equally dense meshes. The results obtained with the integrated method are shown here. Picard iteration between Stokes and heat equations is used to arrive at a steady solution for the non-linear cases 2a and 2b. Meshes with variable grid resolution are used with a typical maximum element size of 10 km and a resolution down to 100 m in the boundary layers. The methodology used here is the same as that used in Van Keken et al. (2002), Van Keken (2003) and Abers et al. (2006).

4. Results

We will focus primarily on the temperature structure at the top of the slab and in the mantle wedge in the tip of the corner flow region. The thermal structure in this area is most relevant for the physical and chemical processes leading to arc volcanism and seismicity. The accurate solution of the equations is also most difficult here due to the formation of the temperature and rheological boundary layers. Since the solution to the temperature equation follows directly from the velocity solution, we find that comparing the temperature fields also provides us with a critical test of the accuracy of the solution of the Stokes equations. We provide one direct comparison of the dynamical solution by focusing on pressure and pressure gradients in the wedge. To compare model results each group contributed the temperature field as discreted values in an equidistant grid with 6 km spacing, which is a 1 × 1 × 101 matrix stored row-wise starting in the top left corner. From this grid we have extracted the following measurements for direct comparison: (1) the temperature difference at the corner point between codes as a function of grid resolution (60, 60 km) and just down-stream from the corner point. This provides therefore one of the most critical tests of accuracy of the numerical codes; (2) the L2 norm of the slab–wedge interface temperature between 0 and 210 km depth defined by

\[ ||T_{slab}|| = \sqrt{\frac{\sum_{i=1}^{36} T_{ii}^2}{36}} \]

and (3) the L2 norm of the temperature in the triangular part of the tip of the wedge, between 54 and 120 km depth:

\[ ||T_{wedge}|| = \sqrt{\frac{\sum_{i=10}^{21} \sum_{j=10}^{21} T_{ij}^2}{78}} \]

We compare these between codes as a function of grid resolution near the corner point in the sections below. We show all results that have been contributed to the benchmark comparison. Some participants did not contribute to all cases.

![Fig. 2. (a) Temperature prediction for case 1a (provided by UM). The bold lines indicate the top of the slab and base of the overriding plate. (b) Close up of the top left part of the model.](image-url)
4.1. Thermal structure: isoviscous cases

The temperature field for the isoviscous case obtained by UM is shown in Fig. 2a with a close-up on the wedge thermal structure in Fig. 2b. The comparison of the three scalar measurements of thermal structure is shown in Fig. 3 for the three isoviscous cases.

There are a number of general trends visible in this comparison. The largest spread is observed for the single temperature measurements (frames a, d, and g). The numerical values tend to converge well and generally overlap within a small temperature variation at the extrapolated highest resolution. All codes agree to within 20°C for grid resolution less than 1 km. The convergence trends for the equidistant grid codes based on finite volume approximations is somewhat poorer than that of the finite element methods (PGC, UM, VT, and WHOI).

Case 1a (frames a–c) is a test of the solution of the heat equation only. Three of the finite element codes tend to overlap with high accuracy (0.1°C) at the highest resolution (see Table 2). A minor systematic offset, that is somewhat stronger in frames b and c, appears for NTU and Brown whereas LDEO trends closely towards the values predicted by PGC, UM, and WHOI.

We have also modeled the thermal structure for this case with the finite difference approximation of Minear and Toksöz (1970), which has been used extensively in studies of the thermal structure of slabs (e.g. Toksöz et al., 1971, 1973; Sleep, 1973; De Jonge et al., 1994). This method does not provide an explicit solution of the wedge flow. Rather, it couples grid size and time-step and explicitly advects temperatures from a set of higher grid points to those just below it followed by a diffusional step with an alternating direction implicit finite difference solver. In the widely available code there is an option to mimic induced flow without explicitly solving the Stokes equations. We find that this code strongly underpredicts the temperature at the slab–wedge interface (e.g. $T_{11,11}$ is 275°C compared to 388°C in the present...
Table 2
Selected thermal quantities for isoviscous cases 1a–1c

<table>
<thead>
<tr>
<th>Case</th>
<th>Code</th>
<th>(T_{11})</th>
<th>(|T_{\text{slab}}|)</th>
<th>(|T_{\text{wedge}}|)</th>
</tr>
</thead>
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<tr>
<td>1a</td>
<td>Brown</td>
<td>393.51</td>
<td>520.14</td>
<td>866.52</td>
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<tr>
<td></td>
<td>LDEO</td>
<td>396.63</td>
<td>506.43</td>
<td>855.58</td>
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<td></td>
<td>NTU</td>
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<td></td>
<td>PGC</td>
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</tr>
<tr>
<td></td>
<td>UM</td>
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<td>503.77</td>
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<td></td>
<td>WHOI</td>
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<tr>
<td>1b</td>
<td>Brown</td>
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<td>493.76</td>
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<td>504.63</td>
<td>853.04</td>
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</table>

\(T_{11}\) is the temperature at (60, 60); \(\|T_{\text{slab}}\|\) is the L2 norm of the slab temperature from 0 to 210 km depth; \(\|T_{\text{wedge}}\|\) is the L2 norm of the temperature in the slab and wedge tip in a triangular area near the wedge tip. All quantities are in °C. Values at highest resolution are listed for each code.

Table 3
Selected thermal quantities for cases 2a–2b

<table>
<thead>
<tr>
<th>Case</th>
<th>Code</th>
<th>(T_{11})</th>
<th>(|T_{\text{slab}}|)</th>
<th>(|T_{\text{wedge}}|)</th>
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<tr>
<td>2a</td>
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<td>1002.85</td>
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<td>606.94</td>
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<td>1003.20</td>
</tr>
<tr>
<td></td>
<td>UM</td>
<td>580.66</td>
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<td>607.26</td>
<td>1003.35</td>
</tr>
<tr>
<td></td>
<td>WHOI</td>
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<td>607.26</td>
<td>1003.35</td>
</tr>
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<td>2b</td>
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<td>NTU</td>
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<td>608.85</td>
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<td>UM</td>
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</tr>
<tr>
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<td>574.84</td>
<td>603.80</td>
<td>995.24</td>
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<td></td>
<td>WHOI</td>
<td>583.11</td>
<td>604.96</td>
<td>1000.05</td>
</tr>
</tbody>
</table>

\(\|T_{\text{slab}}\|\) and \(\|T_{\text{wedge}}\|\) are the L2 norms of the slab temperature and wedge temperature, respectively. \(T_{11}\) is the L2 norm of the temperature at (60, 60) between 0 and 210 km depth.

See Table 2 for definitions.

The temperature difference increases to 165 °C at 210 km depth.

Case 1b (frames d–f) show the results for the isoviscous case with a solution of the Stokes equation that should yield the same flow pattern as that used in case 1a. Except for PGC, the contributing codes used a small ramp in the velocity boundary condition of length \(D\) to mitigate the effect of the pressure singularity. The need for this velocity smoothing is apparent when comparing results for UM with a 2 km ramp (grey circles) to that without (open circles). While the results overlap at very high resolution the convergence behavior is poor and differences in excess of 60 °C are obtained for a grid resolution of less than 4 km. The length of the ramp \(D\) is not prescribed. We have found that this is partly dependent on grid resolution near the corner point (as the ramp should be linear preferably over at least a few grid elements) and that the ramp length should not be too high (since then the lower velocity effects become apparent downstream). With one approach (UM) we have verified that the results shown here are not sensitive to variations in ramp length between 1 and 5 km, provided the resolution near the corner point is sufficiently high. For PGC it was not necessary to use a ramp because of the extremely small elements used near the wedge tip and the high order of the shape functions. For most codes the results trend closely to those obtained in case 1a, except for VT, that interestingly now trends closely to the other finite element methods, and Brown that shows a slightly different systematic offset.

The trends for case 1c (in which case open boundary conditions are used instead of imposing those of the Batchelor solution) are nearly identical to those of case 1b, which strongly suggests that the influence of change in boundary conditions is minimal on the thermal structure near the wedge tip.

Table 2 provides the values predicted by the contributing codes at the highest resolution.

4.2. Thermal structure: variable rheology

The inclusion of temperature- (or temperature- and stress-dependent) rheology causes significantly thinner thermal boundary layers and higher temperatures near the tip of the wedge (Fig. 4; temperature field shown as obtained by UM). This is numerically more challenging and explains the slightly poorer convergence of various codes compared to that of the isoviscous cases (Fig. 5, Table 3). Nevertheless, the agreement at high resolution between various codes is quite good (e.g. less than 1 °C difference for \(T_{11}\) between PGC, UM and WHOI). It is

![Fig. 4](image-url)
interesting to note that the temperature values are not significantly different for the cases that simulate diffusion creep in olivine (case 2a) and those for dislocation creep (case 2b). This indicates that the change in activation energies is compensated for by the non-linear rheology as has been previously suggested (Christensen, 1984).

4.3. Pressure predictions

One critical test of the numerical codes is their ability to accurately predict pressure and pressure gradients. Due to the different order of the differentiation of pressure and velocity in the Stokes equation it is often necessary to approximate pressure with a lower
The position of the two points listed in Table 4 relative to the Gauss points depends on the specific mesh used. The results are therefore more strongly dependent on grid size than for quantities that are linear or quadratic in space.

5. Discussion

The results presented here are part of a multi-year comparison between existing and newly adapted methods for the modeling of the thermal structure of subduction zones. We find in general decent agreement between all codes, and in particular excellent agreement between a number of the finite element methods. We have identified a number of reasons for the observed differences. These include the presence of a velocity discontinuity between \( \vec{x} = (0,0) \) and \( (50,50) \) which makes the solution of the heat equation more challenging, the existence of the pressure singularity caused by the discontinuous velocity boundary condition in the Stokes equation, and the 45° dip of the slab which is more difficult to conform to with finite volume methods. Also, in the case of finite element methods that are based on quadrilaterals with domains that have rectangular layouts (like VT) the elements may get non-optimal aspect ratios which will contribute to the difficulty in achieving high accuracy.

The velocity discontinuity between the slab and overriding plate in the heat equation requires some attention. It may cause principle difficulties with methods that are highly accurate only for smooth velocity fields (like the Smolarkiewicz scheme used by Brown). The finite volume methods benefit from a special treatment of the nodes along this discontinuity. For the finite element methods the discontinuity can be accurately represented by proper integration of the terms in the element stiffness matrix for the discrete heat equation.

We have found that the pressure singularity inherent in the Batchelor analytical solution causes numerical difficulties (Fig. 3d), but that these effects can be efficiently mitigated by removing the discontinuity in the velocity boundary conditions at the corner point (50,50). This is most efficiently and accurately done by including a small ramp in the slab–wedge boundary (Eqs. (13)–(15)).

We have compared a model with a vertically dipping slab to test whether the finite volume methods have more difficulty with a slab (and velocity discontinuity at shallow depths) that cuts across the computational grid. A full set of results is available at http://www.geo.lsa.umich.edu/~keken/subduction/benchmark. We have summarized aspects of this special case in Fig. 7. The accu-

---

Table 4

<table>
<thead>
<tr>
<th>Code</th>
<th>( P_1 )</th>
<th>( P_2 )</th>
<th>( P_{1,1} )</th>
<th>( P_{1,2} )</th>
<th>( P_{2,1} )</th>
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</thead>
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<td>0.0275</td>
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<tr>
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<td>56.86</td>
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<td>0.0293</td>
<td>0.0277</td>
</tr>
</tbody>
</table>

Point 1 corresponds to indices (12,10) and \( \vec{x} = (100, 60) \) and point 2 corresponds to (100,60) and \( \vec{x} = (594, 354) \). Pressure is listed in MPa and pressure gradients in MPa/km.

---

Fig. 6. Comparison of predictions for pressure by UM and VT (frame a) with the analytical values (b). Contours at every 10 MPa are based on the 6 km equidistant grid.
racy and convergence trends are markedly improved. For example, the difference between LDEO and UM was reduced to 1°C from 9°C at 0.5 km resolution and the results are within 10°C for a resolution of 2–3 km (compared to 40°C at the same resolution for case 1a). This strongly suggest that the conformability of the finite element methods provides an attractive aspect for subduction zone modeling.

Acknowledgments

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References


Fig. 7. Limited comparison of the slab temperature at 60 km depth for a case with a vertically dipping slab. The convergence behavior and accuracy of the finite volume methods are greatly improved compared to that of a 45° dipping slab (Fig. 3).


