A community benchmark for compressible mantle convection in a two–dimensional cylindrical domain

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Early numerical models of mantle convection were commonly confined to two– and three–dimensional Cartesian domains, of limited extent. The actual geometry of mantle convection, however, is a three–dimensional spherical shell, with concentric spherical upper and lower boundaries. With improvements in numerical methods and increasing computational resources, global three–dimensional spherical mantle convection models are becoming more common (e.g. Baumgardner, 1985; Bercovici et al., 1989; Tackley et al., 1993; Bunge et al., 1996, 1997; Zhong et al., 2000; McNamara and Zhong, 2005; Tackley, 2008; Zhong et al., 2008; Nakagawa and Tackley, 2008; Davies and Davies, 2009; Schuberth et al., 2009; Wolstencroft et al., 2009; Stadler et al., 2010; Tan et al., 2011; Kronbichler et al., 2012; Burstedde et al., 2013; Davies et al., 2013). However, the use of this geometry for calculations at a realistic convective vigour remains expensive. As a consequence, simplifying geometries are often used, including the axisymmetric spherical shell (e.g. Solheim and Peltier, 1994; van Keken and Yuen, 1995) and the two–dimensional cylinder (e.g. Jarvis, 1993; van Keken and Ballentine, 1998, 1999; van Keken, 2001; Nakagawa and Tackley, 2005). Whilst there has been extensive benchmarking of Cartesian codes, for incompressible (Blankenbach et al., 1989; Travis et al., 1990; Busse et al., 1994; van Keken et al., 1997, 2008) and compressible (King et al., 2010) convection, in both two– and three–dimensions, there has been no benchmark in two–dimensional cylindrical geometry, which is our goal. As with previous community benchmarks, we focus on a comparison between derived quantities of the temperature and velocity fields from a number of carefully designed test cases, including the Nusselt number (Nu) and root–mean–square (RMS) velocity (V_{RMS}). Both incompressible and compressible convection are examined, following a structure very similar to that of King et al. (2010). The computational efficiency of each code is not compared, given the differing computational architectures available to each group.

The outline of this document is as follows: in Section 1, we present the equations and different approximations governing mantle convection. Benchmark cases are presented in Section 2, alongside the diagnostics used for comparing codes. Participants are asked to report all diagnostics, where possible. Codes contributing towards this benchmark are described in Section 3 (please provide a brief description if your code is not currently listed), with preliminary results from four codes: (i) Fluidity (Davies et al., 2011; Kramer et al., 2012); (ii) TerraFERMA (Wilson et al., 2013); (iii) Gaia (Hüttig et al., 2013); and (iv) Cheops (Besserer et al., 2011; Besserer, 2012); presented online at: `https://docs.google.com/spreadsheet/ccc?key=0AruSwf4D-LtMdHFjUHNscWFpR1FWcExyejkzM0lfTUE&usp=sharing#gid=0`. Access to this document will be granted, as requested. A discussion of results will be undertaken when all contributing codes have submitted final diagnostic values.

1 Introduction

1.1 Reference State

Density changes across Earth's mantle result primarily from hydrostatic compression, with density increasing by $\approx 65\%$ from surface to CMB (e.g. Schubert et al., 2001). Variations in density associated with local temperature and pressure perturbations are small in comparison to the spherically averaged density. For a chemically homogeneous mantle, it is therefore appropriate to assume a linearized equation of state, of the form:

$$\begin{aligned} \rho &= \bar{\rho}(\bar{T},\bar{p}) + \rho', \\ &= \bar{\rho}(\bar{T},\bar{p}) + \bar{\rho}(\bar{\chi}_T p' - \bar{\alpha} T'). \end{aligned} \tag{1}$$

Here ρ, p, T, χ_T and α denote density, pressure, temperature, isothermal compressibility and the coefficient of thermal expansion, respectively, whilst over–bars refer to a reference state and primes to departures from it:

$$T = \bar{T} + T', \qquad p = \bar{p} + p'. \tag{2}$$

It is convenient to take the reference state as motionless and steady. Accordingly, for the purposes of this benchmark, we will assume that the reference state varies as a function of depth, $z = r_{max} - r$, only, where r denotes the radius and

r_{max} the outer boundary (i.e. surface) radius. The reference state pressure thus satisfies the hydrostatic approximation:

$$\frac{\partial \bar{p}}{\partial z} = \bar{\rho}\bar{\boldsymbol{g}} \cdot \mathbf{z}, \tag{3}$$

where $\boldsymbol{g}$ is the acceleration of gravity and $\mathbf{z}$ is a radial, downward-pointing unit vector. On Earth, $\boldsymbol{g}$ is a function of position, however, for simplicity, it will be assumed constant herein. We will assume that reference density and reference temperature follow an adiabatic Adams–Williamson equation of state (Birch, 1952), where:

$$\bar{\rho}(z) = \rho_0 \exp\Big(\frac{\alpha_0 g_0}{\gamma_0 c_{p_0}} z\Big) \tag{4}$$

and:

$$\bar{T}(z) = T_s \exp\Big(\frac{\alpha_0 g_0}{c_{p_0}} z\Big). \tag{5}$$

Here, c_p and T_s represent the specific heat capacity at constant pressure and surface temperature, respectively, whilst γ_0 denotes the Grüneisen parameter, given by:

$$\gamma_0 = \frac{\alpha_0}{\rho_0 c_{v_0} \chi_{T_0}}, \tag{6}$$

where c_v denotes the specific heat capacity at constant volume. Variables with a sub-script 0 are constants, used in defining the reference state. Here, they are defined at the domain's outer surface.

1.2 Governing Equations

In contrast to convective flow in other branches of geophysical fluid dynamics, inertial forces are strictly negligible within Earth's mantle (the infinite Prandtl number approximation), which leads to some important differences in the governing equations. Although these equations have been presented elsewhere, they are repeated here for clarity. The equations fully developed in cylindrical coordinates can be found in the classical literature (e.g., Schubert et al., 2001, Chap. 6).

1.2.1 Anelastic Liquid Approximation – ALA

Assuming a linearised equation of state (Eq. 1), the dimensionless form of the conservation of mass equation under the ALA can be expressed as (e.g., Schubert et al., 2001):

$$\nabla \cdot (\bar{\rho}\boldsymbol{u}) = 0, \tag{7}$$

where $\boldsymbol{u}$ is the velocity. Neglecting inertial terms, the force balance equation becomes:

$$\nabla \cdot \left[\mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T - \frac{2}{3}\nabla \cdot \boldsymbol{u}\boldsymbol{I}\right)\right] - \nabla p' + \frac{Di}{\gamma_0}\frac{c_{p_0}}{c_{v_0}}\bar{\rho}\bar{\boldsymbol{g}}\bar{\chi}_T p' - Ra\bar{\rho}\bar{\boldsymbol{g}}\bar{\alpha}T' = 0, \tag{8}$$

where μ denotes the dynamic viscosity, $\boldsymbol{I}$ the identity tensor, Ra the Rayleigh number, and Di the dissipation number given by, respectively:

$$Ra = \frac{\rho_0 \alpha_0 \Delta T g_0 d^3}{\mu_0 \kappa_0}; \qquad Di = \frac{\alpha_0 g_0 d}{c_{p_0}}, \tag{9}$$

with κ denoting the thermal diffusivity, d the length scale and ΔT the temperature scale. Note that the final term in Eq. 8 is expressed in terms of the temperature perturbation, T' (sometimes called the potential temperature). However, it can be expressed in terms of total and reference temperature as $Ra\bar{\rho}\bar{\boldsymbol{g}}\bar{\alpha}(T - \bar{T})$.

Finally, in the absence of internal heating and non-dimensionalizing temperature via:

$$T = \frac{T^{\mathrm{d}} - T_s^{\mathrm{d}}}{\Delta T}, \tag{10}$$

where T^{d} and T_s^{d} indicate dimensional temperature and its surface value, respectively, conservation of energy is expressed as:

$$\bar{\rho}\bar{c}_p \frac{DT'}{Dt} - Di\bar{\alpha}\bar{\rho}\bar{\boldsymbol{g}} \cdot \boldsymbol{u}\,(T' + T_o) = \nabla \cdot \left[\bar{k}\nabla(\bar{T} + T')\right] + \frac{Di}{Ra}\Phi, \tag{11}$$

where $T_o = T_s^{\mathrm{d}}/\Delta T$ is a non-dimensional surface temperature, k is the thermal conductivity and Φ denotes viscous dissipation, given by:

$$\Phi = 2\mu \left|\left|\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T - \frac{2}{3}\nabla \cdot \boldsymbol{u}\boldsymbol{I}\right)\right|\right|^2, \tag{12}$$

where $||\ ||$ stands for the Euclidean norm of a second-order tensor.

Alternatively Eq. 11 can be written in terms of total temperature, as follows:

$$\bar{\rho}\bar{c}_p \frac{DT}{Dt} - Di\bar{\alpha}\bar{\rho}\bar{\boldsymbol{g}} \cdot \boldsymbol{u}\,(T + T_o) = \nabla \cdot \left(\bar{k}\nabla T\right) + \frac{Di}{Ra}\Phi. \tag{13}$$

1.2.2 Truncated Anelastic Liquid Approximation – TALA

In mantle convection, density variations arising from dynamic pressure (p') effects are orders of magnitude smaller than those arising due to temperature. As a consequence, the pressure term in the buoyancy force is sometimes ignored. Accordingly, under the so-called Truncated Anelastic Liquid Approximation, Eq. 8 reduces to:

$$\nabla \cdot \left[\mu\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T - \frac{2}{3}\nabla \cdot \boldsymbol{u}\boldsymbol{I}\right)\right] - \nabla p' - Ra\bar{\rho}\bar{\boldsymbol{g}}\bar{\alpha}T' = 0, \tag{14}$$

The mass and energy equations for TALA remain identical to those for ALA. As some numerical schemes do not explicitly solve for dynamic pressure, use of the TALA approximation has been very popular (e.g. Jarvis and McKenzie, 1980; Ita and King, 1994; Tackley, 1996). However, as demonstrated by Leng and Zhong (2008), neglecting the dynamic pressure effect on buoyancy leads to an energy imbalance in the system and, accordingly, where possible, the ALA should be used. Nonetheless, TALA cases are also examined herein.

1.2.3 Extended Boussinesq Approximation – EBA

Under the EBA, the reference includes simpler (constant) reference density and temperature profiles, i.e. here $\bar{\rho} = 1$ and $\bar{T} = 0$. Furthermore, as in TALA, the influence of dynamic pressure on buoyancy is neglected. Under the EBA, the governing equations thus simplify to:

$$\nabla \cdot \boldsymbol{u} = 0, \tag{15}$$

$$\nabla \cdot \left[\mu\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)\right] - \nabla p' - Ra\bar{\boldsymbol{g}}\bar{\alpha}T' = 0, \tag{16}$$

$$\bar{c}_p \frac{DT'}{Dt} - Di\bar{\alpha}\bar{\boldsymbol{g}} \cdot \boldsymbol{u}(T' + T_o) = \nabla \cdot (\bar{k}\nabla T') + \frac{Di}{Ra}\Phi. \tag{17}$$

As noted by King et al. (2010), comparisons between EBA cases are useful for verifying that terms in the energy equation that scale with the dissipation number, Di, are correctly implemented.

1.2.4 Boussinesq Approximation – BA

Finally, dropping terms that scale with the dissipation number, Di, and requiring $\bar{\alpha} = 1 = \bar{c}_p$ yields the Bousinessq approximation. Under the BA, Eq. 15 remains unchanged, but Eqs. 16 and 17 become, respectively:

$$\nabla \cdot \left[\mu\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T\right)\right] - \nabla p' - Ra\bar{\boldsymbol{g}}T' = 0, \tag{18}$$

$$\frac{DT'}{Dt} = \nabla \cdot (\bar{k}\nabla T'). \tag{19}$$

Test cases using the BA are also examined herein.

2 Benchmark Problems

The test cases selected are an extension of those presented in Blankenbach et al. (1989) and King et al. (2010), modified for a two–dimensional cylindrical domain. We consider the governing equations in their BA, EBA, TALA, and ALA forms. Each case is summarized in Table 1, with key geometrical and physical aspects next described.

Number	Equations	Di	Ra	Rheology	Velocity BCs	Initial Condition (T)
1.1	BA	0.0	10^4	Isoviscous	Zero–slip	$l = 4$
2.1	BA	0.0	10^4	Isoviscous	Free–slip	$l = 4$
2.2	BA	0.0	10^5	Isoviscous	Free–slip	FSS: Case 2.1
2.3	BA	0.0	10^3	$\mu(T)$	Free–slip	FSS: Case 2.1
3.1	EBA	0.25	10^4	Isoviscous	Free–slip	$l = 4$
3.2	EBA	0.25	10^5	Isoviscous	Free–slip	FSS: Case 3.1
3.3	EBA	0.25	10^3	$\mu(T)$	Free–slip	FSS: Case 3.1
3.4	EBA	1.25	10^4	Isoviscous	Free–slip	$l = 4$
3.5	EBA	1.25	10^5	Isoviscous	Free–slip	FSS: Case 3.4
4.1	TALA	0.25	10^4	Isoviscous	Free–slip	$l = 4$
4.2	TALA	0.25	10^5	Isoviscous	Free–slip	FSS: Case 4.1
4.3	TALA	0.25	10^3	$\mu(T)$	Free–slip	FSS: Case 4.1
4.4	TALA	0.75	10^4	Isoviscous	Free–slip	$l = 4$
4.5	TALA	0.75	10^5	Isoviscous	Free–slip	FSS: Case 4.4
4.6	TALA	1.25	10^4	Isoviscous	Free–slip	$l = 4$
4.7	TALA	1.25	10^5	Isoviscous	Free–slip	FSS: Case 4.6
5.1	ALA	0.25	10^4	Isoviscous	Free–slip	$l = 4$
5.2	ALA	0.25	10^5	Isoviscous	Free–slip	FSS: Case 5.1
5.3	ALA	0.25	10^3	$\mu(T)$	Free–slip	FSS: Case 5.1
5.4	ALA	0.75	10^4	Isoviscous	Free–slip	$l = 4$
5.5	ALA	0.75	10^5	Isoviscous	Free–slip	FSS: Case 5.4
5.6	ALA	1.25	10^4	Isoviscous	Free–slip	$l = 4$
5.7	ALA	1.25	10^5	Isoviscous	Free–slip	FSS: Case 5.6

Table 1: Case numbers and descriptions (BCs=boundary conditions). For all cases, $f = r_{min}/r_{max} = 0.55$ and $z = r_{max} - r_{min} = 1$. For initial conditions, l denotes the azimuthal order (i.e. mode) of the perturbation (in case of an initial conductive state), whilst FSS denotes the Final Steady State solution of the specified case.

2.1 Computational Domain

The domain is defined by the radii of the inner (r_{min}) and outer (r_{max}) boundaries. These are chosen such that the non–dimensional depth of the mantle, z = $r_{max} - r_{min} = 1$, and the ratio of the inner and outer radii, $f = r_{min}/r_{max} = 0.55$, thus equalling the ratio between Earth's surface and CMB radii. Specifically, we set $r_{min} = 1.22$ and $r_{max} = 2.22$.

2.2 Boundary Conditions

For the majority of cases, velocity boundary conditions are free-slip at both boundaries. However, we do examine one case with no-slip boundary conditions (Case 1.1: BA-Ra104-Iso-ZS). The domain is heated from below only (no internal heating): both boundaries are kept isothermal and a dimensional temperature contrast ΔT is prescribed between them. As noted by King et al. (2010), temperature boundary conditions require careful consideration for compressible convection. The total temperature contrast across the model, $\Delta T = \Delta\bar{T} + \Delta T'$, comprises an adiabatic contribution from the reference state, $\Delta\bar{T}$, and a super–adiabatic contribution, $\Delta T'$. Boundary conditions differ depending on whether one solves Eq. 11 for T' or Eq. 13 for T. Scaling the temperature through Eq. 10, the non-dimensional form of the reference temperature (Eq. 5) is

$$\bar{T}(z) = T_o \left[\exp(Diz) - 1\right]. \tag{20}$$

As a consequence, because the temperature decomposition (Eq. 2) becomes, in its dimensionless form, $T = \bar{T} + T' + T_o$, strong Dirichlet boundary conditions for Eq. 11 in ALA and TALA cases are

$$\begin{aligned} T'(z=0) &= -T_o, \\ T'(z=1) &= 1 - T_o \exp(Di), \end{aligned} \tag{21}$$

while, for Eq. 13, they are simply

$$\begin{aligned} T(z=0) &= 0, \\ T(z=1) &= 1. \end{aligned} \tag{22}$$

For the purposes of this benchmark, $T_o = 273/3000 = 0.091$. Also note that for BA test cases, where $\bar{T} = 0$ and the value of T_o becomes unimportant (therefore can be fixed at $T_o = 0$) , it is no longer necessary to distinguish between T and T' and boundary conditions for Eq. 19 coincide with 22.

2.3 Material Properties

We examine cases where the Rayleigh number varies from $10^3 - 10^5$, at dissipation numbers of 0.25, 0.75 or 1.25. In all cases, thermodynamic properties (i.e. γ, α, χ_T, c_p, c_v and k) are fixed constants, i.e. the corresponding reference profiles

are here equal to unity. For most cases, we consider a constant viscosity fluid, although in Cases 2.3, 3.3, 4.3 and 5.3, viscosity varies as a function of temperature, according to the relation:

$$\mu(T) = \exp(-\beta T), \tag{23}$$

where $\beta = \ln(1000)$. Note that it is the total temperature, T, inside of the exponential.

2.4 Diagnostic Output

Participants are encouraged to report the following temperature related diagnostics:

$$\text{Volume averaged potential temperature} \quad : \quad \langle T' \rangle = \frac{1}{V} \int_V T' \, dV \tag{24}$$

$$\text{Nusselt number at outer (top) surface} \quad : \quad Nu_{(t)} = \frac{\ln(f)}{2\pi(1-f)} \int_0^{2\pi} \left. \frac{\partial T}{\partial r} \right|_{r=r_{max}} d\theta \tag{25}$$

$$\text{Nusselt number at inner (bottom) surface} \quad : \quad Nu_{(b)} = \frac{f\ln(f)}{2\pi(1-f)} \int_0^{2\pi} \left. \frac{\partial T}{\partial r} \right|_{r=r_{min}} d\theta \tag{26}$$

where V denotes the domain volume, and the integration in Eqs. 25 and 26 is carried out over the cylindrical angular coordinate, θ. Note that our definition of the Nusselt numbers follows Jarvis (1993). Participants are also encouraged to report the following diagnostics, which are related to the velocity field:

$$\text{Radial RMS velocity} \quad : \quad U^r_{RMS} = \left(\frac{1}{V} \int_V u_r^2 \, dV \right)^{1/2} \tag{27}$$

$$\text{Tangential RMS velocity} \quad : \quad U^\theta_{RMS} = \left(\frac{1}{V} \int_V u_\theta^2 \, dV \right)^{1/2} \tag{28}$$

$$\text{Total RMS velocity} \quad : \quad U_{RMS} = \left(\frac{1}{V} \int_V |\boldsymbol{u}|^2 \, dV \right)^{1/2} = \left[\left(U^r_{RMS}\right)^2 + \left(U^\theta_{RMS}\right)^2 \right]^{1/2} \tag{29}$$

$$\text{Maximum outer surface velocity} \quad : \quad U_{max_{(t)}} = \max(|\boldsymbol{u}|)_{(r=r_{max})} = \max(|u_\theta|)_{(r=r_{max})} \tag{30}$$

$$\text{Maximum inner surface velocity} \quad : \quad U_{max_{(b)}} = \max(|\boldsymbol{u}|)_{(r=r_{min})} = \max(|u_\theta|)_{(r=r_{min})} \tag{31}$$

In addition, for EBA, TALA and ALA cases, participants should report:

$$\text{Volume averaged viscous dissipation} \quad : \quad \langle \Psi \rangle = \frac{1}{V} \int_V \frac{Di}{Ra} \Phi \, dV \tag{32}$$

$$\text{Volume averaged work of buoyancy (against gravity)} \quad : \quad \langle W \rangle = \frac{1}{V} \int_V Di \bar{\alpha} \bar{\rho} \bar{\boldsymbol{g}} \cdot \boldsymbol{u}(T' + T_o) \, dV \tag{33}$$

Note that, in the compressible mantle convection litterature, the work (here volumetric power) of buoyancy is often referred to as *adiabatic heating*.

All steady-state diagnostics should be given to 3 decimal places.

3 Contributing Codes

3.1 Fluidity (FLD)

Fluidity is a general purpose computational fluid dynamics code, which was recently extended to solve the Stokes and accompanying field equations that are relevant to geodynamics by Davies et al. (2011) and Kramer et al. (2012). The code uses unstructured simplex meshes, which enable the straightforward representation of complex geometries. In addition, mesh adaptivity is utilized to provide increased resolution in areas of dynamic importance, thus allowing for increased computational efficiency (for further details on the use of mesh adaptivity in geodynamics, see Davies et al., 2007, 2008, 2011; Kronbichler et al., 2012; Burstedde et al., 2013). Fluidity supports both continuous and discontinuous Galerkin finite element discretizations, in addition to control-volume discretizations. However, for the purposes of this benchmark,

the governing equations are discretized using a continuous Galerkin finite element approach. For BA and EBA models, the resulting matrix formulation of Eqs. 15-16 is:

$$\begin{pmatrix} \mathrm{K} & \mathrm{G} \\ \mathrm{G}^T & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{p} \end{pmatrix} = \begin{pmatrix} \underline{f} \\ 0 \end{pmatrix}, \tag{34}$$

where K, G, G^T, $\underline{u}$, $\underline{p}$ and $\underline{f}$ denote the discretised stiffness matrix, gradient operator, divergence operator, and vectors of velocity, pressure and right hand side, respectively (for further details, refer to Davies et al., 2011). For compressible ALA models (Eqs. 7-8), the corresponding matrix equation is modified, as follows:

$$\begin{pmatrix} \mathrm{K} & \mathrm{G}+\mathrm{W} \\ \mathrm{C} & 0 \end{pmatrix} \begin{pmatrix} \underline{u} \\ \underline{p} \end{pmatrix} = \begin{pmatrix} \underline{f} \\ 0 \end{pmatrix}, \tag{35}$$

where the matrix C is the discretised form of Eq. 7 and W accounts for the buoyancy force associated with dynamic pressure. For TALA simulations, the matrix W is ignored.

In all Fluidity results that follow, a P2–P1 velocity–pressure element pair is used for the Stokes system, which consists of piecewise quadratic basis functions (P2) for velocity and piecewise linear basis functions (P1) for pressure. The mass and momentum conservation equations are solved using a Schur Complement Reduction approach: for velocity solves, the Conjugate Gradient (CG) method with an algebraic multigrid preconditioner (GAMG from the PETSc library is used, Balay et al., 1997), with the pressure correction equation solved through the FGMRES Krylov method, preconditioned with a pressure mass matrix, scaled by the local inverse of viscosity (for further details, see May and Moresi, 2008; Davies et al., 2011). We note that in Fluidity the governing equations are discretised and solved for in Cartesian coordinates. Free slip boundary conditions are implemented as a strong boundary condition on the normal component. In a cylindrical geometry this component is not aligned with the Cartesian directions and, accordingly, after discretisation we perform a local transformation (rotation) from Cartesian to boundary-aligned coordinates on each node of the boundary. A particular issue in the idealised cylindrical geometry with free slip boundary conditions, is the existence of a rotational null mode: an arbitrary multiple of $\boldsymbol{u} = (-y, x)$ can be added to the solution whilst still satisfying the governing equations. As a result, the resulting discretised linear system is ill-posed. To circumvent this we remove the rotational mode from the residual at each iteration of the linear solver. This is analogous to the two rotational null modes that exist for the idealised spherical case (Zhong et al., 2008).

For solution of the discretised energy equation, piecewise linear, continuous elements are used. As with the benchmark results presented in Davies et al. (2011), the results presented herein were found to be sufficiently smooth that no stabilization of the Galerkin discretization (e.g. SUPG, Hughes and Brooks, 1982) was required. The GMRES Krylov subspace method is used to solve for temperature with successive over relaxation (SOR) preconditioning and a Crank–Nicholson scheme is used for time–stepping. Non–linear coupling between temperature and velocity is handled via a Picard iteration.

Simulations were run until the infinity norm of the temporal variation of the temperature field became less than 1×10^{-7}.

3.2 TerraFERMA (TF)

TerraFERMA, the Transparent Finite Element Rapid Model Assembler (Wilson et al., 2013), is a general purpose finite element package that harnesses several advanced open-source libraries for its core functionality. FEniCS (Logg et al., 2012a) provides a high level language for describing the weak forms of coupled systems of equations (Alnæs, 2012), and an automatic code generator that produces finite element assembly code (Logg et al., 2012b). PETSc (Balay et al., 1997) provides a wide range of scalable linear and non-linear solvers that can be composed into effective multi-physics preconditioners (Brown et al., 2012). SPuD (Ham et al., 2009, 2011), which is also used by Fluidity, is an application neutral options system that provides both human and machine-readable interfaces based on a single xml schema. TerraFERMA integrates these libraries and provides the user with a framework for exploring multi-physics problems. A single options file fully describes the problem, including all equations, coefficients and solver options. Custom compiled applications are generated from this file but share an infrastructure for services common to all models, e.g. diagnostics, checkpointing and global non-linear convergence monitoring. This maximizes code reusability, reliability and longevity ensuring that scientific results and the methods used to acquire them are transparent and reproducible.

Through FEniCS, TerraFERMA has a range of continuous and discontinuous finite elements available for spatial discretization but in all the tests that follow uses continuous piecewise quadratic and continuous piecewise linear basis functions for velocity and pressure respectively (P2-P1 element pair) and piecewise quadratic functions (P2) for temperature. Temporal discretization is performed using a two-level finite difference scheme. At each timestep, all fields are

solved simultaneously as a coupled system ($\underline{x} = (\underline{u}, \underline{p}, \underline{T})$)using an iterative Newton solver:

$$\mathrm{J}\left(\underline{x}_i\right) \underline{\delta x}_i = -\underline{r}\left(\underline{x}_i\right) \tag{36}$$

where $\underline{\delta x}_i = \underline{x}_{i+1} - \underline{x}_i$ is the change in the variables between iteration i and $i+1$, $\underline{r}\left(\underline{x}_i\right)$ is the residual of the equations and $\mathrm{J}\left(\underline{x}_i\right) = \underline{r}'\left(\underline{x}_i\right)$ is the Jacobian matrix, both at iteration i. The Jacobian matrix:

$$\mathrm{J} = \begin{pmatrix} \mathrm{K} & \mathrm{G}+\mathrm{W} & \mathrm{B}+\mathrm{K_T} \\ \mathrm{C} & 0 & 0 \\ \mathrm{A_u}+\mathrm{D} & 0 & \mathrm{M}+\mathrm{A} \end{pmatrix} \tag{37}$$

is similar to that used in a split scheme (Eq. 35) with extra blocks resulting from the inclusion of temperature (mass and diffusion matrix M, advection matrix A, buoyancy term B, dissipation term D) and due to nonlinear effects (possible temperature dependency of viscosity $\mathrm{K_T}$, velocity dependence of advection $\mathrm{A_u}$). When solving Eq. 36, block preconditioners are used on these physical subblocks of J.

The velocity components are oriented radially and tangentially, allowing free-slip boundary conditions to be applied by restricting the radial component. The resulting tangential null space is removed at each iteration of the linear solve to approximate the inverse of J.

3.3 Gaia

Gaia is a mantle convection code based on a finite-volume discretization of the conservation equations 7, 8 and 13, expressed in Cartesian coordinates. It can handle different geometries, from 2-D and 3-D rectangular boxes to 2-D cylindrical and 3-D spherical shells or full spheres. The computational domain can be meshed with structured or fully unstructured grids representing Voronoi diagrams obtained from a Delaunay triangulation of given sets of generator points (Hüttig and Stemmer, 2008b). Gaia uses a co-located arrangement in which all field variables are defined at the center of each control volume. The momentum and continuity equations 7 and 8 are solved for the primitive variables $\boldsymbol{u}$ and p' by explicitly integrating Eq. 7 for the pressure (e.g. Gerya and Yuen, 2003).

On the one hand, the co-located arrangement of the unknowns presents two main advantages over staggered formulations: it requires the definition of only one set of control volumes, which is shared by all variables, and it permits to easily employ unstructured meshes. Nevertheless, in the latter case and in the presence of spatially varying viscosity, relatively complex interpolation schemes must be introduced for computing second-order cross-derivatives of the velocity field at control volume faces (Hüttig and Stemmer, 2008a). To circumvent this difficulty, we recently introduced a novel formulation of the incompressible Navier-Stokes equations in which we explicitly subtract the term $\mu\nabla\cdot\boldsymbol{u}$ from the diagonal of the deviatoric stress tensor (Hüttig et al., 2013). We showed that this small modification not only leads to the elimination of second-order cross-derivatives, but also to the removal of the net-rotation motion that typically arises in systems with variable viscosity and free-slip boundaries. In this way we avoid the need to explicitly subtract this pure rotational mode from the velocity field at each iteration. In order to treat compressibility, we extended this scheme by writing the deviatoric stress tensor as follows

$$\boldsymbol{\tau} = \mu\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^t - \nabla\cdot\boldsymbol{u}\boldsymbol{I} + \frac{1}{3}\nabla\cdot\boldsymbol{u}\boldsymbol{I}\right) = \mu\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^t - \nabla\cdot\boldsymbol{u}\boldsymbol{I} - \frac{1}{3}\frac{\boldsymbol{u}\cdot\nabla\bar{\rho}}{\bar{\rho}}\boldsymbol{I}\right), \tag{38}$$

where we used Eq. 7 to express $\nabla\cdot\boldsymbol{u}$ in terms of the reference density and its gradient. In this way, it can be easily shown that upon computing the divergence of Eq. 38, second-order cross derivatives of the velocity vanish, so that the advantages of our formulation for incompressible flows are still preserved.

The advection-diffusion equation 13 is solved with a fully implicit, three-levels scheme with second-order accuracy in space and time (Harder and Hansen, 2005). In addition, the non-linear coupling between momentum and energy equations is treated via Picard iterations combined with an under-relaxation scheme, which significantly improves convergence, especially when steady-state solutions are sought for.

Finally, both linear systems arising from the discretization of the conservation equations are solved with the BiCGStab(ℓ) Krylov subspace method (Sleijpen and Fokkema, 1993) (which is particularly well suited for advection-dominated problems) in combination with a simple Jacobi preconditioner.

3.4 Cheops

The code used in this benchmark corresponds to the heat transfer module of a more general thermal-orbital framework, CHEOPS-2D: Coupling Heat transfer and Evolution of the Orbit of Planets and of their Satellites in 2-Dimensional geometry (Besserer et al., in prep.), and will be hereafter referred to as Cheops. Cheops was extensively benchmarked (Besserer, 2012) and presented elsewhere (Besserer et al., 2011). Below is a brief description of its main features.

Cheops's core relies on a single, flexible geometrical framework that enables the user to simulate mantle convection in 2D-Cartesian and cylindrical geometries, as well as in the spherical annulus geometry (Hernlund and Tackley, 2008), under the (E)BA and (T)ALA. Mass, momentum, and energy equations are treated in their primitive variable formulation, through a finite volume approach with an annular, radially refinable orthogonal mesh. Velocities and pressures are defined on a classical staggered arrangement and solved for through a geometric multigrid solver using V- and F-cycles with bilinear, curvature-corrected transfer operators. In particular, pressure prolongation between grid levels, as well as continuity residual restriction are optimized for high viscosity contrasts (Tackley, 2008; Gerya, 2010). The coarse grid discretization is analogous to the fine grid one. The SIMPLER velocity-pressure coupling algorithm (Patankar, 1980, 1981) is used as a smoother for the multigrid solver (Trompert and Hansen, 1996), with spare-matrix Gauss-Seidel relaxation (e.g., Choblet, 2005; Pernice, 2000). This ensures, in particular, an explicit treatment of dynamic pressure (hence of the ALA). Removal of the net-rotation motion in cases with free-slip boundaries is performed by computing the volume-averaged angular velocity in the annular domain and substracting the corresponding solid rotation linear velocity field.

The energy equation, in its potential temperature formulation (i.e. Eq. 11) is discretized through central-difference, second-order-in-space opterators for diffusion. Advection is treated with a high resolution Godunov-like scheme associated with a "superbee" slope limiter (Godunov, 1959; Roe, 1986) to minimize numerical diffusion. Advance in time is performed with a standard explicit, first-order CFL time-stepping, with alternate-flux sub-time steps for advection (e.g., Hourdin and Armengaud, 1999).

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References

Alnæs, M. S. (2012). *UFL: a Finite Element Form Language*, chapter 17. Springer.

Balay, S., Gropp, W. D., McInnes, L. C., and Smith, B. F. (1997). Efficient management of parallelism in object-oriented numerical software libraries. In *Modern software tools for scientific computing*, pages 163–202. Birkhauser Boston Inc.

Baumgardner, J. R. (1985). Three-dimensional treatment of convective flow in the Earth's mantle. *J. Stat. Phys.*, 39:501–511.

Bercovici, D., Schubert, G., and Glatzmaier, G. A. (1989). 3-D spherical models of convection in the Earth's mantle. *Science*, 244:950–955.

Besserer, J. (2012). *Approche Numérique du Couplage par Effets de Marée entre Transferts Thermiques Internes et Évolution Orbitale des Corps Planétaires*. PhD thesis, Université de Nantes. 358 p.

Besserer, J., Mocquet, A., Tobie, G., Choblet, G., Běhounková, M., and Čadek, O. (2011). Coupling tidal effects and heat transfer in planetary bodies. In *EPSC-DPS Joint Meeting 2011*, page 927.

Birch, F. (1952). Elasticity and constitution of the Earth's interior. *J. Geophys. Res.*, 57:227–286.

Blankenbach, B., Busse, F., Christensen, U., Cserepes, L., Gunkel, D., Hansen, U., Harder, H., Jarvis, G., Koch, M., Marquart, G., Moore, D., Olson, P., Schmeling, H., and Schnaubelt, T. (1989). A benchmark comparison for mantle convection codes. *Geophys. J. Int.*, 98:23–38.

Brown, J., Knepley, M. G., May, D. A., McInnes, L. C., and Smith, B. (2012). Composable linear solvers for multiphysics. In *ispdc, 11th International Symposium on Parallel and Distributed Computing*, pages 55–62. IEEE.

Bunge, H.-P., Richards, M. A., and Baumgardner, J. R. (1996). The effect of depth–dependent viscosity on the planform of mantle convection. *Nature*, 279:436–438.

Bunge, H.-P., Richards, M. A., and Baumgardner, J. R. (1997). A sensitivity study of 3-D-spherical mantle convection at 10^8 Rayleigh number: effects of depth-dependent viscosity, heating mode and an endothermic phase change. *J. Geophys. Res.*, 102:11991–12007.

Burstedde, C., Stadler, G., Alisic, L., Wilcox, L. C., Tan, E., Gurnis, M., and Ghattas, O. (2013). Large-scale adaptive mantle convection simulation. *Geophys. J. Int.*, 192:889–906.

Busse, F. H., Christensen, U., Clever, R., Cserepes, L., Gable, C., Giannandrea, E., Guillou, L., Houseman, G., Nataf, H. C., Ogawa, M., Parmentier, M., Sotin, C., and Travis, B. (1994). 3D convection at infinite Prandtl number in Cartesian geometry - a benchmark comparison. *Geophys. Astrophys. Fluid Dyn.*, 75:39–59.

Choblet, G. (2005). Modelling thermal convection with large viscosity gradients in one block of the "cubed sphere". *Journal of Computational Physics*, 205(1):269–291.

Davies, D. R. and Davies, J. H. (2009). Thermally–driven mantle plumes reconcile multiple hot–spot observations. *Earth Planet. Sci. Lett.*, 278:50–54.

Davies, D. R., Davies, J. H., Bollada, P. C., Hassan, O., Morgan, K., and Nithiarasu, P. (2013). A hierarchical mesh refinement technique for global 3D spherical mantle convection modelling. *Geosci. Mod. Dev.*, 6:1095–1107.

Davies, D. R., Davies, J. H., Hassan, O., Morgan, K., and Nithiarasu, P. (2007). Investigations into the applicability of adaptive finite element methods to two-dimensional infinite Prandtl number thermal and thermochemical convection. *Geochem. Geophys. Geosys.*, 8:Q05010.

Davies, D. R., Davies, J. H., Hassan, O., Morgan, K., and Nithiarasu, P. (2008). Adaptive finite element methods in geodynamics: convection dominated mid-ocean ridge and subduction zone simulations. *International Journal of Numerical Methods for Heat & Fluid Flow*, 18:1015–1035.

Davies, D. R., Wilson, C. R., and Kramer, S. C. (2011). Fluidity: a fully unstructured anisotropic adaptive mesh computational modeling framework for geodynamics. *Geochem. Geophys. Geosys.*, 120:Q06001.

Gerya, T. and Yuen, D. (2003). Characteristic-based marker-in-cell method with conservative finite-differences schemes for modelling geological flows with strongly variable transport properties. *Phys. Earth Planet. Inter.*, 140:293–318.

Gerya, T. V. (2010). *Numerical Geodynamic Modelling*. Cambridge University Press, Cambridge (UK).

Godunov, S. K. (1959). A finite difference scheme for numerical computation of discontinuous solutions of equations of fluid dynamics. *Matematicheskii Sbornik (N.S.)*, 47(89)(3):271–306.

Ham, D. A., Farrell, P. E., Gorman, G. J., Maddison, J. R., Wilson, C. R., Kramer, S. C., Shipton, J., Collins, G. S., Cotter, C. J., and Piggott, M. D. (2009). Spud 1.0: generalising and automating the user interfaces of scientific computer models. *Geoscientific Model Development*, 2(1):33–42.

Ham, D. A., Farrell, P. E., Gorman, G. J., Maddison, J. R., Wilson, C. R., Kramer, S. C., Shipton, J., Collins, G. S., Cotter, C. J., and Piggott, M. D. (2011). SPuD manual. Technical report, Imperial College London.

Harder, H. and Hansen, U. (2005). A finite-volume solution method for thermal convection and dynamo problems in spherical shells. *Geophys. J. Int.*, 161:522–532.

Hernlund, J. W. and Tackley, P. J. (2008). Modeling mantle convection in the spherical annulus. *Physics of the Earth and Planetary Interiors*, 171(1-4):48–54.

Hourdin, F. and Armengaud, A. (1999). The use of finite-volume methods for atmospheric advection of trace species. Part I: Test of various formulations in a general circulation model. *Monthly Weather Review*, 127(5):822–837.

Hughes, T. J. R. and Brooks, A. (1982). Streamline upwind Petrov-Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations. *Comp. Meth. Appl. Mech. Eng.*, 32:199–259.

Hüttig, C. and Stemmer, K. (2008a). Finite volume discretization for dynamic viscosities on Voronoi grids. *Phys. Earth Planet. Inter.*, 171:137–146.

Hüttig, C. and Stemmer, K. (2008b). The spiral grid: A new approach to discretize the sphere and its application to mantle convection. *Geochem. Geophys. Geosys.*, 9(2):Q02018.

Hüttig, C., Tosi, N., and Moore, W. B. (2013). An improved formulation of the incompressible Navier-Stokes equations with variable viscosity. *Phys. Earth Planet. Inter.*, 220:11–18.

Ita, J. and King, S. D. (1994). Sensitivity of convection with an endothermic phase change to the form of governing equations, initial conditions, boundary conditions, and equation of state. *J. Geophys. Res*, 99:915–919.

Jarvis, G. T. (1993). Effects of curvature on two–dimensional models of mantle convection: cylindrical polar coordinates. *J. Geophys. Res.*, 98:4477–4485.

Jarvis, G. T. and McKenzie, D. P. (1980). Convection in a compressible fluid with infinite Prandtl number. *J. Fluid Mech.*, 96:515–583.

King, S. D., Lee, C., van Keken, P. E., Leng, W., Zhong, S., Tan, E., Tosi, N., and Kameyama, M. C. (2010). A community benchmark for 2-D Cartesian compressible convection in Earth's mantle. *Geophys. J. Int.*, 180:73–87.

Kramer, S. C., Wilson, C. R., and Davies, D. R. (2012). An implicit free-surface algorithm for geodynamical simulations. *Phys. Earth Planet. Int.*, 194:25–37.

Kronbichler, M., Heister, T., and Bangerth, W. (2012). High accuracy mantle convection simulation through modern numerical methods. *Geophys. J. Int.*, 191:12–29.

Leng, W. and Zhong, S. (2008). Viscous heating, adiabatic heating and energetic consistency in compressible mantle convection. *Geophys. J. Int.*, 173:693–702.

Logg, A., Mardal, K.-A., and Wells, G. N. (2012a). *Automated Solution of Differential Equations by the Finite Element Method*. Springer.

Logg, A., Ølgaard, K. B., Rognes, M. E., and Wells, G. N. (2012b). *FFC: the FEniCS Form Compiler*, chapter 11. Springer.

May, D. and Moresi, L. (2008). Preconditioned iterative methods for stokes flow problems arising in computational geodynamics. *Phys. Earth Planet. Int.*, 171:33–47.

McNamara, A. K. and Zhong, S. (2005). Thermo–chemical structures beneath Africa and the Pacific Ocean. *Nature*, 437:1136–1139.

Nakagawa, T. and Tackley, P. J. (2005). The interaction between the post-perovskite phase change and a thermo-chemical boundary layer near the core-mantle boundary. *Earth Planet. Sci. Lett.*, 238:204–216.

Nakagawa, T. and Tackley, P. J. (2008). Lateral variations in CMB heat flux and deep mantle seismic velocity caused by a thermal-chemical-phase boundary layer in 3D spherical convection. *Earth Planet. Sci. Lett.*, 271:348–358.

Patankar, S. V. (1980). *Numerical Heat Transfer and Fluid Flow*. Hemisphere, Washington, D.C. (USA).

Patankar, S. V. (1981). A calculation procedure for two-dimensional elliptic situations. *Numerical Heat Transfer, Part A: Applications*, 4(4):409–425.

Pernice, M. (2000). A hybrid multigrid method for the steady-state incompressible Navier-Stokes equations. *Electronic Transactions on Numerical Analysis*, 10:74–91.

Roe, P. L. (1986). Characteristic-based schemes for the Euler equations. *Annual Review of Fluid Mechanics*, 18:337–365.

Schubert, G., Turcotte, D. L., and Olson, P. (2001). *Mantle convection in the Earth and planets*. Cambridge University Press.

Schuberth, B. S. A., H.-P. Bunge, Steinle-Neumann, G., Moder, C., and Oeser, J. (2009). Thermal versus elastic heterogeneity in high-resolution mantle circulation models with pyrolite composition: high plume excess temperatures in the lowermost mantle. *Geochem. Geophy. Geosyst.*, 10:Q01W01.

Sleijpen, G. L. G. and Fokkema, D. R. (1993). BiCGstab(ℓ) for linear equations involving unsymmetric matrices with complex spectrum. *Electron. Trans. Numer. Anal.*, 1(11):2000.

Solheim, L. P. and Peltier, W. R. (1994). Avalanche effects in phase transition modulated convection - a model of Earth's mantle. *J. Geophys. Res.*, 99:6997–7018.

Stadler, G., Gurnis, M., Burstedde, C., Wilcox, L. C., Alisic, L., and Ghattas, O. (2010). The dynamics of plate tectonics and mantle flow: from local to global scales. *Science*, 329:1033–1038.

Tackley, P. J. (1996). Effects of strongly variable viscosity on three–dimensional compressible convection in planetary mantles. *J. Geophys. Res.*, 101:3311–3332.

Tackley, P. J. (2008). Modelling compressible mantle convection with large viscosity contrasts in a three-dimensional spherical shell using the Yin-Yang grid. *Phys. Earth Planet. Int.*, 171:7–18.

Tackley, P. J., Stevenson, D. J., Glatzmaier, G. A., and Schubert, G. (1993). Effects of an endothermic phase transition at 670 km depth in a spherical model of convection in the Earth's mantle. *Nature*, 361:699–704.

Tan, E., Leng, W., Zhong, S., and Gurins, M. (2011). On the location of plumes and mobility of thermo–chemical structures with high bulk modulus in the 3-D compressible mantle. *Geochem. Geophys. Geosys.*, 12:Q07005.

Travis, B. J., Anderson, C., Baumgardner, J. R., Gable, C. W., Hager, B. H., O'Connell, R. J., Olson, P., Raefsky, A., and Schubert, G. (1990). A benchmark comparison of numerical methods for infinite Prandtl number thermal convection in two–dimensional Cartesian geometry. *Geophys. Astrophys. Fluid Dyn.*, 55:137–160.

Trompert, R. A. and Hansen, U. (1996). The application of a finite volume multigrid method to three-dimensional flow problems in a highly viscous fluid with a variable viscosity. *Geophysical and Astrophysical Fluid Dynamics*, 83(3):261–291.

van Keken, P. E. (2001). Cylindrical scaling for dynamical cooling models of the Earth. *Phys. Earth. Planet. Int.*, 124:119–130.

van Keken, P. E. and Ballentine, C. J. (1998). Whole–mantle versus layered mantle convection and the role of a high–viscosity lower mantle in terrestrial volatile evolution. *Earth Planet. Sci. Lett.*, 156:19–32.

van Keken, P. E. and Ballentine, C. J. (1999). Dynamical models of mantle volatile evolution and the role of phase transitions and temperature–dependent rheology. *J. Geophys. Res.*, 104:7137–7151.

van Keken, P. E., Currie, C., King, S. D., Behn, M. D., Cagnioncle, A., He, J., Katz, R. F., Lin, S., Parmentier, E. M., Spiegelman, M., and Wang, K. (2008). A community benchmark for subduction zone modeling. *Phys. Earth Planet. Int.*, 171:187–197.

van Keken, P. E., King, S. D., Schmeling, H., Christensen, U. R., Neumeister, D., and Doin, M. P. (1997). A comparison of methods for the modeling of thermo–chemical convection. *J. Geophys. Res.*, 102:22477–22495.

van Keken, P. E. and Yuen, D. A. (1995). Dynamical influences of high viscosity in the lower mantle induced by the steep melting curve of perovskite: effects of curvature and time–dependence. *J. Geophys. Res.*, 100:15233–15248.

Wilson, C. R., Spiegelman, M., and van Keken, P. E. (2013). TerraFERMA: the transparent finite element rapid model assembler for multiphysics problems in the Earth sciences. *Geochem. Geophys. Geosys.*, submitted.

Wolstencroft, M., Davies, J. H., and Davies, D. R. (2009). Nusselt-Rayleigh number scaling for spherical shell Earth mantle simulation up to a Rayleigh number of 10^9. *Phys. Earth Planet. Int.*, 176:132–141.

Zhong, S., McNamara, A., Tan, E., Moresi, L., and Gurnis, M. (2008). A benchmark study on mantle convection in a 3-D spherical shell using CitcomS. *Geochem. Geophys. Geosys.*, 9:Q10017.

Zhong, S., Zuber, M. T., Moresi, L., and Gurnis, M. (2000). Role of temperature-dependent viscosity and surface plates in spherical shell models of mantle convection. *J. Geophys. Res.*, 105:PP. 11,063–11,082.