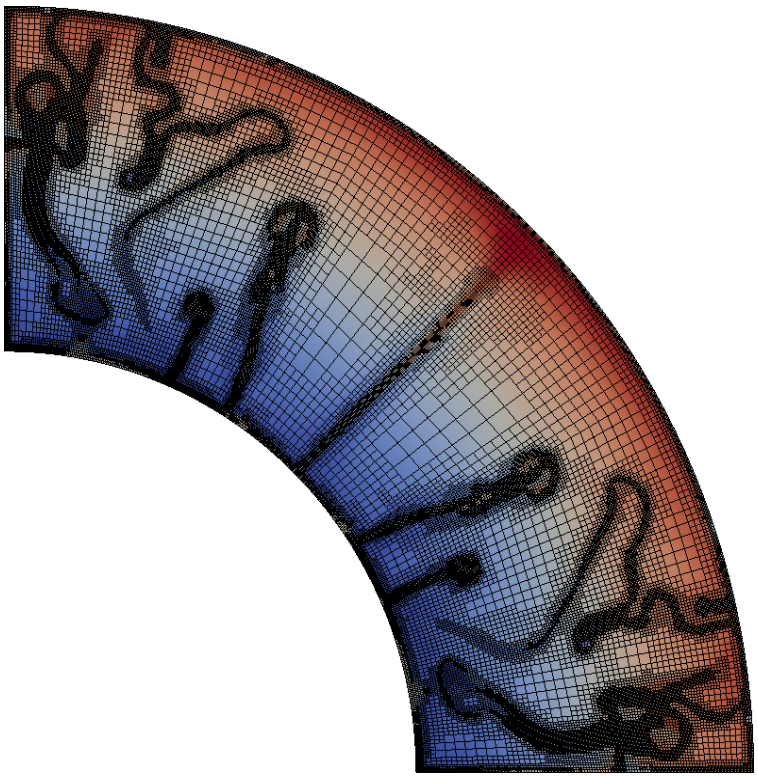

Aspect

Advanced Solver for Problems in Earth's ConvecTion

Preview release, version 0.8
(generated from subversion: *Revision* : 1621)

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1 Introduction

ASPECT — short for Advanced Solver for Problems in Earth's ConvecTion — is a code intended to solve the equations that describe thermally driven convection with a focus on doing so in the context of convection in the earth mantle. It is primarily developed by computational scientists at Texas A&M University based on the following principles:

- *Usability and extensibility:* Simulating mantle convection is a difficult problem characterized not only by complicated and nonlinear material models but, more generally, by a lack of understanding which parts of a much more complicated model are really necessary to simulate the defining features of the problem. To name just a few examples:
  - Mantle convection is often solved in a spherical shell geometry, but the earth is not a sphere – its true shape on the longest lengthscales is dominated by polar oblateness, but deviations from spherical shape relevant to convection patterns may go down to the lengthscales of mountain belts, mid-ocean ridges or subduction trenches. Furthermore, processes outside the mantle like crustal depression during glaciations can change the geometry as well.
  - Rocks in the mantle flow on long time scales, but on shorter time scales they behave more like a visco-elasto-plastic material as they break and as their crystalline structure heals again. The mathematical models discussed in Section 2 can therefore only be approximations.
  - If pressures are low and temperatures high enough, rocks melt, leading to all sorts of new and interesting behavior.

  This uncertainty in what problem one actually wants to solve requires a code that is easy to extend by users to support the community in determining what the essential features of convection in the earth mantle are. Achieving this goal also opens up possibilities outside the original scope, such as the simulation of convection in exoplanets or the icy satellites of the gas giant planets in our solar system.
- *Modern numerical methods:* We build ASPECT on numerical methods that are at the forefront of research in all areas – adaptive mesh refinement, linear and nonlinear solvers, stabilization of transport-dominated processes. This implies complexity in our algorithms, but also guarantees highly accurate solutions while remaining efficient in the number of unknowns and with CPU and memory resources.
- *Parallelism:* Many convection processes of interest are characterized by small features in large domains – for example, mantle plumes of a few tens of kilometers diameter in a mantle almost 3,000 km deep. Such problems can not be solved on a single computer but require dozens or hundreds of processors to work together. ASPECT is designed from the start to support this level of parallelism.
- *Building on others' work:* Building a code that satisfies above criteria from scratch would likely require several 100,000 lines of code. This is outside what any one group can achieve on academic time scales. Fortunately, most of the functionality we need is already available in the form of widely used, actively maintained, and well tested and documented libraries, and we leverage these to make ASPECT a much smaller and easier to understand system. Specifically, ASPECT builds immediately on top of the DEAL.II library (see http://www.dealii.org/) for everything that has to do with finite elements, geometries, meshes, etc.; and, through DEAL.II on Trilinos (see http://trilinos.sandia.gov/) for parallel linear algebra and on P4EST (see http://www.p4est.org/) for parallel mesh handling.

Combining all of these aspects into one code makes for an interesting challenge. We hope to have achieved our goal of providing a useful tool to the geodynamics community and beyond!

Note: ASPECT is a community project. As such, we encourage contributions from the community to improve this code over time. Natural candidates for such contributions are implementations of new plugins as discussed in Section 7.2 since they are typically self-contained and do not require much knowledge of the details of the remaining code. Obviously, however, we also encourage contributions to the core functionality in any form! If you have something that might be of general interest, please contact us.

Note: ASPECT will only solve problems relevant to the community if we get feedback from the community on things that are missing or necessary for what you want to do. Let us know by personal email to the developers, or the mantle convection or `aspect-devel` mailing lists hosted at http://geodynamics.org/cgi-bin/mailman/listinfo/aspect-devel!

1.1 Referencing Aspect

As with all scientific work, funding agencies have a reasonable expectation that if we ask for continued funding for this work, we need to demonstrate relevance. To this end, we ask that if you publish results that were obtained to some part using ASPECT, you cite the following, canonical reference for this software:

```
@Article{KHB12,
  author =        {Martin Kronbichler and Timo Heister and Wolfgang Bangerth},
  title =         {High Accuracy Mantle Convection Simulation through Modern Numerical Methods},
  journal =       {Geophysics Journal International},
  year =          2012,
  volume =        191,
  pages =         {12--29}}
```

1.2 Acknowledgments

The development of ASPECT has been funded through a variety of grants to the authors. Most immediately, it has been supported through the Computational Infrastructure in Geodynamics (CIG-II) grant (National Science Foundation Award No. EAR-0949446, via The University of California – Davis) but the initial portions have also been supported by the original CIG grant (National Science Foundation Award No. EAR-0426271, via The California Institute of Technology). In addition, the libraries upon which ASPECT builds heavily have been supported through many other grants that are equally gratefully acknowledged.

2 Equations, models, coefficients

2.1 Basic equations

ASPECT solves a system of equations in a $d = 2$- or $d = 3$-dimensional domain Ω that describes the motion of a highly viscous fluid driven by differences in the gravitational force due to a density that depends on the temperature. In the following, we largely follow the exposition of this material in Schubert, Turcotte and Olson [STO01].

Specifically, we consider the following set of equations for velocity $\mathbf{u}$, pressure p and temperature T, as well as a set of advected quantities c_i that we call *compositional fields*:

To be finished. Wouldn't the last term need to have a minus sign? drho/dT is negative...

$$-\nabla\cdot\left[2\eta\left(\varepsilon(\mathbf{u})-\frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{1}\right)\right]+\nabla p=\rho\mathbf{g} \qquad \text{in } \Omega, \tag{1}$$

$$\nabla\cdot(\rho\mathbf{u})=0 \qquad \text{in } \Omega, \tag{2}$$

$$\begin{aligned}\rho C_p\left(\frac{\partial T}{\partial t}+\mathbf{u}\cdot\nabla T\right)-\nabla\cdot k\nabla T &= \rho H\\ &\quad+2\eta\left(\varepsilon(\mathbf{u})-\frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{1}\right):\left(\varepsilon(\mathbf{u})-\frac{1}{3}(\nabla\cdot\mathbf{u})\mathbf{1}\right) \qquad (3)\\ &\quad+\frac{\partial\rho}{\partial T}T\mathbf{u}\cdot\mathbf{g} \qquad \text{in } \Omega,\end{aligned}$$

$$\frac{\partial c_i}{\partial t}+\mathbf{u}\cdot\nabla T=0 \qquad \text{in } \Omega, i=1\ldots C \tag{4}$$

where $\varepsilon(\mathbf{u})=\frac{1}{2}(\nabla\mathbf{u}+\nabla\mathbf{u}^T)$ is the symmetric gradient of the velocity (often called the *strain rate*).

In this set of equations, (1) and (2) represent the compressible Stokes equations in which $\mathbf{u}=\mathbf{u}(\mathbf{x},t)$ is the velocity field and $p=p(\mathbf{x},t)$ the pressure field. Both fields depend on space $\mathbf{x}$ and time t. Fluid flow is driven by the gravity force that acts on the fluid and that is proportional to both the density of the fluid and the strength of the gravitational pull.

Coupled to this Stokes system is equation (3) for the temperature field $T=T(\mathbf{x},t)$ that contains heat conduction terms as well as advection with the flow velocity $\mathbf{u}$. The right hand side terms of this equation correspond to

- internal heat production for example due to radioactive decay;
- friction heating;
- adiabatic compression of material; as written, this term assumes that the the overall pressure is dominated by the hydrostatic pressure, in which case the variation of the total pressure can be expressed by gravity and density.

The equations ASPECT currently solves do not include phase change terms, see Section 8.

The final set equations, (4), describes the motion of a set of advected quantities $c_i(\mathbf{x},t), i=1\ldots C$. We call these *compositional fields* because we think of them as spatially and temporally varying concentrations of different elements, minerals, or other constituents of the composition of the material that convects. As such, these fields participate actively in determining the values of the various coefficients of these equations. On the other hand, ASPECT also allows the definition of material models that are independent of these compositional fields, making them passively advected quantities. Several of the cookbooks in Section 6 consider compositional fields in this way, i.e., essentially as tracer quantities that only keep track of where material came from.

These equations are augmented by boundary conditions that can either be of Dirichlet-, Neumann, or tangential type on subsets of the boundary $\Gamma=\partial\Omega$:

$$\mathbf{u}=0 \qquad \text{on } \Gamma_{0,\mathbf{u}}, \tag{5}$$

$$\mathbf{n}\cdot\mathbf{u}=0 \qquad \text{on } \Gamma_{\|,\mathbf{u}}, \tag{6}$$

$$T=T_{\text{prescribed}} \qquad \text{on } \Gamma_{D,T}, \tag{7}$$

$$\mathbf{n}\cdot k\nabla T=0 \qquad \text{on } \Gamma_{N,T}. \tag{8}$$

$$c_i=0 \qquad \text{on } \Gamma_{in}=\{\mathbf{x}:\mathbf{u}\cdot\mathbf{n}<0\}. \tag{9}$$

Here, $\Gamma_{0,\mathbf{u}}$ corresponds to parts of the boundary on which the velocity is fixed to be zero, $\Gamma_{\|,\mathbf{u}}$ to parts of the boundary on which the velocity may be nonzero but must be parallel to the boundary, $\Gamma_{D,T}$ to places where the temperature is prescribed (for example at the inner and outer boundaries of the earth mantle), and finally $\Gamma_{N,T}$ to places where the temperature is unknown but the heat flux across the boundary is zero

(for example on symmetry surfaces if only a part of the shell that constitutes the domain the Earth mantle occupies is simulated). We require that one of these boundary conditions hold at each point for both velocity and temperature, i.e., $\Gamma_{0,\mathbf{u}} \cup \Gamma_{\|,\mathbf{u}} = \Gamma$ and $\Gamma_{D,T} \cup \Gamma_{N,T} = \Gamma$. No boundary conditions have to be posed for the compositional fields at those parts of the boundary where flow is either tangential to the boundary or points outward.

ASPECT solves these equations in essentially the form stated. In particular, the form given in (1) implies that the pressure p we compute is in fact the *total pressure*, i.e., the sum of hydrostatic pressure and dynamic pressure (however, see Section 2.4 for more information on this, as well as the extensive discussion of this issue in [KHB12]). Consequently, it allows the direct use of this pressure when looking up pressure dependent material parameters.

2.2 Coefficients

The equations above contain a significant number of coefficients that we will discuss in the following. In the most general form, many of these coefficients depend nonlinearly on the solution variables pressure p, temperature T and, in the case of the viscosity, on the strain rate $\varepsilon(\mathbf{u})$. If compositional fields $\mathfrak{c} = \{c_1, \ldots, c_C\}$ are present (i.e., if $C > 0$), coefficients may also depend on them. Alternatively, they may be parameterized as a function of the spatial variable $\mathbf{x}$. ASPECT allows both kinds of parameterizations.

Note: One of the next versions of ASPECT will actually iterate out nonlinearities in the material description. However, in the current version, we simply evaluate all nonlinear dependence of coefficients at the solution variables from the previous time step or a solution suitably extrapolated from the previous time steps.

Note that below we will discuss examples of the dependence of coefficients on other quantities; which dependence is actually implemented in the code is a different matter. As we will discuss in Section 5 and 7, some versions of these models are already implemented and can be selected from the input parameter file; others are easy to add to ASPECT by providing self-contained descriptions of a set of coefficients that the rest of the code can then use without a need for further modifications.

Concretely, we consider the following coefficients and dependencies:

- *The viscosity* $\eta = \eta(p, T, \varepsilon(\mathbf{u}), \mathfrak{c}, \mathbf{x})$*:* Units $\mathrm{Pa} \cdot \mathrm{s} = \mathrm{kg}\frac{1}{\mathrm{m} \cdot \mathrm{s}}$.

  The viscosity is the proportionality factor that relates total forces (external gravity minus pressure gradients) and fluid velocities $\mathbf{u}$. The simplest models assume that η is constant, with the constant often chosen to be on the order of 10^{21}Pa s.

  More complex (and more realistic) models assume that the viscosity depends on pressure, temperature and strain rate. Since this dependence is often difficult to quantify, one modeling approach is to make η spatially dependent.

- *The density* $\rho = \rho(p, T, \mathfrak{c}, \mathbf{x})$*:* Units $\frac{\mathrm{kg}}{\mathrm{m}^3}$.

  In general, the density depends on pressure and temperature, both through pressure compression, thermal expansion, and phase changes the material may undergo as it moves through the pressure-temperature phase diagram.

  The simplest parameterization for the density is to assume a linear dependence on temperature, yielding the form $\rho(T) = \rho_{\mathrm{ref}}[1 - \beta(T - T_{\mathrm{ref}})]$ where ρ_{ref} is the reference density at temperature T_{ref} and β is the linear thermal expansion coefficient. For the earth mantle, typical values for this parameterization would be $\rho_{\mathrm{ref}} = 3300\frac{\mathrm{kg}}{\mathrm{m}^3}$, $T_{\mathrm{ref}} = 293\mathrm{K}$, $\beta = 2 \cdot 10^{-5}\frac{1}{\mathrm{K}}$.

- *The gravity vector* $\mathbf{g} = \mathbf{g}(\mathbf{x})$*:* Units $\frac{\mathrm{m}}{\mathrm{s}^2}$.

  Simple models assume a radially inward gravity vector of constant magnitude (e.g., the surface gravity of Earth, $9.81\frac{\mathrm{m}}{\mathrm{s}^2}$), or one that can be computed analytically assuming a homogenous mantle density.

A physically self-consistent model would compute the gravity vector as $\mathbf{g} = -\nabla\varphi$ with a gravity potential φ that satisfies $-\Delta\varphi = 4\pi G\rho$ with the density ρ from above and G the universal constant of gravity. This would provide a gravity vector that changes as a function of time. Such a model is not currently implemented.

- *The specific heat capacity* $C_p = C_p(p, T, \mathfrak{c}, \mathbf{x})$*:* Units $\frac{\mathrm{J}}{\mathrm{kg}\cdot\mathrm{K}} = \frac{\mathrm{m}^2}{\mathrm{s}^2\cdot\mathrm{K}}$.

  The specific heat capacity denotes the amount of energy needed to increase the temperature of one kilogram of material by one degree. Wikipedia lists a value of 790 $\frac{\mathrm{J}}{\mathrm{kg}\cdot\mathrm{K}}$ for granite[1] For the earth mantle, a value of 1250 $\frac{\mathrm{J}}{\mathrm{kg}\cdot\mathrm{K}}$ is within the range suggested by the literature.

- *The thermal conductivity* $k = k(p, T, \mathfrak{c}, \mathbf{x})$*:* Units $\frac{\mathrm{W}}{\mathrm{m}\cdot\mathrm{K}} = \frac{\mathrm{kg}\cdot\mathrm{m}}{\mathrm{s}^3\cdot\mathrm{K}}$.

  The thermal conductivity denotes the amount of thermal energy flowing through a unit area for a given temperature gradient. It depends on the material and as such will from a physical perspective depend on pressure and temperature due to phase changes of the material as well as through different mechanisms for heat transport (see, for example, the partial transparency of perovskite, the most abundant material in the earth mantle, at pressures above around 120 GPa [BRV+04]).

  As a rule of thumb for its order of magnitude, wikipedia quotes values of 1.83–2.90$\frac{\mathrm{W}}{\mathrm{m}\cdot\mathrm{K}}$ for sandstone and 1.73–3.98$\frac{\mathrm{W}}{\mathrm{m}\cdot\mathrm{K}}$ for granite.[2] The values in the mantle are almost certainly higher than this though probably not by much. The exact value is not really all that important: heat transport through convection is several orders of magnitude more important than through thermal conduction.

- *The intrinsic specific heat production* $H = H(\mathbf{x})$*:* Units $\frac{\mathrm{W}}{\mathrm{kg}} = \frac{\mathrm{m}^2}{\mathrm{s}^3}$.

  This term denotes the intrinsic heating of the material, for example due to the decay of radioactive material. As such, it depends not on pressure or temperature, but may depend on the location due to different chemical composition of material in the earth mantle. The literature suggests a value of $\gamma = 7.4 \cdot 10^{-12}\frac{\mathrm{W}}{\mathrm{kg}}$.

2.3 Dimensional or non-dimensionalized equations?

Equations (1)–(3) are stated in the physically correct form. One would usually interpret them in a way that the various coefficients such as the viscosity, density and thermal conductivity η, ρ, κ are given in their correct physical units, typically expressed in a system such as the meter, kilogram, second (MKS) system that is part of the SI system. This is certainly how we envision ASPECT to be used: with geometries, material models, boundary conditions and initial values to be given in their correct physical units. As a consequence, when ASPECT prints information about the simulation onto the screen, it typically does so by using a postfix such as `m/s` to indicate a velocity or `W/m^2` to indicate a heat flux.

Note: For convenience, output quantities are sometimes provided in units meters per *year* instead of meters per *second* (velocities) or in *years* instead of *seconds* (the current time, the time step size); this conversion happens at the time output is generated, and is not part of the solution process. Whether this conversion should happen is determined by the flag "`Use years in output instead of seconds`" in the input file, see Section 5.2. Obviously, this conversion from seconds to years only makes sense if the model is described in physical units rather than in non-dimensionalized form, see below.

That said, in reality, ASPECT has no preferred system of units as long as every material constant, geometry, time, etc., are all expressed in the same system. In other words, it is entirely legitimate to

[1] See http://en.wikipedia.org/wiki/Specific_heat.

[2] See http://en.wikipedia.org/wiki/Thermal_conductivity and http://en.wikipedia.org/wiki/List_of_thermal_conductivities.

implement geometry and material models in which the dimension of the domain is one, density and viscosity are one, and the density variation as a function of temperature is scaled by the Rayleigh number – i.e., to use the usual non-dimensionalization of the Boussinesq equations. Some of the cookbooks in Section 6 use this non-dimensional form; for example, the simplest cookbook in Section 6.1.1 as well as the SolCx, SolKz and inclusion benchmarks in Sections 6.3.1, are such cases. Whenever this is the case, output showing units `m/s` or `W/m^2` clearly no longer have a literal meaning. Rather, the unit postfix must in this case simply be interpreted to mean that the number that precedes the first is a velocity and a heat flux in the second case.

In other words, whether a computation uses physical or non-dimensional units really depends on the geometry, material, initial and boundary condition description of the particular case under consideration – ASPECT will simply use whatever it is given. Whether one or the other is the more appropriate description is a decision we purposefully leave to the user. There are of course good reasons to use non-dimensional descriptions of realistic problems, rather than to use the original form in which all coefficients remain in their physical units. On the other hand, there are also downsides:

- Non-dimensional descriptions, such as when using the Rayleigh number to indicate the relative strength of convective to diffusive thermal transport, have the advantage that they allow to reduce a system to its essence. For example, it is clear that we get the same behavior if one increases both the viscosity and the thermal expansion coefficient by a factor of two because the resulting Rayleigh number; similarly, if we were to increase the size of the domain by 2 and thermal diffusion coefficient by a factor of 8. In both of these cases, the non-dimensional equations are exactly the same. On the other hand, the equations in their physical unit form are different and one may not see that the result of this variations in coefficients will be exactly the same as before. Using non-dimensional variables therefore reduces the space of independent parameters one may have to consider when doing parameter studies.

- From a practical perspective, equations (1)–(3) are often ill-conditioned in their original form: the two sides of each equation have physical units different from those of the other equations, and their numerical values are often vastly different.[3] Of course, these values can not be compared: they have different physical units, and the ratios between these values depends on whether we choose to measure lengths in meters or kilometers, for example. Nevertheless, when implementing these equations in software, at one point or another, we have to work with numbers and at this point the physical units are lost. If one does not take care at this point, it is easy to get software in which all accuracy is lost due to round-off errors. On the other hand, non-dimensionalization typically avoids this since it normalizes all quantities so that values that appear in computations are typically on the order of one.

- On the downside, the numbers non-dimensionalized equations produce are not immediately comparable to ones we know from physical experiments. This is of little concern if all we have to do is convert every output number of our program back to physical units. On the other hand, it is more difficult and a source of many errors if this has to be done inside the program, for example, when looking up the viscosity as a pressure-, temperature- and strain-rate-dependent function: one first has to convert pressure, temperature and strain rate from non-dimensional to physical units, look up the corresponding viscosity in a table, and then convert the viscosity back to non-dimensional quantities. Getting this right at every one of the dozens or hundreds of places inside a program, using the correct (but distinct) conversion factors for each of these quantities, is a challenge and a source of errors.

- From a mathematical viewpoint, it is typically clear how an equation needs to be non-dimensionalized if all coefficients are constant. However, how is one to normalize the equations if, as is the case in the earth mantle, the viscosity varies by several orders of magnitude? In cases like these, one has to choose a reference viscosity, density, etc. While the resulting non-dimensionalization retains the universality of parameters in the equations, as discussed above, it is not entirely clear that this would also retain the numerical stability if the reference values are poorly chosen.

[3] To illustrate this, consider convection in the Earth as a back-of-the-envelope example. With the length scale of the mantle $L = 3 \cdot 10^6\ m$, viscosity $\eta = 10^{24}\ kg/m/s$, density $\rho = 3 \cdot 10^3\ kg/m^3$ and a typical velocity of $U = 0.1\ m/year = 3 \cdot 10^{-9}\ m/s$, we get that the friction term in (1) has size $\eta U/L^2 \approx 3 \cdot 10^2\ kg/m/s^3$. On the other hand, the term $\nabla \cdot (\rho u)$ in the continuity equation (2) has size $\rho U/L \approx 3 \cdot 10^{-12}\ kg/s/m^3$. In other words, their *numerical values* are 14 orders of magnitude apart.

As a consequency of such considerations, most codes in the past have used non-dimensionalized models. This was aided by the fact that until recently and with notable exceptions, many models had constant coefficients and the difficulties associated with variable coefficients were not a concern. On the other hand, our goal with ASPECT is for it to be a code that solves realistic problems using complex models and that is easy to use. Thus, we allow users to input models in physical or non-dimensional units, at their discretion. We believe that this makes the description of realistic models simpler. On the other hand, ensuring numerical stability is not something users should have to be concerned about, and is taken care of in the implementation of ASPECT's core (see the corresponding section in [KHB12]).

2.4 Static or dynamic pressure?

One could reformulate equation (1) somewhat. To this end, let us say that we would want to represent the pressure p as the sum of two parts that we will call static and dynamic, $p = p_s + p_d$. If we assume that p_s is already given, then we can replace (1) by

$$-\nabla \cdot 2\eta\nabla\mathbf{u} + \nabla p_d = \rho\mathbf{g} - \nabla p_s.$$

One typically chooses p_s as the pressure one would get if the whole medium were at rest – i.e., as the hydrostatic pressure. This pressure can be computed noting that (1) reduces to

$$\nabla p_s = \rho(p_s, T_s, \mathbf{x})\mathbf{g}$$

in the absence of any motion where T_s is some static temperature field (see also Section 2.6). This, our rewritten version of (1) would look like this:

$$-\nabla \cdot 2\eta\nabla\mathbf{u} + \nabla p_d = \left[\rho(p, T, \mathbf{x}) - \rho(p_s, T_s, \mathbf{x})\right]\mathbf{g}.$$

In this formulation, it is clear that the quantity that drives the fluid flow is in fact the *buoyancy* caused by the *variation* of densities, not the density itself.

This reformulation has a number of advantages and disadvantages:

- One can notice that in many realistic cases, the dynamic component p_d of the pressure is orders of magnitude smaller than the static component p_s. For example, in the earth, the two are separated by around 6 orders of magnitude at the bottom of the earth mantle. Consequently, if one wants to solve the linear system that arises from discretization of the original equations, one has to solve it a significant degree of accuracy (6–7 digits) to get the dynamic part of the pressure correct to even one digit. This entails a very significant numerical effort, and one that is not necessary if we can split the pressure in a way so that the pre-computed static pressure p_s (or, rather, the density using the static pressure and temperature from which p_s results) absorbs the dominant part and one only has to compute the remaining, dynamic pressure to 2 or 3 digits of accuracy, rather than the corresponding 7–8 for the total pressure.

- On the other hand, the pressure p_d one computes this way is not immediately comparable to quantities that we use to look up pressure-dependent quantities such as the density. Rather, one needs to first find the static pressure as well (see Section 2.6) and add the two together before they can be used to look up material properties or to compare them with experimental results. Consequently, if the pressure a program outputs (either for visualization, or in the internal interfaces to parts of the code where users can implement pressure- and temperature-dependent material properties) is only the dynamic component, then all of the consumers of this information need to convert it into the total pressure when comparing with physical experiments. Since any code implementing realistic material models has a great many of these places, there is a large potential for inadvertant errors and bugs.

- Finally, the definition of a reference density $\rho(p_s, T_s, \mathbf{x})$ derived from static pressures and temperatures is only simple if we have incompressible models and under the assumption that the temperature-induced density variations are small compared to the overall density. In this case, we can choose

$\rho(p_s, T_s, \mathbf{x}) = \rho_0$ with a constant reference density ρ_0. On the other hand, for more complicated models, it is not a priori clear which density to choose since we first need to compute static pressures and temperatures – quantities that satisfy equations that introduce boundary layers, may include phase changes releasing latent heat, and where the density may have discontinuities at certain depths, see Section 2.6.

Thus, if we compute adiabatic pressures and temperatures $\bar{p}_s, \bar{T}_s$ under the assumption of a thermal boundary layer worth 900 Kelvin at the top, and we get a corresponding density profile $\bar{\rho} = \rho(\bar{p}_s, \bar{T}_s, \mathbf{x})$, but after running for a few million years the temperature turns out to be so that the top boundary layer has a jump of only 800 Kelvin with corresponding adiabatic pressures and temperatures $\hat{p}_s, \hat{T}_s$, then a more appropriate density profile would be $\hat{\rho} = \rho(\hat{p}_s, \hat{T}_s, \mathbf{x})$.

The problem is that it may well be that the erroneously computed density profile $\hat{\rho}$ does *not* lead to a separation where $|p_d| \ll |p_s|$ because, especially if the material undergoes phase changes, there will be entire areas of the computational domain in which $|\rho - \hat{\rho}_s| \ll |\rho|$ but $|\rho - \bar{\rho}_s| \not\ll |\rho|$. Consequently the benefits of lesser requirements on the iterative linear solver would not be realized.

We do note that most of the codes available today and that we are aware of split the pressure into static and dynamic parts nevertheless, either internally or require the user to specify the density profile as the difference between the true and the hydrostatic density. This may, in part, be due to the fact that historically most codes where written to solve problems in which the medium was considered incompressible, i.e., where the definition of a static density was simple.

On the other hand, we intend ASPECT to be a code that can solve more general models for which this definition is not as simple. As a consequence, we have chosen to solve the equations as stated originally – i.e., we solve for the *full* pressure rather than just its *dynamic* component. With most traditional methods, this would lead to a catastrophic loss of accuracy in the dynamic pressure since it is many orders of magnitude smaller than the total pressure at the bottom of the earth mantle. We avoid this problem in ASPECT by using a cleverly chosen iterative solver that ensures that the full pressure we compute is accurate enough so that the dynamic pressure can be extracted from it with the same accuracy one would get if one were to solve for only the dynamic component. The methods that ensure this are described in detail in [KHB12] and in particular in the appendix of that paper.

2.5 Pressure normalization

The equations described above, (1)–(3), only determine the pressure p up to an additive constant. On the other hand, since the pressure appears in the definition of many of the coefficients, we need a pressure that has some sort of *absolute* definition. A physically useful definition would be to normalize the pressure in such a way that the average pressure along the "surface" has a prescribed value where the geometry description (see Section 7.2.2) has to determine which part of the boundary of the domain is the "surface" (we call a part of the boundary the "surface" if its depth is "close to zero").

Typically, one will choose this average pressure to be zero, but there is a parameter "`Surface pressure`" in the input file (see Section 5.2) to set it to a different value. One may want to do that, for example, if one wants to simulate the earth mantle without the overlying lithosphere. In that case, the "surface" would be the interface between mantle and lithosphere, and the average pressure at the surface to which the solution of the equations will be normalized should in this case be the hydrostatic pressure at the bottom of the lithosphere.

An alternative is to normalize the pressure in such a way that the *average* pressure throughout the domain is zero or some constant value. This is not a useful approach for most geodynamics applications but is common in benchmarks for which analytic solutions are available. Which kind of normalization is chosen is determined by the "`Pressure normalization`" flag in the input file, see Section 5.2.

2.6 Initial conditions and the adiabatic pressure/temperature

Equations (1)–(3) require us to pose initial conditions for the temperature, and this is done by selecting one of the existing models for initial conditions in the input parameter file, see Section 5.21. The equations themselves do not require that initial conditions are specified for the velocity and pressure variables (since there are no time derivatives on these variables in the model).

Nevertheless, a nonlinear solver will have difficulty converging to the correct solution if we start with a completely unphysical pressure for models in which coefficients such as density ρ and viscosity η depend on the pressure and temperature. To this end, ASPECT computes pressure and temperature fields $p_{\text{ad}}(z), T_{\text{ad}}(z)$ that satisfy adiabatic conditions:

$$\rho C_p \frac{\mathrm{d}}{\mathrm{d}z} T_{\text{ad}}(z) = \frac{\partial \rho}{\partial T} T_{\text{ad}}(z) g_z, \tag{10}$$

$$\frac{\mathrm{d}}{\mathrm{d}z} p_{\text{ad}}(z) = \rho g_z, \tag{11}$$

where strictly speaking g_z is the magnitude of the vertical component of the gravity vector field, but in practice we take the magnitude of the entire gravity vector.

These equations can be integrated numerically starting at $z = 0$, using the depth dependent gravity field and values of the coefficients $\rho = \rho(p, T, z), C_p = C_p(p, T, z)$. As starting conditions at $z = 0$ we choose a pressure $p_{\text{ad}}(0)$ equal to the average surface pressure (often chosen to be zero, see Section 2.5), and an adiabatic surface temperature $T_{\text{ad}}(0)$ that is also selected in the input parameter file.

Note: The adiabatic surface temperature is often chosen significantly higher than the actual surface temperature. For example, on earth, the actual surface temperature is on the order of 290 K, whereas a reasonable adiabatic surface temperature is maybe 1200 K. The reason is that the bulk of the mantle is more or less in thermal equilibrium with a thermal profile that corresponds to the latter temperature, whereas the very low actual surface temperature and the very high bottom temperature at the core-mantle boundary simply induce a thermal boundary layer. Since the temperature and pressure profile we compute using the equations above are simply meant to be good starting points for nonlinear solvers, it is important to choose this profile in such a way that it covers most of the mantle well; choosing an adiabatic surface temperature of 290 K would yield a temperature and pressure profile that is wrong almost throughout the entire mantle.

2.7 Numerical methods

There is no shortage in the literature for methods to solve the equations outlined above. The methods used by ASPECT use the following, interconnected set of strategies in the implementation of numerical algorithms:

- *Mesh adaptation:* Mantle convection problems are characterized by widely disparate length scales (from plate boundaries on the order of kilometers or even smaller, to the scale of the entire earth). Uniform meshes can not resolve the smallest length scale without an intractable number of unknowns. Fully adaptive meshes allow resolving local features of the flow field without the need to refine the mesh globally. Since the location of plumes that require high resolution change and move with time, meshes also need to be adapted every few time steps.

- *Accurate discretizations:* The Boussinesq problem upon which most models for the earth mantle are based has a number of intricacies that make the choice of discretization non-trivial. In particular, the finite elements chosen for velocity and pressure need to satisfy the usual compatibility condition for saddle point problems. This can be worked around using pressure stabilization schemes for low-order discretizations, but high-order methods can yield better accuracy with fewer unknowns and offer more reliability. Equally important is the choice of a stabilization method for the highly advection-dominated temperature equation. ASPECT uses a nonlinear artificial diffusion method for the latter.

- *Efficient linear solvers:* The major obstacle in solving the Boussinesq system is the saddle-point nature of the Stokes equations. Simple linear solvers and preconditioners can not efficiently solve this system in the presence of strong heterogeneities or when the size of the system becomes very large. ASPECT uses an efficient solution strategy based on a block triangular preconditioner utilizing an algebraic multigrid that provides optimal complexity even up to problems with hundreds of millions of unknowns.

- *Parallelization of all of the steps above:* Global mantle convection problems frequently require extremely large numbers of unknowns for adequate resolution in three dimensional simulations. The only realistic way to solve such problems lies in parallelizing computations over hundreds or thousands of processors. This is made more complicated by the use of dynamically changing meshes, and it needs to take into account that we want to retain the optimal complexity of linear solvers and all other operations in the program.

- *Modularity of the code:* A code that implements all of these methods from *scratch* will be unwieldy, unreadable and unusable as a community resource. To avoid this, we build our implementation on widely used and well tested libraries that can provide researchers interested in extending it with the support of a large user community. Specifically, we use the DEAL.II library [BHK07, BHK12] for meshes, finite elements and everything discretization related; the TRILINOS library [HBH+05, H+11] for scalable and parallel linear algebra; and P4EST [BWG11] for distributed, adaptive meshes. As a consequence, our code is freed of the mundane tasks of defining finite element shape functions or dealing with the data structures of linear algebra, can focus on the high-level description of what is supposed to happen, and remains relatively compact. The code will also automatically benefit from improvements to the underlying libraries with their much larger development communities. ASPECT is extensively documented to enable other researchers to understand, test, use, and extend it.

Rather than detailing the various techniques upon which ASPECT is built, we refer to the paper by Kronbichler, Heister and Bangerth [KHB12] that gives a detailed description and rationale for the various building blocks.

2.8 Simplifications of the basic equations

There are two common variations to equations (1)–(3) that are frequently used and that make the system much simpler to solve and analyze: assuming that the fluid is incompressible (the Boussinesq approximation) and a linear dependence of the density on the temperature with constants that are otherwise independent of the solution variables. These are discussed in the following; ASPECT has run-time parameters that allow both of these simpler models to be used.

2.8.1 The Boussinesq approximation: Incompressibility

The original Boussinesq approximation assumes that the density can be considered constant in all occurrences in the equations with the exception of the buoyancy term on the right hand side of (1). The primary result of this assumption is that the continuity equation (2) will now read

$$\nabla \cdot \mathbf{u} = 0.$$

This makes the equations *much* simpler to solve: First, because the divergence operation in this equation is the transpose of the gradient of the pressure in the momentum equation (1), making the system of these two equations symmetric. And secondly, because the two equations are now linear in pressure and velocity (assuming that the viscosity η and the density ρ are considered fixed). In addition, one can drop all terms involving $\nabla \cdot \mathbf{u}$ from the left hand side of the momentum equation (1) as well as from the shear heating term on the right hand side of (3); while dropping these terms does not affect the solution of the equations, it makes assembly of linear systems faster. In addition, in the incompressible case, one needs to neglect the adiabatic heating term $\frac{\partial \rho}{\partial T} T \mathbf{u} \cdot \mathbf{g}$ on the right hand side of (3).

From a physical perspective, the assumption that the density is constant in the continuity equation but variable in the momentum equation is of course inconsistent. However, it is justified if the variation is small since the momentum equation can be rewritten to read

$$-\nabla \cdot 2\eta\varepsilon(\mathbf{u}) + \nabla p_d = (\rho - \rho_0)\mathbf{g},$$

where p_d is the *dynamic* pressure and ρ_0 is the constant reference density. This makes it clear that the true driver of motion is in fact the *deviation* of the density from its background value, however small this value is: the resulting velocities are simply proportional to the density variation, not to the absolute magnitude of the density.

As such, the Boussinesq approximation can be justified. On the other hand, given the real pressures and temperatures at the bottom of the earth mantle, it is arguable whether the density can be considered to be almost constant. Most realistic models predict that the density of mantle rocks increases from somewhere around 3300 at the surface to over 5000 kilogram per cubic meters at the core mantle boundary, due to the increasing lithostatic pressure. While this appears to be a large variability, if the density changes slowly with depth, this is not in itself an indication that the Boussinesq approximation will be wrong. To this end, consider that the continuity equation can be rewritten as $\frac{1}{\rho}\nabla\cdot(\rho\mathbf{u}) = 0$, which we can multiply out to obtain

$$\nabla \cdot \mathbf{u} + \frac{1}{\rho}\mathbf{u}\cdot\nabla\rho = 0.$$

The question whether the Boussinesq approximation is valid is then whether the second term (the one omitted in the Boussinesq model) is small compared to the first. To this end, consider that the velocity can change completely over length scales of maybe 10 km, so that $\nabla \cdot \mathbf{u} \approx \|u\|/10\text{km}$. On the other hand, given a smooth dependence of density on pressure, the length scale for variation of the density is the entire earth mantle, i.e., $\frac{1}{\rho}\mathbf{u}\cdot\nabla\rho \approx \|u\|0.5/3000\text{km}$ (given a variation between minimal and maximal density of 0.5 times the density itself). In other words, for a smooth variation, the contribution of the compressibility to the continuity equation is very small. This may be different, however, for models in which the density changes rather abruptly, for example due to phase changes at mantle discontinuities.

In summary, models that use the approximation of incompressibility solve the following set of equations instead of (1)–(3):

$$-\nabla \cdot [2\eta\varepsilon(\mathbf{u})] + \nabla p = \rho\mathbf{g} \qquad \text{in } \Omega, \tag{12}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega, \tag{13}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) - \nabla\cdot k\nabla T = \rho H + 2\eta\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}) \qquad \text{in } \Omega, \tag{14}$$

where the coefficients $\eta, \rho, \mathbf{g}, C_p$ may possible depend on the solution variables.

Note: As we will see in Section 7, it is easy to add new material models to ASPECT. Each model can decide whether it wants to use the Boussinesq approximation or not. The description of the models in Section 5.26 also gives an answer which of the models already implemented uses the approximation or considers the material sufficiently compressible to go with the fully compressible continuity equation.

2.8.2 Almost linear models

A further simplification can be obtained if one assumes that all coefficients with the exception of the density do not depend on the solution variables but are, in fact, constant. In such models, one typically assumes that the density satisfies a relationship of the form $\rho = \rho(T) = \rho_0(1 - \beta(T - T_0))$ with a small thermal expansion

coefficient β and a reference density ρ_0 that is attained at temperature T_0. Since the thermal expansion is considered small, this naturally leads to the following variant of the Boussinesq model discussed above:

$$
\begin{aligned}
-\nabla \cdot [2\eta\varepsilon(\mathbf{u})] + \nabla p &= \rho_0(1-\beta(T-T_0))\mathbf{g} && \text{in } \Omega,\\
\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega,\\
\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) - \nabla\cdot k\nabla T &= \rho H + 2\eta\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}) && \text{in } \Omega,
\end{aligned}
$$

If the gravitational acceleration $\mathbf{g}$ results from a gravity potential φ via $\mathbf{g} = -\nabla\varphi$, then one can rewrite the equations above in the following, commonly used form:[4]

$$
\begin{aligned}
-\nabla \cdot [2\eta\varepsilon(\mathbf{u})] + \nabla p_d &= -\beta\rho_0 T\mathbf{g} && \text{in } \Omega, && (15)\\
\nabla \cdot \mathbf{u} &= 0 && \text{in } \Omega, && (16)\\
\rho C_p \left(\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T\right) - \nabla\cdot k\nabla T &= \rho H + 2\eta\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u}) && \text{in } \Omega, && (17)
\end{aligned}
$$

where $p_d = p + \rho_0(1+\beta T_0)\varphi$ is the dynamic pressure, as opposed to the total pressure $p = p_d + p_s$ that also includes the hydrastatic pressure $p_s = -\rho_0(1+\beta T_0)\varphi$. Note that the right hand side forcing term in (15) is now only the deviation of the gravitational force from the force that would act if the material were at temperature T_0.

Under the assumption that all other coefficients are constant, one then arrives at equations in which the only nonlinear terms are the advection term, $\mathbf{u}\cdot\nabla T$, and the shear friction, $2\eta\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})$, in the temperature equation (17). This facilitates the use of a particular class of time stepping scheme in which one does not solve the whole set of equations at once, iterating out nonlinearities as necessary, but instead in each time step solves first the Stokes system with the previous time step's temperature, and then uses the so-computed velocity to solve the temperature equation. These kind of time stepping schemes are often referred to as *IMPES* methods (they originate in the porous media flow community, where the acronym stands for *Im*plicit *P*ressure, *E*xplicit *S*aturation). For details see [KHB12].

Note: In ASPECT 0.1, using the IMPES scheme is the only available option. However, in later versions we will implement a fully nonlinear scheme that treats the equations as coupled, and one will be able to choose between the two variants using a run-time parameter.

3 Installation

This is a brief explanation of how to install all the required software and ASPECT itself.

3.1 Prerequisites

ASPECT builds on a few other libraries that are widely used in the computational science area and that provide most of the lower-level functionality such as finite element descriptions or parallel linear algebra. Specifically, it builds on DEAL.II which in turn uses Trilinos and P4EST. These need to be installed first before you can compile and run ASPECT. All of these libraries can readily be installed in a user's home directory, without the need to modify the overall system directories.

The following steps should guide you through the installation of these prerequisites:

[4] Note, however, that ASPECT does not solve the equations in the form given in (15)–(17). Rather, it takes the original form with the real density, not the variation of the density. That said, you can use the formulation (15)–(17) by implementing a material model (see Section 7.2.1) in which the density in fact has the form $\rho(T) = \beta\rho_0 T$ even though this is not physical.

1. *Trilinos:* Trilinos can be downloaded from http://trilinos.sandia.gov/. At the current time we recommend Trilinos Version 10.12.x.[5] For installation instructions see the deal.II README file on installing Trilinos and PETSc. Note that you have to configure with MPI by using

   ```
   TPL_ENABLE_MPI:BOOL=ON
   ```

   in the call to cmake. After that, run `make install`.

2. P4EST*:* Download and install P4EST as described in the deal.II p4est installation instructions. This is done using the `p4est-setup.sh`; do not use the P4EST stand-alone installation instructions.

3. DEAL.II*:* The current version of ASPECT requires DEAL.II version 7.3.0 or later. This version can be downloaded and installed from `https://code.google.com/p/dealii/downloads/list`.

   You may want to set the environment variable[6] `DEAL_DIR` to the directory where you checked out DEAL.II.

4. *Configuring and compiling* DEAL.II*:* Now it is time to configure DEAL.II. To this end, follow the DEAL.II installation instructions. Remember to point the `./configure` script to the paths where you installed p4est and Trilinos and make sure you use MPI compilers. A typical command line would look like this:

   ```
   ./configure CXX=mpicxx --enable-mpi --disable-threads \
      --with-trilinos=/u/username/bin/trilinos-10.12.2 \
      --with-p4est=/u/username/bin/p4est-0.3.3.8
   ```

   if the Trilinos and P4EST packages have been installed in the subdirectory `/u/username/bin`. Make sure the configuration succeeds and detects the MPI compilers correctly. For more information see the documentation of DEAL.II.

   Now you are ready to compile DEAL.II by running `make all`. If you have multiple processor cores, feel free to do `make all -jN` where `N` is the number of processors in your machine to accelerate the process.

5. *Testing your installation:* Test that your installation works by running the `step-32` example that you can find in `$DEAL_DIR/examples/step-32`. Compile by running `make` and run with `mpirun -n 2 ./step-32`.

3.2 Obtaining Aspect and initial configuration

The development version of ASPECT can be downloaded by executing the command

```
svn checkout https://svn.aspect.dealii.org/trunk/aspect
```

If `$DEAL_DIR` points to your DEAL.II installation, there is no further configuration that needs to be done, otherwise you need to edit the `Makefile` accordingly.

3.3 Compiling Aspect and generating documentation

After downloading ASPECT and having built the libraries it builds on, you can compile it by typing

```
make
```

[5] Other versions of Trilinos like 10.6.x and 10.8.x have bugs that make these versions unusable for our purpose. The DEAL.II ReadMe file provides a list of versions that are known to work without bugs with DEAL.II.

[6] For bash this would be adding the line `export DEAL_DIR=/path/to/deal.ii/` to the file `~/.bashrc`.

on the command line (or `make -jN` if you have multiple processors in your machine, where `N` is the number of processors). This builds the ASPECT executable which will reside in the `lib/` subdirectory and will be named `lib/aspect-2d` or `lib/aspect-3d`, depending on the space dimension you compile for (see Section 4.2 for more information on this). If you intend to modify ASPECT for your own experiments, you may want to also generate documentation about the source code. This can be done using the command

```
make doc
```

which assumes that you have the `doxygen` documentation generation tool installed. Most linux distributions have packages for `doxygen`. The result will be the file `doc/doxygen/index.html` that is the starting point for exploring the documentation.

4 Running Aspect

4.1 Overview

After compiling ASPECT as described above, you should have an executable file in the `lib/` subdirectory. It can be called as follows:

```
./lib/aspect parameter-file.prm
```

or, if you want to run the program in parallel, using something like

```
mpirun -np 32 ./lib/aspect parameter-file.prm
```

to run with 32 processors. In either case, the argument denotes the (path and) name of a file that contains input parameters. When you download ASPECT, you should already have a sample input file in the top-level directory that gives you an idea of the parameters that can be set. A full description of all parameters is given in Section 5.

Running the program should produce output that will look something like this (numbers will all be different, of course):

```
Number of active cells: 1,536 (on 5 levels)
Number of degrees of freedom: 20,756 (12,738+1,649+6,369)

*** Timestep 0:  t=0 years

   Rebuilding Stokes preconditioner...
   Solving Stokes system... 30+3 iterations.
   Solving temperature system... 8 iterations.

Number of active cells: 2,379 (on 6 levels)
Number of degrees of freedom: 33,859 (20,786+2,680+10,393)

*** Timestep 0:  t=0 years

   Rebuilding Stokes preconditioner...
   Solving Stokes system... 30+4 iterations.
   Solving temperature system... 8 iterations.

   Postprocessing:
     Writing graphical output: output/solution-00000
     RMS, max velocity:        0.0946 cm/year, 0.183 cm/year
     Temperature min/avg/max:  300 K, 3007 K, 6300 K
     Inner/outer heat fluxes:  1.076e+05 W, 1.967e+05 W

*** Timestep 1:  t=1.99135e+07 years

   Solving Stokes system... 30+3 iterations.
   Solving temperature system... 8 iterations.
```

```
   Postprocessing:
     Writing graphical output: output/solution-00001
     RMS, max velocity:         0.104 cm/year, 0.217 cm/year
     Temperature min/avg/max:   300 K, 3008 K, 6300 K
     Inner/outer heat fluxes:   1.079e+05 W, 1.988e+05 W

*** Timestep 2:  t=3.98271e+07 years

   Solving Stokes system... 30+3 iterations.
   Solving temperature system... 8 iterations.

   Postprocessing:
     RMS, max velocity:         0.111 cm/year, 0.231 cm/year
     Temperature min/avg/max:   300 K, 3008 K, 6300 K
     Inner/outer heat fluxes:   1.083e+05 W, 2.01e+05 W

*** Timestep 3:  t=5.97406e+07 years

...
```

This output was produced by a parameter file that, among other settings, contained the following values:

```
set Dimension                              = 2
set End time                               = 2e9
set Output directory                       = output

subsection Geometry model
  set Model name                           = spherical shell
end

subsection Mesh refinement
  set Initial global refinement            = 4
  set Initial adaptive refinement          = 1
end

subsection Postprocess
  set List of postprocessors               = all
end
```

In other words, these run-time parameters specify that we should start with a geometry that represents a spherical shell (see Sections 5.15 and 5.17 for details). The coarsest mesh is refined 4 times globally, i.e., every cell is refined into four children (or eight, in 3d) 4 times. This yields the initial number of 1,536 cells on a mesh hierarchy that is 5 levels deep. We then solve the problem there once and, based on the number of adaptive refinement steps at the initial time set in the parameter file, use the solution so computed to refine the mesh once adaptively (yielding 2,379 cells on 6 levels) on which we start the computation over at time $t = 0$.

Within each time step, the output indicates the number of iterations performed by the linear solvers, and we generate a number of lines of output by the postprocessors that were selected (see Section 5.40). Here, we have selected to run all postprocessors that are currently implemented in ASPECT which includes the ones that evaluate properties of the velocity, temperature, and heat flux as well as a postprocessor that generates graphical output for visualization.

While the screen output is useful to monitor the progress of a simulation, it's lack of a structured output makes it not useful for later plotting things like the evolution of heat flux through the core-mantle boundary. To this end, ASPECT creates additional files in the output directory selected in the input parameter file (here, the `output/` directory relative to the directory in which ASPECT runs). In a simple case, this will look as follows:

```
aspect> ls -l output/
total 780
-rw------- 1 b    9863 Dec  1 15:13 parameters.prm
```

```
-rw------- 1 b 306562 Dec  1 15:13 solution-00000.0000.vtu
-rw------- 1 b  97057 Nov 30 05:58 solution-00000.0001.vtu
...
-rw------- 1 b   1061 Dec  1 15:13 solution-00000.pvtu
-rw------- 1 b     35 Dec  1 15:13 solution-00000.visit
-rw------- 1 b 306530 Dec  1 15:13 solution-00001.0000.vtu
-rw------- 1 b   1061 Dec  1 15:13 solution-00001.pvtu
-rw------- 1 b     35 Dec  1 15:13 solution-00001.visit
...
-rw-r--r-- 1 b    997 Dec  1 15:13 solution.pvd
-rw------- 1 b    924 Dec  1 15:13 statistics
```

The purpose of these files is as follows:

- *A listing of all run-time parameters:* The `output/parameters.prm` file contains a complete listing of all run-time parameters. In particular, this includes the one that have been specified in the input parameter file passed on the command line, but it also includes those parameters for which defaults have been used. It is often useful to save this file together with simulation data to allow for the easy reproduction of computations later on.

- *Graphical output files:* One of the postprocessors you select when you say "all" in the parameter files is the one that generates output files that represent the solution at certain time steps. The screen output indicates that it has run at time step 0, producing output files of the form `output/solution-00000`. At the current time, the default is that ASPECT generates this output in VTK format[7] as that is widely used by a number of excellent visualization packages and also supports parallel visualization.[8] If the program has been run with multiple MPI processes, then the list of output files will look as shown above, with the base `solution-x.y` denoting that this the `x`th time we create output files and that the file was generated by the `y`th processor.

  VTK files can be visualized by many of the large visualization packages. In particular, the Visit and ParaView programs, both widely used, can read the files so created. However, while VTK has become a de-facto standard for data visualization in scientific computing, there doesn't appear to be an agreed upon way to describe which files jointly make up for the simulation data of a single time step (i.e., all files with the same `x` but different `y` in the example above). Visit and Paraview both have their method of doing things, through `.pvtu` and `.visit` files. To make it easy for you to view data, ASPECT simply creates both kinds of files in each time step in which graphical data is produced.

  The final file of this kind, `solution.pvd` is a file that describes to Paraview which `solution-xxxx.pvtu` jointly form a complete simulation by listing the `.pvtu` files of all timesteps together with the simulation time to which they correspond. To visualize an entire simulation, not just a single time step, it is therefore simplest to just load this `solution.pvd` file.

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  For more on visualization, see Section 4.4.

- *A statistics file:* The `output/statistics` file contains statistics collected during each time step, both from within the simulator (e.g., the current time for a time step, the time step length, etc.) as well as from the postprocessors that run at the end of each time step. The file is essentially a table that allows for the simple production of time trends. In the example above, it looks like this:

[7] The output is in fact in the VTU version of the VTK file format. This is the XML-based version of this file format in which contents are compressed. Given that typical file sizes for 3d simulation are substantial, the compression saves a significant amount of disk space.

[8] The underlying DEAL.II package actually supports output in around a dozen different formats, but most of them are not very useful for large-scale, 3d, parallel simulations. If you need a different format than VTK, you can select this using the run-time parameters discussed in Section 5.43.

```
# 1: Time step number
# 2: Time (years)
# 3: Iterations for Stokes solver
# 4: Time step size (year)
# 5: Iterations for temperature solver
# 6: Visualization file name
# 7: RMS velocity (m/year)
# 8: Max. velocity (m/year)
# 9: Minimal temperature (K)
# 10: Average temperature (K)
# 11: Maximal temperature (K)
# 12: Average nondimensional temperature (K)
# 13: Core-mantle heat flux (W)
# 14: Surface heat flux (W)
0 0.0000e+00 33 2.9543e+07 8                          "" 0.0000 0.0000    0.0000     0.0000 ...
0 0.0000e+00 34 1.9914e+07 8 output/solution-00000 0.0946 0.1829 300.0000 3007.2519 ...
1 1.9914e+07 33 1.9914e+07 8 output/solution-00001 0.1040 0.2172 300.0000 3007.8406 ...
2 3.9827e+07 33 1.9914e+07 8                          "" 0.1114 0.2306 300.0000 3008.3939 ...
```

The actual columns you have in your statistics file may differ from the ones above, but the format of this file should be obvious. Since the hash mark is a comment marker in many programs (for example, `gnuplot` ignores lines in text files that start with a hash mark), it is simple to plot these columns as time series. Alternatively, the data can be imported into a spreadsheet and plotted there.

> **Note:** As noted in Section 2.1, ASPECT can be thought to compute in the meter-kilogram-second (MKS, or SI) system. Unless otherwise noted, the quantities in the output file are therefore also in MKS units.

A simple way to plot the contents of this file is shown in Section 4.4.2.

- *Depth average statistics:* Similar to the `output/statistics` file, Aspect can generate depth-average statistics into `output/depthaverage.plt`. This is done by the "depth average" postprocessor and the user can control how often this file is updated.

  The data is written in text format that can be easily displayed by e.g. gnuplot. For an example, see Figure 1. The plot shows how an initially linear temperatur profile forms upper and lower boundary layers.

4.2 Selecting between 2d and 3d runs

ASPECT can solve both two- and three-dimensional problems. You select which one you want by putting a line like the following into the parameter file (see Section 5):

```
set Dimension                              = 2
```

Internally, dealing with the dimension builds on a feature in DEAL.II, upon which ASPECT is based, that is called *dimension-independent programming*. In essence, what this does is that you write your code only once in a way so that the space dimension is a variable (or, in fact, a template parameter) and you can compile the code for either 2d or 3d. The advantage is that codes can be tested and debugged in 2d where simulations are relatively cheap, and the same code can then be re-compiled and executed in 3d where simulations would otherwise be prohibitively expensive for finding bugs; it is also a useful feature when scoping out whether certain parameter settings will have the desired effect by testing them in 2d first, before running them in 3d. This feature is discussed in detail in the DEAL.II tutorial program step-4. Like there, all the functions and classes in ASPECT are compiled for both 2d and 3d. Which dimension is actually called internally depends on what you have set in the input file, but in either case, the machine code generated for 2d and 3d results from the same source code and should, thus, contain the same set of features and bugs. Running in 2d and

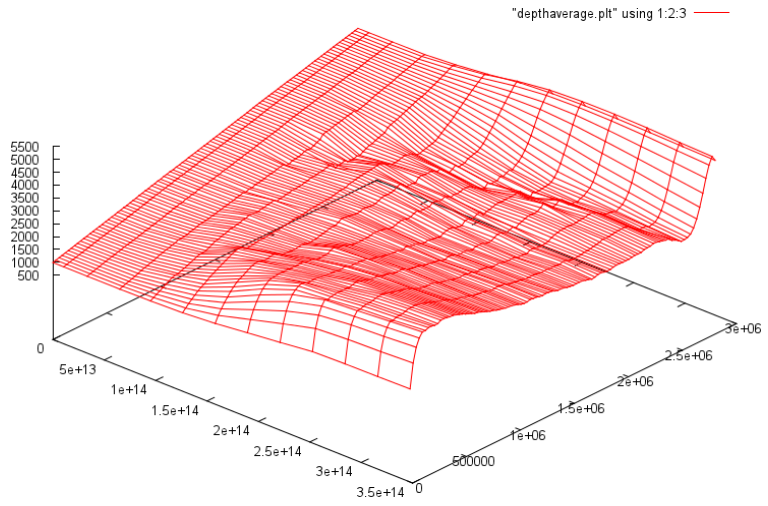


Figure 1: *Example output for depth average statistics. On the left axis are 13 time steps, on the right is the depth (from the top at 0 to the bottom of the mantle on the far right), and the upwards pointing axis is the average temperature. This plot is created by calling* `splot "depthaverage.plt" using 1:2:3 with lines` *in gnuplot.*

3d should therefore yield comparable results. Be prepared to wait much longer for computations to finish in the latter case, however.

4.3 Debug or optimized mode

ASPECT utilizes a DEAL.II feature called *debug mode*. By default, ASPECT uses debug mode, i.e., it calls a version of the DEAL.II library that contain lots of checks for the correctness of function arguments, the consistency of the internal state of data structure, etc. If you program with DEAL.II, for example to extend ASPECT, it has been our experience over the years that, by number, most programming errors are of the kind where one forgets to initialize a vector, one accesses data that has not been updated, one tries to write into a vector that has ghost elements, etc. If not caught, the result of these bugs is that parts of the program use invalid data (data written into ghost elements is not communicated to other processors), that operations simply make no sense (adding vectors of different length), that memory is corrupted (writing past the end of an array) or, in rare and fortunate cases, that the program simply crashes.

Debug mode is designed to catch most of these errors: It enables some 7,300 assertions (as of late 2011) in DEAL.II where we check for errors like the above and, if the condition is violated, abort the program with a detailed message that shows the failed check, the location in the source code, and a stacktrace how the program got there. The downside of debug mode is, of course, that it makes the program much slower – depending on application by a factor of 4–10. An example of the speedup one can get is shown in Section 6.1.1.

ASPECT by default uses debug mode because most users will want to play with the source code, and because it is also a way to verify that the compilation process worked correctly. If you have verified that the program runs correctly with your input parameters, for example by letting it run for the first 10 time steps, then you can switch to optimized mode by editing the top of the `Makefile` and following the steps to build and run in Section 3.3; alternatively, you can just build the entire application using the command `make debug-mode=off`.

> **Note:** It goes without saying that if you make significant modifications to the program, you should do the first runs in debug mode to verify that your program still works as expected.

4.4 Visualizing results

Among the postprocessors that can be selected in the input parameter file (see Sections 4.1 and 5.43) are some that can produce files in a format that can later be used to generate a graphical visualization of the solution variables $\mathbf{u}, p$ and T at select time steps, or of quantities derived from these variables (for the latter, see Section 7.2.8).

By default, the files that are generated are in VTU format, i.e., the XML-based, compressed format defined by the VTK library, see http://public.kitware.com/VTK/. This file format has become a broadly accepted pseudo-standard that many visualization program support, including two of the visualization programs used most widely in computational science: Visit (see http://www.llnl.gov/visit/) and ParaView (see http://www.paraview.org/HTML/Index.html). The VTU format has a number of advantages beyond being widely distributed:

- It allows for compression, keeping files relatively small even for sizeable computations.
- It is a structured XML format, allowing other programs to read it without too much trouble.
- It has a degree of support for parallel computations where every processor would only write that part of the data to a file that this processor in fact owns, avoiding the need to communicate all data to a single processor that then generates a single file. This requires a master file for each time step that then contains a reference to the individual files that together make up the output of a single time step. Unfortunately, there doesn't appear to be a standard for these master records; however, both ParaView and Visit have defined a format that each of these programs understand and that requires placing a file with ending `.pvtu` or `.visit` into the same directory as the output files from each processor. Section 4.1 gives an example of what can be found in the output directory.

Note: You can select other formats for output than VTU, see the run-time parameters in Section 5.43. However, none of the numerous formats currently implemented in deal.II other than the VTK/VTU formats allows for splitting up data over multiple files in case of parallel computations, thus making subsequent visualization of the entire volume impossible. Furthermore, given the amount of data Aspect can produce, the compression that is part of the VTU format is an important part of keeping data manageable.

4.4.1 Visualization the graphical output using *Visit*

In the following, let us discuss the process of visualizing a 2d computation using Visit. The steps necessary for other visualization programs will obviously differ but are, in principle, similar.

To this end, let us consider a simulation of convection in a box-shaped, 2d region (see the "cookbooks" section, Section 6, and in particular Section 6.1.1 for the input file for this particular model). We can run the program with 4 processors using

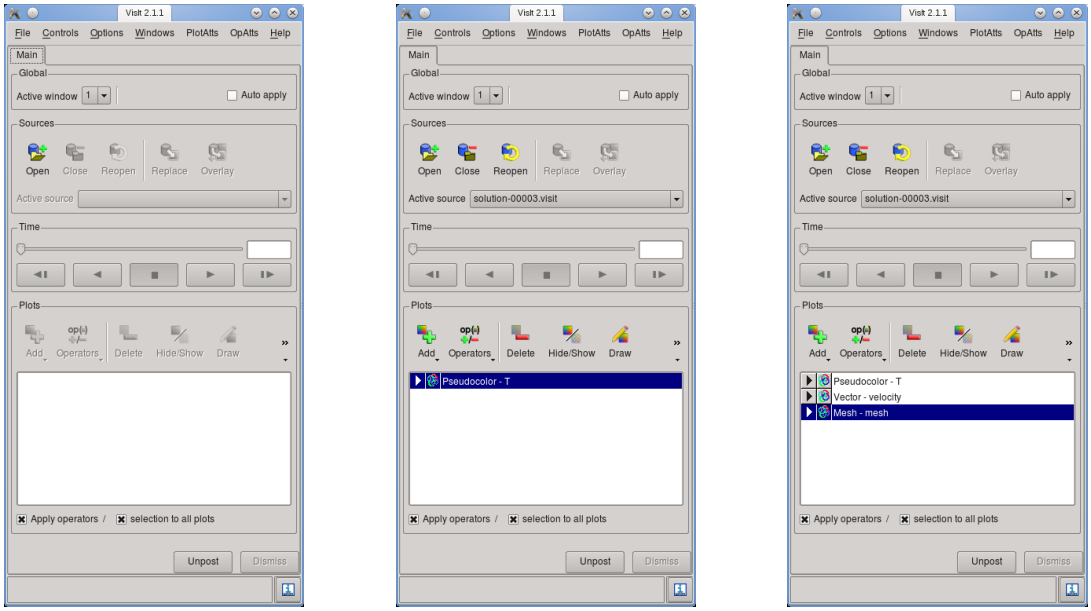
```
mpirun -np 4 ./lib/aspect-2d box.prm
```

Letting the program run for a while will result in several output files as discussed in Section 4.1 above.

In order to visualize one time step, follow these steps:[9]

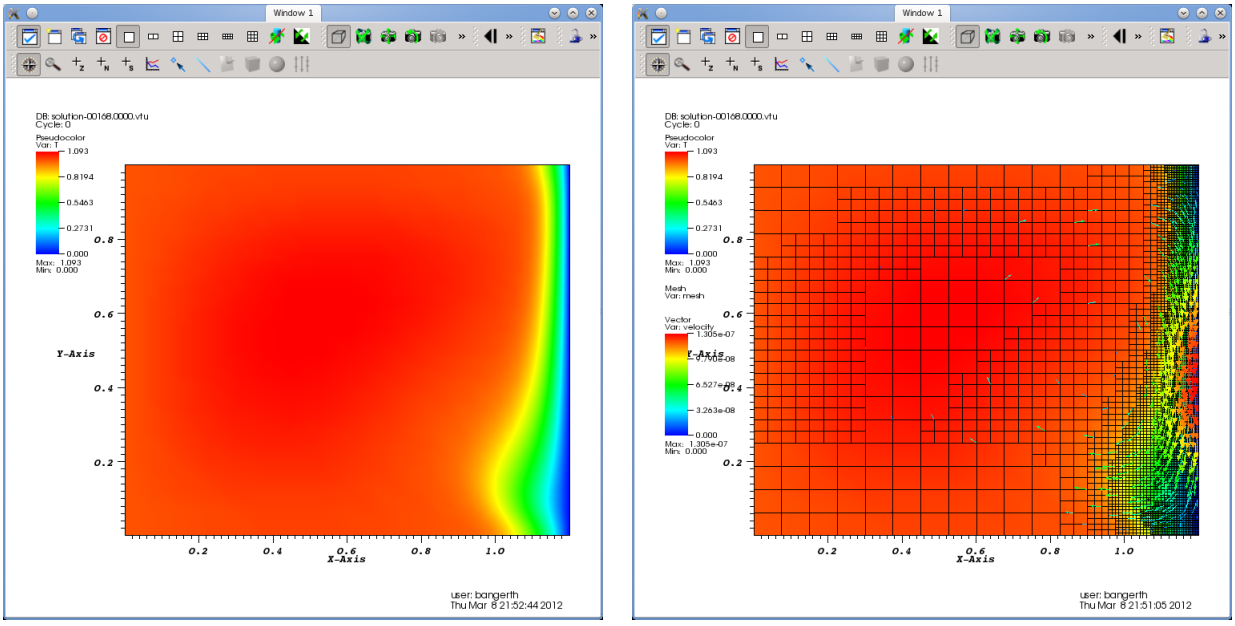
- *Selecting input files:* As mentioned above, in parallel computations we usually generate one output file per processor in each time step for which visualization data is produced (see, however, Section 4.4.3). To tell Visit which files together make up one time step, Aspect creates a `solution-NNNNN.visit` file in the output directory. To open it, start Visit, click on the "Open" button in the "Sources" area of its main window (see Fig. 2(a)) and select the file you want. Alternatively, you can also select files using the "File > Open" menu item, or hit the corresponding keyboard short-cut. After adding an input source, the "Sources" area of the main window should list the selected file name.

[9] The instructions and screenshots were generated with Visit 2.1. Later versions of Visit differ slightly in the arrangement of components of the graphical user interface, but the workflow and general idea remains unchanged.



(a) (b) (c)

Figure 2: *Main window of Visit, illustrating the different steps of adding content to a visualization.*



(a) (b)

Figure 3: *Display window of Visit, showing a single plot and one where different data is overlaid.*

- *Selecting what to plot:* ASPECT outputs all sorts of quantities that characterize the solution, such as temperature, pressure, velocity, and many others on demand (see Section 5.43). Once an input file has been opened, you will want to add graphical representations of some of this data to the still empty canvas. To this end, click on the "Add" button of the "Plots" area. The resulting menu provides a number of different kinds of plots. The most important for our purpose are: (i) "Pseudocolor" allows the visualization of a scalar field (e.g., temperature, pressure, density) by using a color field. (ii) "Vector" displays a vector-valued field (e.g., velocity) using arrows. (iii) "Mesh" displays the mesh. The "Contour", "Streamline" and "Volume" options are also frequently useful, in particular in 3d.

  Let us choose the "Pseudocolor" item and select the temperature field as the quantity to plot. Your main window should now look as shown in Fig. 2(b). Then hit the "Draw" button to make Visit generate data for the selected plots. This will yield a picture such as shown in Fig. 3(a) in the display window of Visit.

- *Overlaying data:* Visit can overlay multiple plots in the same view. To this end, add another plot to the view using again the "Add" button to obtain the menu of possible plots, then the "Draw" button to actually draw things. For example, if we add velocity vectors and the mesh, the main window looks as in Fig. 2(c) and the main view as in Fig. 3(b).

- *Adjusting how data is displayed:* Without going into too much detail, if you double click onto the name of a plot in the "Plots" window, you get a dialog in which many of the properties of this plot can be adjusted. Further details can be changed by using "Operators" on a plot.

- *Making the output prettier:* As can be seen in Fig. 3, Visit by default puts a lot of clutter around the figure – the name of the user, the name of the input file, color bars, axes labels and ticks, etc. This may be useful to explore data in the beginning but does not yield good pictures for presentations or publications. To reduce the amount of information displayed, go to the "Controls > Annotations" menu item to get a dialog in which all of these displays can be selectively switched on and off.

- *Saving figures:* To save a visualization into a file that can then be included into presentations and publications, go to the menu item "File > Save window". This will create successively numbered files in the directory from which Visit was started each time a view is saved. Things like the format used for these files can be chosen using the "File > Set save options" menu item. We have found that one can often get better looking pictures by selecting the "Screenshot" method in this dialog.

More information on all of these topis can be found in the Visit documentation, see `http://www.llnl.gov/visit/`. We have also recorded video lectures demonstrating this process interactively at `http://www.youtube.com/watch?v=3ChnUxqtt08` for Visit, and at `http://www.youtube.com/watch?v=w-65jufR-bc` for Paraview.

4.4.2 Visualizing statistical data

In addition to the graphical outputdiscussed above, ASPECT produces a statistics file that collects information produced during each time step. For the remainder of this section, let us assume that we have run ASPECT with the input file discussed in Section 6.1.1, simulating convection in a box. After running ASPECT, you will find a file called `statistics` in the output directory that, at the time of writing this, looked like this: This file has a structure that looks like this:

```
# 1: Time step number
# 2: Time (seconds)
# 3: Number of mesh cells
# 4: Number of Stokes degrees of freedom
# 5: Number of temperature degrees of freedom
# 6: Iterations for temperature solver
# 7: Iterations for Stokes solver
# 8: Time step size (seconds)
```

```
# 9: RMS velocity (m/s)
# 10: Max. velocity (m/s)
# 11: Minimal temperature (K)
# 12: Average temperature (K)
# 13: Maximal temperature (K)
# 14: Average nondimensional temperature (K)
# 15: Outward heat flux through boundary with indicator 0 (W)
# 16: Outward heat flux through boundary with indicator 1 (W)
# 17: Outward heat flux through boundary with indicator 2 (W)
# 18: Outward heat flux through boundary with indicator 3 (W)
# 19: Visualization file name
   0 0.0000e+00 256 2467 1089  1 22 1.2225e-02 1.79038621e+00 2.54812273e+00 ...
   1 1.2225e-02 256 2467 1089 40 16 3.7409e-03 5.88727814e+00 8.34299267e+00 ...
   2 1.5966e-02 256 2467 1089 25 15 2.0249e-03 1.08925316e+01 1.54185045e+01 ...
   3 1.7991e-02 256 2467 1089 19 15 1.3658e-03 1.61586242e+01 2.28690070e+01 ...
   4 1.9357e-02 256 2467 1089 16 14 1.0291e-03 2.14311381e+01 3.03519178e+01 ...
   5 2.0386e-02 256 2467 1089 14 14 8.2853e-04 2.65966688e+01 3.76989179e+01 ...
```

In other words, it first lists what the individual columns mean with a hash mark at the beginning of the line and then has one line for each time step in which the individual columns list what has been explained above. In the example shown here, the first time step appears twice because we use a mesh that starts out globally refined and we then start the entire computation over again on a once adaptively refined mesh (see the parameters in Section 5.38 for how to do that).

This file is easy to visualize. For example, one can import it as a whitespace separated file into a spreadsheet such as Microsoft Excel or OpenOffice/LibreOffice Calc and then generate graphs of one column against another. Or, maybe simpler, there is a multitude of simple graphing programs that do not need the overhead of a full fledged spreadsheet engine and simply plot graphs. One that is particularly simple to use and available on every major platform is `Gnuplot`. It is extensively documented at http://www.gnuplot.info/.

`Gnuplot` is a command line program in which you enter commands that plot data or modify the way data is plotted. When you call it, you will first get a screen that looks like this:

```
/home/user/aspect/output$ gnuplot

        G N U P L O T
        Version 4.6 patchlevel 0     last modified 2012-03-04
        Build System: Linux x86_64

        Copyright (C) 1986-1993, 1998, 2004, 2007-2012
        Thomas Williams, Colin Kelley and many others

        gnuplot home:     http://www.gnuplot.info
        faq, bugs, etc:   type "help FAQ"
        immediate help:   type "help"  (plot window: hit 'h')

Terminal type set to 'qt'
gnuplot>
```

At the prompt on the last line, you can then enter commands. Given the description of the individual columns given above, let us first try to plot the heat flux through boundary 2 (which in this case is the bottom boundary of the box), i.e., column 17, as a function of time (column 2). This can be achieved using the following command:

```
plot "statistics" using 2:17
```

The left panel of Fig. 4 shows what `Gnuplot` will display in its output window. There are many things one can configure in these plots (see the `Gnuplot` manual referenced above). For example, let us assume that we want to add labels to the x- and y-axes, use not just points but lines and points for the curves, restrict the time axis to the range $[0, 0.2]$ and the heat flux axis to $[-10 : 10]$, plot not only the flux through the

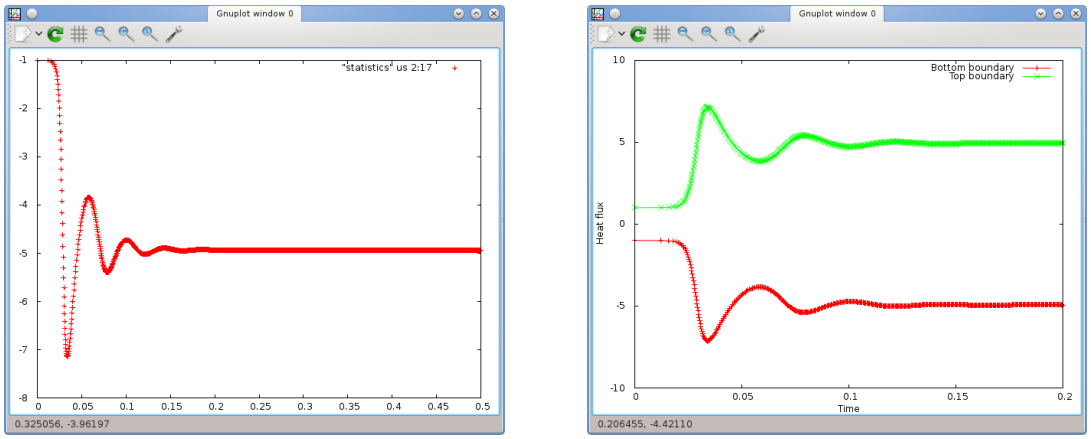


Figure 4: *Visualizing the statistics file obtained from the example in Section 6.1.1 using* **Gnuplot***: Output using simple commands.*

bottom but also through the top boundary (column 18) and finally add a key to the figure, then the following commands achieve this:

```
set xlabel "Time"
set ylabel "Heat flux"
set style data linespoints
plot [0:0.2][-10:10] "statistics" using 2:17 title "Bottom boundary", \
                     "statistics" using 2:18 title "Top boundary"
```

If a line gets too long, you can continue it by ending it in a backslash as above. This is rarely used on the command line but useful when writing the commands above into a script file, see below. We have done it here to get the entire command into the width of the page.

For those who are lazy, **Gnuplot** allows to abbreviate things in many different ways. For example, one can abbreviate most commands. Furthermore, one does not need to repeat the name of an input file if it is the same as the previous one in a plot command. Thus, instead of the commands above, the following abbreviated form would have achieved the same effect:

```
se xl "Time"
se yl "Heat flux"
se sty da lp
pl [:0.2][-10:10] "statistics" us 2:17 t "Bottom boundary", "" us 2:18 t "Top boundary"
```

This is of course unreadable at first but becomes useful once you become more familiar with the command offered by this program.

Once you have gotten the commands that create the plot you want right, you probably want to save it into a file. **Gnuplot** can write output in many different formats. For inclusion in publications, either **eps** or **png** are the most common. In the latter case, the commands to achieve this are

```
set terminal png
set output "heatflux.png"
replot
```

The last command will simply generate the same plot again but this time into the given file. The result is a graphics file similar to the one shown in Fig. 6 on page 71.

Note: After setting output to a file, *all* following plot commands will want to write to this file. Thus, if you want to create more plots after the one just created, you need to reset output back to the screen. On linux, this is done using the command `set terminal X11`. You can then continue experimenting with plots and when you have the next plot ready, switch back to output to a file.

What makes `Gnuplot` so useful is that it doesn't just allow entering all these commands at the prompt. Rather, one can write them all into a file, say `plot-heatflux.gnuplot`, and then, on the command line, call

```
gnuplot plot-heatflux.gnuplot
```

to generate the `heatflux.png` file. This comes in handy if one wants to create the same plot for multiple simulations while playing with parameters of the physical setup. It is also a very useful tool if one wants to generate the same kind of plot again later with a different data set, for example when a reviewer requested additional computations to be made for a paper or if one realizes that one has forgotten or misspelled an axis label in a plot.[10]

`Gnuplot` has many many more features we have not even touched upon. For example, it is equally happy to produce three-dimensional graphics, and it also has statistics modules that can do things like curve fits, statistical regression, and many more operations on the data you provide in the columns of an input file. We will not try to cover them here but instead refer to the manual at http://www.gnuplot.info/. You can also get a good amount of information by typing `help` at the prompt, or a command like `help plot` to get help on the `plot` command.

4.4.3 Large data issues for parallel computations

Among the challenges in visualizing the results of parallel computations is dealing with the large amount of data. The first bottleneck this presents is during run-time when ASPECT wants to write the visualization data of a time step to disk. Using the compressed VTU format, ASPECT generates on the order of 10 bytes of output for each degree of freedom in 2d and more in 3d; thus, output of a single time step can run into the range of gigabytes that somehow have to get from compute nodes to disk. This stresses both the cluster interconnect as well as the data storage array.

There are essentially two strategies supported by ASPECT for this scenario:

- If your cluster has a fast interconnect, for example Infiniband, and if your cluster has a fast, distributed file system, then ASPECT can produce output files that are already located in the correct output directory (see the options in Section 5.2) on the global file system. ASPECT uses MPI I/O calls to this end, ensuring that the local machines do not have to access these files using slow NFS-mounted global file systems.

- If your cluster has a slow interconnect, e.g., if it is simply a collection of machines connected via ethernet, then writing data to a central file server may block the rest of the program for a while. On the other hand, if your machines have fast local storage for temporary file systems, then ASPECT can write data first into such a file and then move it in the background to its final destination while already continuing computations. To select this mode, set the appropriate variables discussed in Section 5.43. Note, however, that this scheme only makes sense if every machine on which MPI processes run has fast local disk space for temporary storage.

[10] In my own work, I usually save the ASPECT input file, the `statistics` output file and the `Gnuplot` script along with the actual figure I want to include in a paper. This way, it is easy to either re-run an entire simulation, or just tweak the graphic at a later time. Speaking from experience, you will not believe how often one wants to tweak a figure long after it was first created. In such situations it is outstandingly helpful if one still has both the actual data as well as the script that generated the graphic.

Note: An alternative would be if every processor directly writes its own files into the global output directory (possibly in the background), without the intermediate step of the temporary file. In our experience, file servers are quickly overwhelmed when encountering a few hundred machines wanting to open, fill, flush and close their own file via NFS mounted file system calls, sometimes completely blocking the entire cluster environment for extended periods of time.

4.5 Checkpoint/restart support

If you do long runs, especially when using parallel computations, there are a number of reasons to periodically save the state of the program:

- If the program crashes for whatever reason, the entire computation may be lost. A typical reason is that a program has exceeded the requested wallclock time allocated by a batch scheduler on a cluster.
- Most of the time, no realistic initial conditions for strongly convecting flow are available. Consequently, one typically starts with a somewhat artificial state and simply waits for a long while till the convective state enters the phase where it shows its long-term behavior. However, getting there may take a good amount of CPU time and it would be silly to always start from scratch for each different parameter setting. Rather, one would like to start such parameter studies with a saved state that has already passed this initial, unphysical, transient stage.

To this end, ASPECT creates a set of files in the output directory (selected in the parameter file) every 50 time steps in which the entire state of the program is saved so that a simulation can later be continued at this point. The previous checkpoint files will then be deleted. To resume operations from the last saved state, you need to set the `Resume computation` flag in the input parameter file to `true`, see Section 5.2.

Note: It is not imperative that the parameters selected in the input file are exactly the same when resuming a program from a saved state than what they were at the time when this state was saved. For example, one may want to choose a different parametrization of the material law, or add or remove postprocessors that should be run at the end of each time step. Likewise, the end time, the times at which some additional mesh refinement steps should happen, etc., can be different.
Yet, it is clear that some other things can't be changed: For example, the geometry model that was used to generate the coarse mesh and describe the boundary must be the same before and after resuming a computation. Likewise, you can not currently restart a computation with a different number of processors than initially used to checkpoint the simulation. Not all invalid combinations are easy to detect, and ASPECT may not always realize immediate what is going on if you change a setting that can't be changed. However, you will almost invariably get non-sensical results after some time.

5 Run-time input parameters

5.1 Overview

What ASPECT computes is driven by two things:

- The models implemented in ASPECT. This includes the geometries, the material laws, or the initial conditions currently supported. Which of these models are currently implemented is discussed below; Section 7 discusses in great detail the process of implementing additional models.
- Which of the implemented models is selected, and what their run-time parameters are. For example, you could select a model that prescribes constant coefficients throughout the domain from all the material models currently implemented; you could then select appropriate values for all of these constants.

Both of these selections happen from a parameter file that is read at run time and whose name is specified on the command line. (See also Section 4.1.)

In this section, let us give an overview of what can be selected in the parameter file. Specific parameters, their default values, and allowed values for these parameters are documented in the following subsections. An index with page numbers for all run-time parameters can be found on page 118.

5.1.1 The structure of parameter files

Most of the run-time behavior of ASPECT is driven by a parameter file that looks in essence like this:

```
set Dimension                              = 2
set Resume computation                     = false
set End time                               = 1e10
set CFL number                             = 1.0
set Output directory                       = bin

subsection Mesh refinement
  set Initial adaptive refinement = 1
  set Initial global refinement   = 4
end

subsection Material model
  set Model name                           = simple

  subsection Simple model
    set Reference density                  = 3300
    set Reference temperature              = 293
    set Viscosity                          = 5e24
  end
end

...
```

Some parameters live at the top level, but most parameters are grouped into subsections. An input parameter file is therefore much like a file system: a few files live in the root directory; others are in a nested hierarchy of sub-directories. And just as with files, parameters have both a name (the thing to the left of the equals sign) and a content (what's to the right).

All parameters you can list in this input file have been *declared* in ASPECT. What this means is that you can't just list anything in the input file with entries that are unknown simply being ignored. Rather, if your input file contains a line setting a parameter that is unknown to something, you will get an error message. Likewise, all declared parameters have a description of possible values associated with them – for example, some parameters must be non-negative integers (the number of initial refinement steps), can either be true or false (whether the computation should be resumed from a saved state), or can only be a single element from a selection (the name of the material model). If an entry in your input file doesn't satisfy these constraints, it will be rejected at the time of reading the file (and not when a part of the program actually accesses the value and the programmer has taken the time to also implement some error checking at this location). Finally, because parameters have been declared, you do not *need* to specify a parameter in the input file: if a parameter isn't listed, then the program will simply use the default provided when declaring the parameter.

5.1.2 Categories of parameters

The parameters that can be provided in the input file can roughly be categorized into the following groups:

- Global parameters (see Section 5.2): These parameters determine the overall behavior of the program. Primarily they describe things like the output directory, the end time of the simulation, or whether the computation should be resumed from a previously saved state.

- Parameters for certain aspects of the numerical algorithm: These describe, for example, the specifics of the spatial discretization. In particular, this is the case for parameters concerning the polynomial degree of the finite element approximation (Section 5.13), some details about the stabilization (Section 5.14), and how adaptive mesh refinement is supposed to work (Section 5.38).

- Parameters that describe certain global aspects of the equations to be solved: This includes, for example, a description if certain terms in the model should be omitted or not. See Section 5.39 for the list of parameters in this category.

- Parameters that characterize plugins: Certain behaviors of ASPECT are described by what we call *plugins* – self-contained parts of the code that describe one particular aspect of the simulation. An example would be which of the implemented material models to use, and the specifics of this material model. The sample parameter file above gives an indication of how this works: within a subsection of the file that pertains to the material models, one can select one out of several plugins (or, in the case of the postprocessors, any number, including none, of the available plugins), and one can then specify the specifics of this model in a sub-subsection dedicated to this particular model.

  A number of components of ASPECT are implemented via plugins. These are, together with the sections in which their parameters are declared:

  - The material model: Sections 5.26 and following.
  - The geometry: Sections 5.15 and following.
  - The gravity description: Sections 5.18 and following.
  - Initial conditions for the temperature: Sections 5.21 and following.
  - Temperature boundary conditions: Sections 5.3 and following.
  - Postprocessors: Sections 5.40 and following for most postprocessors, section 5.43 and following for postprocessors related to visualization.

The details of parameters in each of these categories can be found in the sections linked to above. Some of them will also be used in the cookbooks in Section 6.

5.2 Global parameters

- *Parameter name:* `Adiabatic surface temperature`

  Value: 0

  Default: 0

  Description: In order to make the problem in the first time step easier to solve, we need a reasonable guess for the temperature and pressure. To obtain it, we use an adiabatic pressure and temperature field. This parameter describes what the 'adiabatic' temperature would be at the surface of the domain (i.e. at depth zero). Note that this value need not coincide with the boundary condition posed at this point. Rather, the boundary condition may differ significantly from the adiabatic value, and then typically induce a thermal boundary layer. For more information, see the section in the manual that discusses the general mathematical model.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `CFL number`

  Value: 1.0

  Default: 1.0

  Description: In computations, the time step k is chosen according to $k = c \min_K \frac{h_K}{\|u\|_{\infty,K} p_T}$ where h_K is the diameter of cell K, and the denominator is the maximal magnitude of the velocity on cell K times

the polynomial degree p_T of the temperature discretization. The dimensionless constant c is called the CFL number in this program. For time discretizations that have explicit components, c must be less than a constant that depends on the details of the time discretization and that is no larger than one. On the other hand, for implicit discretizations such as the one chosen here, one can choose the time step as large as one wants (in particular, one can choose $c > 1$) though a CFL number significantly larger than one will yield rather diffusive solutions. Units: None.

Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Composition solver tolerance`

  Value: 1e-12

  Default: 1e-12

  Description: The relative tolerance up to which the linear system for the composition system gets solved. See 'linear solver tolerance' for more details.

  Possible values: [Double 0...1 (inclusive)]

- *Parameter name:* `Dimension`

  Value: 2

  Default: 2

  Description: The number of space dimensions you want to run this program in.

  Possible values: [Integer range 2...4 (inclusive)]

- *Parameter name:* `End time`

  Value: 5e6

  Default: 1e8

  Description: The end time of the simulation. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Linear solver tolerance`

  Value: 1e-7

  Default: 1e-7

  Description: A relative tolerance up to which linear systems in each time or nonlinear step should be solved. The absolute tolerance will then be the norm of the right hand side of the equation times this tolerance. A given tolerance value of 1 would mean that a zero solution vector is an acceptable solution since in that case the norm of the residual of the linear system equals the norm of the right hand side. A given tolerance of 0 would mean that the linear system has to be solved exactly, since this is the only way to obtain a zero residual.

  In practice, you should choose the value of this parameter to be so that if you make it smaller the results of your simulation do not change any more (qualitatively) whereas if you make it larger, they do. For most cases, the default value should be sufficient. However, for cases where the static pressure is much larger than the dynamic one, it may be necessary to choose a smaller value.

  Possible values: [Double 0...1 (inclusive)]

- *Parameter name:* `Nonlinear iteration`

  Value: false

  Default: false

Description: A flag indicating whether the Stokes+Advection equation should be solved once per time step (false) or resolved using a fixed-point iteration (true).

Possible values: [Bool]

- *Parameter name:* `Nonlinear solver scheme`

  Value: IMPES

  Default: IMPES

  Description: The kind of scheme used to resolve the nonlinearity in the system. 'IMPES' is the classical IMplicit Pressure Explicit Saturation scheme in which ones solves the temperatures and Stokes equations exactly once per time step, one after the other. The 'iterated IMPES' scheme iterates this decoupled approach by alternating the solution of the temperature and Stokes systems. The 'iterated Stokes' scheme solves the temperature equation once at the beginning of each time step and then iterates out the solution of the Stokes equation.

  Possible values: [Selection IMPES—iterated IMPES—iterated Stokes]

- *Parameter name:* `Output directory`

  Value: output

  Default: output

  Description: The name of the directory into which all output files should be placed. This may be an absolute or a relative path.

  Possible values: [DirectoryName]

- *Parameter name:* `Pressure normalization`

  Value: surface

  Default: surface

  Description: If and how to normalize the pressure after the solution step. This is necessary because depending on boundary conditions, in many cases the pressure is only determined by the model up to a constant. On the other hand, we often would like to have a well-determined pressure, for example for table lookups of material properties in models or for comparing solutions. If the given value is 'surface', then normalization at the end of each time steps adds a constant value to the pressure in such a way that the average pressure at the surface of the domain is zero; the surface of the domain is determined by asking the geometry model whether a particular face of the geometry has a zero or small 'depth'. If the value of this parameter is 'volume' then the pressure is normalized so that the domain average is zero. If 'no' is given, the no pressure normalization is performed.

  Possible values: [Selection surface—volume—no]

- *Parameter name:* `Resume computation`

  Value: false

  Default: false

  Description: A flag indicating whether the computation should be resumed from a previously saved state (if true) or start from scratch (if false).

  Possible values: [Bool]

- *Parameter name:* `Start time`

  Value: 0

  Default: 0

Description: The start time of the simulation. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Surface pressure`

  Value: 0

  Default: 0

  Description: The mathematical equations that describe thermal convection only determine the pressure up to an arbitrary constant. On the other hand, for comparison and for looking up material parameters it is important that the pressure be normalized somehow. We do this by enforcing a particular average pressure value at the surface of the domain, where the geometry model determines where the surface is. This parameter describes what this average surface pressure value is supposed to be. By default, it is set to zero, but one may want to choose a different value for example for simulating only the volume of the mantle below the lithosphere, in which case the surface pressure should be the lithostatic pressure at the bottom of the lithosphere. For more information, see the section in the manual that discusses the general mathematical model.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Temperature solver tolerance`

  Value: 1e-12

  Default: 1e-12

  Description: The relative tolerance up to which the linear system for the temperature system gets solved. See 'linear solver tolerance' for more details.

  Possible values: [Double 0...1 (inclusive)]

- *Parameter name:* `Timing output frequency`

  Value: 100

  Default: 100

  Description: How frequently in timesteps to output timing information. This is generally adjusted only for debugging and timing purposes.

  Possible values: [Integer range 0...2147483647 (inclusive)]

- *Parameter name:* `Use conduction timestep`

  Value: false

  Default: false

  Description: Mantle convection simulations are often focused on convection dominated systems. However, these codes can also be used to investigate systems where heat conduction plays a dominant role. This parameter indicates whether the simulator should also use heat conduction in determining the length of each time step.

  Possible values: [Bool]

- *Parameter name:* `Use years in output instead of seconds`

  Value: false

  Default: true

  Description: When computing results for mantle convection simulations, it is often difficult to judge the order of magnitude of results when they are stated in MKS units involving seconds. Rather, some kinds of results such as velocities are often stated in terms of meters per year (or, sometimes, centimeters per

year). On the other hand, for non-dimensional computations, one wants results in their natural unit system as used inside the code. If this flag is set to 'true' conversion to years happens; if it is 'false', no such conversion happens.

Possible values: [Bool]

5.3 Parameters in section `Boundary temperature model`

- *Parameter name:* `Model name`

  Value: box

  Default:

  Description: Select one of the following models:

  'box': A model in which the temperature is chosen constant on all the sides of a box.

  'spherical constant': A model in which the temperature is chosen constant on the inner and outer boundaries of a spherical shell. Parameters are read from subsection 'Sherical constant'.

  'Tan Gurnis': A model for the Tan/Gurnis benchmark.

  Possible values: [Selection box—spherical constant—Tan Gurnis]

5.4 Parameters in section `Boundary temperature model/Box`

- *Parameter name:* `Bottom temperature`

  Value: 0

  Default: 0

  Description: Temperature at the bottom boundary (at minimal z-value). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Left temperature`

  Value: 1

  Default: 1

  Description: Temperature at the left boundary (at minimal x-value). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Right temperature`

  Value: 0

  Default: 0

  Description: Temperature at the right boundary (at maximal x-value). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Top temperature`

  Value: 0

  Default: 0

  Description: Temperature at the top boundary (at maximal x-value). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

5.5 Parameters in section `Boundary temperature model/Spherical constant`

- *Parameter name:* `Inner temperature`

  Value: 6000

  Default: 6000

  Description: Temperature at the inner boundary (core mantle boundary). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Outer temperature`

  Value: 0

  Default: 0

  Description: Temperature at the outer boundary (lithosphere water/air). Units: K.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

5.6 Parameters in section `Boundary velocity model`

5.7 Parameters in section `Boundary velocity model/Function`

- *Parameter name:* `Function constants`

  Value:

  Default:

  Description: Sometimes it is convenient to use symbolic constants in the expression that describes the function, rather than having to use its numeric value everywhere the constant appears. These values can be defined using this parameter, in the form 'var1=value1, var2=value2, ...'.

  A typical example would be to set this runtime parameter to 'pi=3.1415926536' and then use 'pi' in the expression of the actual formula. (That said, for convenience this class actually defines both 'pi' and 'Pi' by default, but you get the idea.)

  Possible values: [Anything]

- *Parameter name:* `Function expression`

  Value: 0; 0

  Default: 0; 0

  Description: The formula that denotes the function you want to evaluate for particular values of the independent variables. This expression may contain any of the usual operations such as addition or multiplication, as well as all of the common functions such as 'sin' or 'cos'. In addition, it may contain expressions like 'if(x¿0, 1, -1)' where the expression evaluates to the second argument if the first argument is true, and to the third argument otherwise. For a full overview of possible expressions accepted see the documentation of the fparser library.

  If the function you are describing represents a vector-valued function with multiple components, then separate the expressions for individual components by a semicolon.

  Possible values: [Anything]

- *Parameter name:* `Variable names`

  Value: x,y,t

  Default: x,y,t

  Description: The name of the variables as they will be used in the function, separated by commas. By default, the names of variables at which the function will be evaluated is 'x' (in 1d), 'x,y' (in 2d) or

'x,y,z' (in 3d) for spatial coordinates and 't' for time. You can then use these variable names in your function expression and they will be replaced by the values of these variables at which the function is currently evaluated. However, you can also choose a different set of names for the independent variables at which to evaluate your function expression. For example, if you work in spherical coordinates, you may wish to set this input parameter to 'r,phi,theta,t' and then use these variable names in your function expression.

Possible values: [Anything]

5.8 Parameters in section `Boundary velocity model/GPlates model`

- *Parameter name:* `Data directory`

  Value: data/velocity-boundary-conditions/gplates/

  Default: data/velocity-boundary-conditions/gplates/

  Description: The path to the model data.

  Possible values: [DirectoryName]

- *Parameter name:* `Point one`

  Value: 1.570796,0.0

  Default: 1.570796,0.0

  Description: Point that determines the plane in which a 2D model lies in. Has to be in the format 'a,b' where a and b are theta (polar angle) and phi in radians.

  Possible values: [Anything]

- *Parameter name:* `Point two`

  Value: 1.570796,1.570796

  Default: 1.570796,1.570796

  Description: Point that determines the plane in which a 2D model lies in. Has to be in the format 'a,b' where a and b are theta (polar angle) and phi in radians.

  Possible values: [Anything]

- *Parameter name:* `Time step`

  Value: 3.1558e13

  Default: 3.1558e13

  Description: Time step between following velocity files. Default is one million years expressed in SI units.

  Possible values: [Anything]

- *Parameter name:* `Velocity file name`

  Value: phi_test.

  Default: phi_test.

  Description: The file name of the material data. Provide file in format: (Velocity file name).

  Possible values: [Anything]

- *Parameter name:* `Velocity file start time`

  Value: 0.0

  Default: 0.0

  Description: Time at which the velocity file with number 0 shall be loaded.Previous to this time, a no-slip boundary condition is assumed.

  Possible values: [Anything]

5.9 Parameters in section `Checkpointing`

- *Parameter name:* `Steps between checkpoint`

  Value: 50

  Default: 0

  Description: The number of timesteps between performing checkpoints. If 0 and time between checkpoint is not specified, checkpointing will not be performed. Units: None.

  Possible values: [Integer range 0...2147483647 (inclusive)]

- *Parameter name:* `Time between checkpoint`

  Value: 0

  Default: 0

  Description: The wall time between performing checkpoints. If 0, will use the checkpoint step frequency instead. Units: Seconds.

  Possible values: [Integer range 0...2147483647 (inclusive)]

5.10 Parameters in section `Compositional fields`

- *Parameter name:* `List of normalized fields`

  Value:

  Default:

  Description: A list of integers smaller than or equal to the number of compositional fields. All compositional fields in this list will be normalized before the first timestep. The normalization is implemented in the following way: First, the sum of the fields to be normalized is calculated at every point and the global maximum is determined. Second, the compositional fields to be normalized are divided by this maximum.

  Possible values: [List list of ¡[Integer range 0...2147483647 (inclusive)]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Number of fields`

  Value: 0

  Default: 0

  Description: The number of fields that will be advected along with the flow field, excluding velocity, pressure and temperature.

  Possible values: [Integer range 0...2147483647 (inclusive)]

5.11 Parameters in section `Compositional initial conditions`

- *Parameter name:* `Model name`

  Value: function

  Default: function

  Description: Select one of the following models:

  'function': Composition is given in terms of an explicit formula

  Possible values: [Selection function]

5.12 Parameters in section `Compositional initial conditions/Function`

- *Parameter name:* `Function constants`

  Value:

  Default:

  Description: Sometimes it is convenient to use symbolic constants in the expression that describes the function, rather than having to use its numeric value everywhere the constant appears. These values can be defined using this parameter, in the form 'var1=value1, var2=value2, ...'.

  A typical example would be to set this runtime parameter to 'pi=3.1415926536' and then use 'pi' in the expression of the actual formula. (That said, for convenience this class actually defines both 'pi' and 'Pi' by default, but you get the idea.)

  Possible values: [Anything]

- *Parameter name:* `Function expression`

  Value: 0

  Default: 0

  Description: The formula that denotes the function you want to evaluate for particular values of the independent variables. This expression may contain any of the usual operations such as addition or multiplication, as well as all of the common functions such as 'sin' or 'cos'. In addition, it may contain expressions like 'if(x¿0, 1, -1)' where the expression evaluates to the second argument if the first argument is true, and to the third argument otherwise. For a full overview of possible expressions accepted see the documentation of the fparser library.

  If the function you are describing represents a vector-valued function with multiple components, then separate the expressions for individual components by a semicolon.

  Possible values: [Anything]

- *Parameter name:* `Variable names`

  Value: x,y,t

  Default: x,y,t

  Description: The name of the variables as they will be used in the function, separated by commas. By default, the names of variables at which the function will be evaluated is 'x' (in 1d), 'x,y' (in 2d) or 'x,y,z' (in 3d) for spatial coordinates and 't' for time. You can then use these variable names in your function expression and they will be replaced by the values of these variables at which the function is currently evaluated. However, you can also choose a different set of names for the independent variables at which to evaluate your function expression. For example, if you work in spherical coordinates, you may wish to set this input parameter to 'r,phi,theta,t' and then use these variable names in your function expression.

  Possible values: [Anything]

5.13 Parameters in section `Discretization`

- *Parameter name:* `Composition polynomial degree`

  Value: 2

  Default: 2

  Description: The polynomial degree to use for the composition variable(s). Units: None.

  Possible values: [Integer range 1...2147483647 (inclusive)]

- *Parameter name:* `Stokes velocity polynomial degree`

  Value: 2

  Default: 2

  Description: The polynomial degree to use for the velocity variables in the Stokes system. The polynomial degree for the pressure variable will then be one less in order to make the velocity/pressure pair conform with the usual LBB (Babuska-Brezzi) condition. In other words, we are using a Taylor-Hood element for the Stoeks equations and this parameter indicates the polynomial degree of it. Units: None.

  Possible values: [Integer range 1...2147483647 (inclusive)]

- *Parameter name:* `Temperature polynomial degree`

  Value: 2

  Default: 2

  Description: The polynomial degree to use for the temperature variable. Units: None.

  Possible values: [Integer range 1...2147483647 (inclusive)]

- *Parameter name:* `Use locally conservative discretization`

  Value: false

  Default: false

  Description: Whether to use a Stokes discretization that is locally conservative at the expense of a larger number of degrees of freedom (true), or to go with a cheaper discretization that does not locally conserve mass, although it is globally conservative (false).

  When using a locally conservative discretization, the finite element space for the pressure is discontinuous between cells and is the polynomial space P_{-q} of polynomials of degree q in each variable separately. Here, q is one less than the value given in the parameter "Stokes velocity polynomial degree". As a consequence of choosing this element, it can be shown if the medium is considered incompressible that the computed discrete velocity field $\mathbf{u}_h$ satisfies the property $\int_{\partial K} \mathbf{u}_h \cdot \mathbf{n} = 0$ for every cell K, i.e., for each cell inflow and outflow exactly balance each other as one would expect for an incompressible medium. In other words, the velocity field is locally conservative.

  On the other hand, if this parameter is set to "false", then the finite element space is chosen as Q_q. This choice does not yield the local conservation property but has the advantage of requiring fewer degrees of freedom. Furthermore, the error is generally smaller with this choice.

  For an in-depth discussion of these issues and a quantitative evaluation of the different choices, see [KHB12].

  Possible values: [Bool]

5.14 Parameters in section `Discretization/Stabilization parameters`

- *Parameter name:* `alpha`

  Value: 2

  Default: 2

  Description: The exponent α in the entropy viscosity stabilization. Units: None.

  Possible values: [Double 1...2 (inclusive)]

- *Parameter name:* `beta`

  Value: 0.078

  Default: 0.078

  Description: The β factor in the artificial viscosity stabilization. An appropriate value for 2d is 0.078 and 0.117 for 3d. Units: None.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `cR`

  Value: 0.5

  Default: 0.33

  Description: The c_R factor in the entropy viscosity stabilization. Units: None.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.15 Parameters in section `Geometry model`

- *Parameter name:* `Model name`

  Value: box

  Default:

  Description: Select one of the following models:

  'box': A box geometry parallel to the coordinate directions. The extent of the box in each coordinate direction is set in the parameter file. The box geometry labels its 2*dim sides as follows: in 2d, boundary indicators 0 through 3 denote the left, right, bottom and top boundaries; in 3d, boundary indicators 0 through 5 indicate left, right, front, back, bottom and top boundaries. See also the documentation of the deal.II class "GeometryInfo".

  'spherical shell': A geometry representing a spherical shell or a pice of it. Inner and outer radii are read from the parameter file in subsection 'Spherical shell'.

  Possible values: [Selection box—spherical shell]

5.16 Parameters in section `Geometry model/Box`

- *Parameter name:* `X extent`

  Value: 1.2

  Default: 1

  Description: Extent of the box in x-direction. Units: m.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Y extent`

  Value: 1

  Default: 1

  Description: Extent of the box in y-direction. Units: m.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Z extent`

  Value: 1

  Default: 1

  Description: Extent of the box in z-direction. This value is ignored if the simulation is in 2d Units: m.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.17 Parameters in section `Geometry model/Spherical shell`

- *Parameter name:* `Inner radius`

  Value: 3481000

  Default: 3481000

  Description: Inner radius of the spherical shell. Units: m.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Opening angle`

  Value: 360

  Default: 360

  Description: Opening angle in degrees of the section of the shell that we want to build. Units: degrees.

  Possible values: [Double 0...360 (inclusive)]

- *Parameter name:* `Outer radius`

  Value: 6336000

  Default: 6336000

  Description: Outer radius of the spherical shell. Units: m.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.18 Parameters in section `Gravity model`

- *Parameter name:* `Model name`

  Value: vertical

  Default:

  Description: Select one of the following models:

  'radial constant': A gravity model in which the gravity direction is radially inward and at constant magnitude. The magnitude is read from the parameter file in subsection 'Radial constant'.

  'radial earth-like': A gravity model in which the gravity direction is radially inward and with a magnitude that matches that of the earth at the core-mantle boundary as well as at the surface and in between is physically correct under the assumption of a constant density.

  'vertical': A gravity model in which the gravity direction is vertically downward and at a constant magnitude by default equal to one.

  Possible values: [Selection radial constant—radial earth-like—vertical]

5.19 Parameters in section `Gravity model/Radial constant`

- *Parameter name:* `Magnitude`

  Value: 30

  Default: 30

  Description: Magnitude of the gravity vector in m/s^2. The direction is always radially outward from the center of the earth.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.20 Parameters in section `Gravity model/Vertical`

- *Parameter name:* `Magnitude`

  Value: 1

  Default: 1

  Description: Value of the gravity vector in m/s^2 directed along negative y (2D) or z (3D) axis.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.21 Parameters in section `Initial conditions`

- *Parameter name:* `Model name`

  Value: perturbed box

  Default:

  Description: Select one of the following models:

  'adiabatic': Temperature is prescribed as an adiabatic profile with upper and lower thermal boundary layers,whose ages are given as input parameters.

  'perturbed box': An initial temperature field in which the temperature is perturbed slightly from an otherwise constant value equal to one. The perturbation is chosen in such a way that the initial temperature is constant to one along the entire boundary.

  'function': Temperature is given in terms of an explicit formula

  'spherical hexagonal perturbation': An initial temperature field in which the temperature is perturbed following a six-fold pattern in angular direction from an otherwise spherically symmetric state.

  'spherical gaussian perturbation': An initial temperature field in which the temperature is perturbed by a single Gaussian added to an otherwise spherically symmetric state. Additional parameters are read from the parameter file in subsection 'Spherical gaussian perturbation'.

  Possible values: [Selection adiabatic—perturbed box—function—spherical hexagonal perturbation—spherical gaussian perturbation]

5.22 Parameters in section `Initial conditions/Adiabatic`

- *Parameter name:* `Age bottom boundary layer`

  Value: 0e0

  Default: 0e0

  Description: The age of the lower thermal boundary layer, used for the calculationof the half-space cooling model temperature. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Age top boundary layer`

  Value: 0e0

  Default: 0e0

  Description: The age of the upper thermal boundary layer, used for the calculationof the half-space cooling model temperature. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Amplitude`

  Value: 0e0

  Default: 0e0

  Description: The amplitude (in K) of the initial spherical temperature perturbationat the bottom of the model domain. This perturbation will be added tothe adiabatic temperature profile, but not to the bottom thermalboundary layer. Instead, the maximum of the perturbation and the bottomboundary layer temperature will be used.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Position`

  Value: center

  Default: center

  Description: Where the initial temperature perturbation should be placed (in the center or at the boundary of the model domain).

  Possible values: [Selection center—boundary]

- *Parameter name:* `Radius`

  Value: 0e0

  Default: 0e0

  Description: The Radius (in m) of the initial spherical temperature perturbationat the bottom of the model domain.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Subadiabaticity`

  Value: 0e0

  Default: 0e0

  Description: If this value is larger than 0, the initial temperature profile willnot be adiabatic, but subadiabatic. This value gives the maximal deviation from adiabaticity. Set to 0 for an adiabatic temperature profile. Units: K. The function object in the Function subsectionrepresents the compositional fields that will be used as a reference profile for calculating the thermal diffusivity.The function depends only on depth.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.23 Parameters in section `Initial conditions/Adiabatic/Function`

- *Parameter name:* `Function constants`

  Value:

  Default:

  Description: Sometimes it is convenient to use symbolic constants in the expression that describes the function, rather than having to use its numeric value everywhere the constant appears. These values can be defined using this parameter, in the form 'var1=value1, var2=value2, ...'.

  A typical example would be to set this runtime parameter to 'pi=3.1415926536' and then use 'pi' in the expression of the actual formula. (That said, for convenience this class actually defines both 'pi' and 'Pi' by default, but you get the idea.)

  Possible values: [Anything]

- *Parameter name:* `Function expression`

  Value: 0

  Default: 0

  Description: The formula that denotes the function you want to evaluate for particular values of the independent variables. This expression may contain any of the usual operations such as addition or multiplication, as well as all of the common functions such as 'sin' or 'cos'. In addition, it may contain expressions like 'if(x¿0, 1, -1)' where the expression evaluates to the second argument if the first argument is true, and to the third argument otherwise. For a full overview of possible expressions accepted see the documentation of the fparser library.

  If the function you are describing represents a vector-valued function with multiple components, then separate the expressions for individual components by a semicolon.

  Possible values: [Anything]

- *Parameter name:* `Variable names`

  Value: x,t

  Default: x,t

  Description: The name of the variables as they will be used in the function, separated by commas. By default, the names of variables at which the function will be evaluated is 'x' (in 1d), 'x,y' (in 2d) or 'x,y,z' (in 3d) for spatial coordinates and 't' for time. You can then use these variable names in your function expression and they will be replaced by the values of these variables at which the function is currently evaluated. However, you can also choose a different set of names for the independent variables at which to evaluate your function expression. For example, if you work in spherical coordinates, you may wish to set this input parameter to 'r,phi,theta,t' and then use these variable names in your function expression.

  Possible values: [Anything]

5.24 Parameters in section `Initial conditions/Function`

- *Parameter name:* `Function constants`

  Value:

  Default:

  Description: Sometimes it is convenient to use symbolic constants in the expression that describes the function, rather than having to use its numeric value everywhere the constant appears. These values can be defined using this parameter, in the form 'var1=value1, var2=value2, ...'.

A typical example would be to set this runtime parameter to 'pi=3.1415926536' and then use 'pi' in the expression of the actual formula. (That said, for convenience this class actually defines both 'pi' and 'Pi' by default, but you get the idea.)

Possible values: [Anything]

- *Parameter name:* `Function expression`

  Value: 0

  Default: 0

  Description: The formula that denotes the function you want to evaluate for particular values of the independent variables. This expression may contain any of the usual operations such as addition or multiplication, as well as all of the common functions such as 'sin' or 'cos'. In addition, it may contain expressions like 'if(x¿0, 1, -1)' where the expression evaluates to the second argument if the first argument is true, and to the third argument otherwise. For a full overview of possible expressions accepted see the documentation of the fparser library.

  If the function you are describing represents a vector-valued function with multiple components, then separate the expressions for individual components by a semicolon.

  Possible values: [Anything]

- *Parameter name:* `Variable names`

  Value: x,y,t

  Default: x,y,t

  Description: The name of the variables as they will be used in the function, separated by commas. By default, the names of variables at which the function will be evaluated is 'x' (in 1d), 'x,y' (in 2d) or 'x,y,z' (in 3d) for spatial coordinates and 't' for time. You can then use these variable names in your function expression and they will be replaced by the values of these variables at which the function is currently evaluated. However, you can also choose a different set of names for the independent variables at which to evaluate your function expression. For example, if you work in spherical coordinates, you may wish to set this input parameter to 'r,phi,theta,t' and then use these variable names in your function expression.

  Possible values: [Anything]

5.25 Parameters in section `Initial conditions/Spherical gaussian perturbation`

- *Parameter name:* `Amplitude`

  Value: 0.01

  Default: 0.01

  Description: The amplitude of the perturbation.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Angle`

  Value: 0e0

  Default: 0e0

  Description: The angle where the center of the perturbation is placed.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Filename for initial geotherm table`

  Value: initial_geotherm_table

  Default: initial_geotherm_table

  Description: The file from which the initial geotherm table is to be read. The format of the file is defined by what is read in source/initial_conditions/spherical_shell.cc.

  Possible values: [FileName (Type: input)]

- *Parameter name:* `Non-dimensional depth`

  Value: 0.7

  Default: 0.7

  Description: The non-dimensional radial distance where the center of the perturbation is placed.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Sigma`

  Value: 0.2

  Default: 0.2

  Description: The standard deviation of the Gaussian perturbation.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Sign`

  Value: 1

  Default: 1

  Description: The sign of the perturbation.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

5.26 Parameters in section `Material model`

- *Parameter name:* `Model name`

  Value: simple

  Default:

  Description: Select one of the following models:

  'SolCx': A material model that corresponds to the 'SolCx' benchmark defined in Duretz et al., G-Cubed, 2011.

  'SolKz': A material model that corresponds to the 'SolKz' benchmark defined in Duretz et al., G-Cubed, 2011.

  'Inclusion': A material model that corresponds to the 'Inclusion' benchmark defined in Duretz et al., G-Cubed, 2011.

  'simple': A simple material model that has constant values for all coefficients but the density and viscosity. This model uses the formulation that assumes an incompressible medium despite the fact that the density follows the law $\rho(T) = \rho_0(1-\beta(T-T_{\text{ref}})$. The temperature dependency of viscosity is switched off by default and follows the formula$\eta(T) = \eta_0 * e^{\eta_T * \Delta T/T_{\text{ref}})}$.The value for the components of this formula and additional parameters are read from the parameter file in subsection 'Simple model'.

  'Steinberger': lookup viscosity from the paper of Steinberger/Calderwood2006 and material data from a database generated by Perplex. The database builds upon the thermodynamic database by Stixrude 2011 and assumes a pyrolitic composition by Ringwood 1988.

'table': A material model that reads tables of pressure and temperature dependent material coefficients from files. The default values for this model's runtime parameters use a material description taken from the paper *Complex phase distribution and seismic velocity structure of the transition zone: Convection model predictions for a magnesium-endmember olivine-pyroxene mantle* by Michael H.G. Jacobs and Arie P. van den Berg, Physics of the Earth and Planetary Interiors, Volume 186, Issues 1-2, May 2011, Pages 36–48. See http://www.sciencedirect.com/science/article/pii/S0031920111000422.

'Tan Gurnis': A simple compressible material model based on a benchmark from the paper of Tan/Gurnis (2007). This does not use the temperature equation, but has a hardcoded temperature.

Possible values: [Selection SolCx—SolKz—Inclusion—simple—Steinberger—table—Tan Gurnis]

5.27 Parameters in section `Material model/Inclusion`

- *Parameter name:* `Viscosity jump`

  Value: 1e3

  Default: 1e3

  Description: Viscosity in the Inclusion.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.28 Parameters in section `Material model/Simple model`

- *Parameter name:* `Composition viscosity prefactor`

  Value: 1.0

  Default: 1.0

  Description: A linear dependency of viscosity on composition. Dimensionless prefactor.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Density differential for compositional field 1`

  Value: 0

  Default: 0

  Description: If compositional fields are used, then one would frequently want to make the density depend on these fields. In this simple material model, we make the following assumptions: if no compositional fields are used in the current simulation, then the density is simply the usual one with its linear dependence on the temperature. If there are compositional fields, then the density only depends on the first one in such a way that the density has an additional term of the kind $+\Delta\rho\, c_1(\mathbf{x})$. This parameter describes the value of $\Delta\rho$. Units: kg/m^3/unit change in composition.

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Reference density`

  Value: 1

  Default: 3300

  Description: Reference density ρ_0. Units: kg/m^3.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Reference specific heat`

  Value: 1250

  Default: 1250

Description: The value of the specific heat cp. Units: $J/kg/K$.

Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Reference temperature`

  Value: 1

  Default: 293

  Description: The reference temperature T_0. Units: K.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Thermal conductivity`

  Value: 1e-6

  Default: 4.7

  Description: The value of the thermal conductivity k. Units: $W/m/K$.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Thermal expansion coefficient`

  Value: 2e-5

  Default: 2e-5

  Description: The value of the thermal expansion coefficient β. Units: $1/K$.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Thermal viscosity exponent`

  Value: 0.0

  Default: 0.0

  Description: The temperature dependence of viscosity. Dimensionless exponent.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Viscosity`

  Value: 1

  Default: 5e24

  Description: The value of the constant viscosity. Units: $kg/m/s$.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.29 Parameters in section `Material model/SolCx`

- *Parameter name:* `Background density`

  Value: 0

  Default: 0

  Description: Density value upon which the variation of this testcase is overlaid. Since this background density is constant it does not affect the flow pattern but it adds to the total pressure since it produces a nonzero adiabatic pressure if set to a nonzero value.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Viscosity jump`

  Value: 1e6

  Default: 1e6

  Description: Viscosity in the right half of the domain.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.30 Parameters in section `Material model/Steinberger model`

- *Parameter name:* `Bilinear interpolation`

  Value: true

  Default: true

  Description: whether to use bilinear interpolation to compute material properties (slower but more accurate).

  Possible values: [Bool]

- *Parameter name:* `Data directory`

  Value: data/material-model/steinberger/

  Default: data/material-model/steinberger/

  Description: The path to the model data.

  Possible values: [DirectoryName]

- *Parameter name:* `Latent heat`

  Value: false

  Default: false

  Description: whether to include latent heat effects in thecalculation of thermal expansivity and specific heat.Following the approach of Nakagawa et al. 2009.

  Possible values: [Bool]

- *Parameter name:* `Lateral viscosity file name`

  Value: temp_viscosity_prefactor.txt

  Default: temp_viscosity_prefactor.txt

  Description: The file name of the lateral viscosity data.

  Possible values: [Anything]

- *Parameter name:* `Material file names`

  Value: pyr-ringwood88.txt

  Default: pyr-ringwood88.txt

  Description: The file names of the material data. List with as many components as activecompositional fields (material data is assumed tobe in order with the ordering of the fields).

  Possible values: [List list of ¡[Anything]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Radial viscosity file name`

  Value: radial_visc.txt

  Default: radial_visc.txt

  Description: The file name of the radial viscosity data.

  Possible values: [Anything]

5.31 Parameters in section `Material model/Table model`

- *Parameter name:* `Composition`
  Value: standard
  Default: standard
  Description: The Composition of the model.
  Possible values: [Anything]

- *Parameter name:* `Compressible`
  Value: true
  Default: true
  Description: whether the model is compressible.
  Possible values: [Bool]

- *Parameter name:* `ComputePhases`
  Value: false
  Default: false
  Description: whether to compute phases.
  Possible values: [Bool]

- *Parameter name:* `Gravity`
  Value: 30
  Default: 30
  Description: The value of the gravity constant.Units: m/s^2.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Path to model data`
  Value: data/material-model/table/
  Default: data/material-model/table/
  Description: The path to the model data.
  Possible values: [DirectoryName]

- *Parameter name:* `Reference density`
  Value: 3300
  Default: 3300
  Description: Reference density ρ_0. Units: kg/m^3.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Reference specific heat`
  Value: 1250
  Default: 1250
  Description: The value of the specific heat *cp*. Units: $J/kg/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Reference temperature`
  Value: 293
  Default: 293
  Description: The reference temperature T_0. Units: K.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Thermal conductivity`
  Value: 4.7
  Default: 4.7
  Description: The value of the thermal conductivity k. Units: $W/m/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Thermal expansion coefficient`
  Value: 2e-5
  Default: 2e-5
  Description: The value of the thermal expansion coefficient β. Units: $1/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.32 Parameters in section `Material model/Table model/Viscosity`

- *Parameter name:* `Reference Viscosity`
  Value: 5e24
  Default: 5e24
  Description: The value of the constant viscosity. Units: $kg/m/s$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Viscosity Model`
  Value: Exponential
  Default: Exponential
  Description: Viscosity Model
  Possible values: [Anything]
- *Parameter name:* `Viscosity increase lower mantle`
  Value: 1e0
  Default: 1e0
  Description: The Viscosity increase (jump) in the lower mantle.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.33 Parameters in section `Material model/Table model/Viscosity/Composite`

- *Parameter name:* `Activation energy diffusion`
  Value: 335e3
  Default: 335e3
  Description: activation energy for diffusion creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Activation energy dislocation`
  Value: 540e3
  Default: 540e3
  Description: activation energy for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Activation volume diffusion`
  Value: 4.0e-6
  Default: 4.0e-6
  Description: activation volume for diffusion creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Activation volume dislocation`
  Value: 14.0e-6
  Default: 14.0e-6
  Description: activation volume for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Prefactor diffusion`
  Value: 1.92e-11
  Default: 1.92e-11
  Description: prefactor for diffusion creep (1e0/prefactor)*exp((activation_energy+activation_volume*pressure)/(R*temp
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Prefactor dislocation`
  Value: 2.42e-10
  Default: 2.42e-10
  Description: prefactor for dislocation creep (1e0/prefactor)*exp((activation_energy+activation_volume*pressure)/(R*te
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Stress exponent`
  Value: 3.5
  Default: 3.5
  Description: stress exponent for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.34 Parameters in section `Material model/Table model/Viscosity/Diffusion`

- *Parameter name:* `Activation energy diffusion`
  Value: 335e3
  Default: 335e3
  Description: activation energy for diffusion creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Activation volume diffusion`
  Value: 4.0e-6
  Default: 4.0e-6
  Description: activation volume for diffusion creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Prefactor diffusion`
  Value: 1.92e-11
  Default: 1.92e-11
  Description: prefactor for diffusion creep (1e0/prefactor)*exp((activation_energy+activation_volume*pressure)/(R*temp
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.35 Parameters in section `Material model/Table model/Viscosity/Dislocation`

- *Parameter name:* `Activation energy dislocation`
  Value: 335e3
  Default: 335e3
  Description: activation energy for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Activation volume dislocation`
  Value: 4.0e-6
  Default: 4.0e-6
  Description: activation volume for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Prefactor dislocation`
  Value: 1.92e-11
  Default: 1.92e-11
  Description: prefactor for dislocation creep (1e0/prefactor)*exp((activation_energy+activation_volume*pressure)/(R*te
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Stress exponent`
  Value: 3.5
  Default: 3.5
  Description: stress exponent for dislocation creep
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.36 Parameters in section `Material model/Table model/Viscosity/Exponential`

- *Parameter name:* `Exponential P`
  Value: 1
  Default: 1
  Description: multiplication factor or Pressure exponent
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Exponential T`
  Value: 1
  Default: 1
  Description: multiplication factor or Temperature exponent
  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.37 Parameters in section `Material model/Tan Gurnis model`

- *Parameter name:* `Di`
  Value: 0.5
  Default: 0.5
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Reference density`
  Value: 3300
  Default: 3300
  Description: Reference density ρ_0. Units: kg/m^3.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Reference specific heat`
  Value: 1250
  Default: 1250
  Description: The value of the specific heat cp. Units: $J/kg/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Reference temperature`
  Value: 293
  Default: 293
  Description: The reference temperature T_0. Units: K.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Thermal conductivity`
  Value: 4.7
  Default: 4.7
  Description: The value of the thermal conductivity k. Units: $W/m/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]
- *Parameter name:* `Thermal expansion coefficient`
  Value: 2e-5
  Default: 2e-5
  Description: The value of the thermal expansion coefficient β. Units: $1/K$.
  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Viscosity`

  Value: 5e24

  Default: 5e24

  Description: The value of the constant viscosity. Units: $kg/m/s$.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `a`

  Value: 0

  Default: 0

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `gamma`

  Value: 1

  Default: 1

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `wavenumber`

  Value: 1

  Default: 1

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.38 Parameters in section `Mesh refinement`

- *Parameter name:* `Additional refinement times`

  Value:

  Default:

  Description: A list of times so that if the end time of a time step is beyond this time, an additional round of mesh refinement is triggered. This is mostly useful to make sure we can get through the initial transient phase of a simulation on a relatively coarse mesh, and then refine again when we are in a time range that we are interested in and where we would like to use a finer mesh. Units: each element of the list has units years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [List list of ¡[Double 0...1.79769e+308 (inclusive)]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Coarsening fraction`

  Value: 0.05

  Default: 0.05

  Description: The fraction of cells with the smallest error that should be flagged for coarsening.

  Possible values: [Double 0...1 (inclusive)]

- *Parameter name:* `Initial adaptive refinement`

  Value: 1

  Default: 2

  Description: The number of adaptive refinement steps performed after initial global refinement but while still within the first time step.

  Possible values: [Integer range 0...2147483647 (inclusive)]

- *Parameter name:* `Initial global refinement`

  Value: 4

  Default: 2

  Description: The number of global refinement steps performed on the initial coarse mesh, before the problem is first solved there.

  Possible values: [Integer range 0...2147483647 (inclusive)]

- *Parameter name:* `Normalize individual refinement criteria`

  Value: true

  Default: true

  Description: If multiple refinement criteria are specified in the "Strategy" parameter, then they need to be combined somehow to form the final refinement indicators. This is done using the method described by the "Refinement criteria merge operation" parameter which can either operate on the raw refinement indicators returned by each strategy (i.e., dimensional quantities) or using normalized values where the indicators of each strategy are first normalized to the interval $[0,1]$ (which also makes them non-dimensional). This parameter determines whether this normalization will happen.

  Possible values: [Bool]

- *Parameter name:* `Refinement criteria merge operation`

  Value: max

  Default: max

  Description: If multiple mesh refinement criteria are computed for each cell (by passing a list of more than element to the `Strategy` parameter in this section of the input file) then one will have to decide which one should win when deciding which cell to refine. The operation that selects from these competing criteria is the one that is selected here. The options are:

  - `plus`: Add the various error indicators together and refine those cells on which the sum of indicators is largest.
  - `max`: Take the maximum of the various error indicators and refine those cells on which the maximal indicators is largest.

  The refinement indicators computed by each strategy are modified by the "Normalize individual refinement criteria" and "Refinement criteria scale factors" parameters.

  Possible values: [Selection plus—max]

- *Parameter name:* `Refinement criteria scaling factors`

  Value:

  Default:

  Description: A list of scaling factors by which every individual refinement criterion will be multiplied by. If only a single refinement criterion is selected (using the "Strategy" parameter, then this parameter has no particular meaning. On the other hand, if multiple criteria are chosen, then these factors are used to weigh the various indicators relative to each other.

  If "Normalize individual refinement criteria" is set to true, then the criteria will first be normalized to the interval $[0,1]$ and then multiplied by the factors specified here. You will likely want to choose the factors to be not too far from 1 in that case, say between 1 and 10, to avoid essentially disabling those criteria with small weights. On the other hand, if the criteria are not normalized to $[0,1]$ using the parameter mentioned above, then the factors you specify here need to take into account the relative numerical size of refinement indicators (which in that case carry physical units).

You can experimentally play with these scaling factors by choosing to output the refinement indicators into the graphical output of a run.

If the list of indicators given in this parameter is empty, then this indicates that they should all be chosen equal to one. If the list is not empty then it needs to have as many entries as there are indicators chosen in the "Strategy" parameter.

Possible values: [List list of ¡[Double 0...1.79769e+308 (inclusive)]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Refinement fraction`

  Value: 0.3

  Default: 0.3

  Description: The fraction of cells with the largest error that should be flagged for refinement.

  Possible values: [Double 0...1 (inclusive)]

- *Parameter name:* `Run postprocessors on initial refinement`

  Value: false

  Default: false

  Description: Whether or not the postproccessors should be run at the end of each of ths initial adaptive refinement cycles at the of the simulation start.

  Possible values: [Bool]

- *Parameter name:* `Strategy`

  Value: thermal energy density

  Default: thermal energy density

  Description: A comma separated list of mesh refinement criteria that will be run whenever mesh refinement is required. The results of each of these criteria will, i.e., the refinement indicators they produce for all the cells of the mesh will then be normalized to a range between zero and one and the results of different criteria will then be merged through the operation selected in this section.

  The following criteria are available:

  'composition': A mesh refinement criterion that computes refinement indicators from the compositional fields. If there is more than one compositional field, then it simply takes the sum of the indicators computed from each of the compositional field.

  'density': A mesh refinement criterion that computes refinement indicators from a field that describes the spatial variability of the density, ρ. Because this quantity may not be a continuous function (ρ and C_p may be discontinuous functions along discontinuities in the medium, for example due to phase changes), we approximate the gradient of this quantity to refine the mesh. The error indicator defined here takes the magnitude of the approximate gradient and scales it by $h_K^{1+d/2}$ where h_K is the diameter of each cell and d is the dimension. This scaling ensures that the error indicators converge to zero as $h_K \to 0$ even if the energy density is discontinuous, since the gradient of a discontinuous function grows like $1/h_K$.

  'temperature': A mesh refinement criterion that computes refinement indicators from the temperature field.

  'thermal energy density': A mesh refinement criterion that computes refinement indicators from a field that describes the spatial variability of the thermal energy density, $\rho C_p T$. Because this quantity may not be a continuous function (ρ and C_p may be discontinuous functions along discontinuities in the medium, for example due to phase changes), we approximate the gradient of this quantity to refine the mesh. The error indicator defined here takes the magnitude of the approximate gradient and scales it by $h_K^{1.5}$ where h_K is the diameter of each cell. This scaling ensures that the error indicators converge

to zero as $h_K \to 0$ even if the energy density is discontinuous, since the gradient of a discontinuous function grows like $1/h_K$.

'velocity': A mesh refinement criterion that computes refinement indicators from the velocity field.

Possible values: [MultipleSelection composition—density—temperature—thermal energy density—velocity]

- *Parameter name:* `Time steps between mesh refinement`

  Value: 5

  Default: 10

  Description: The number of time steps after which the mesh is to be adapted again based on computed error indicators. If 0 then the mesh will never be changed.

  Possible values: [Integer range 0...2147483647 (inclusive)]

5.39 Parameters in section `Model settings`

- *Parameter name:* `Fixed temperature boundary indicators`

  Value: 0, 1

  Default:

  Description: A comma separated list of integers denoting those boundaries on which the temperature is fixed and described by the boundary temperature object selected in its own section of this input file. All boundary indicators used by the geometry but not explicitly listed here will end up with no-flux (insulating) boundary conditions.

  This parameter only describes which boundaries have a fixed temperature, but not what temperature should hold on these boundaries. The latter piece of information needs to be implemented in a plugin in the BoundaryTemperature group, unless an existing implementation in this group already provides what you want.

  Possible values: [List list of ¡[Integer range 0...2147483647 (inclusive)]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Include adiabatic heating`

  Value: false

  Default: false

  Description: Whether to include adiabatic heating into the model or not. From a physical viewpoint, adiabatic heating should always be used but may be undesirable when comparing results with known benchmarks that do not include this term in the temperature equation.

  Possible values: [Bool]

- *Parameter name:* `Include shear heating`

  Value: false

  Default: true

  Description: Whether to include shear heating into the model or not. From a physical viewpoint, shear heating should always be used but may be undesirable when comparing results with known benchmarks that do not include this term in the temperature equation.

  Possible values: [Bool]

- *Parameter name:* `Prescribed velocity boundary indicators`

  Value:

  Default:

  Description: A comma separated list denoting those boundaries on which the velocity is tangential but prescribed, i.e., where external forces act to prescribe a particular velocity. This is often used to prescribe a velocity that equals that of overlying plates.

  The format of valid entries for this parameter is that of a map given as "key1: value1, key2: value2, key3: value3, ..." where each key must be a valid boundary indicator and each value must be one of the currently implemented boundary velocity models.

  Note that the no-slip boundary condition is a special case of the current one where the prescribed velocity happens to be zero. It can thus be implemented by indicating that a particular boundary is part of the ones selected using the current parameter and using "zero velocity" as the boundary values. Alternatively, you can simply list the part of the boundary on which the velocity is to be zero with the parameter "Zero velocity boundary indicator" in the current parameter section.

  Possible values: [Map map of ¡[Integer range 0...255 (inclusive)]:[Selection inclusion—function—gplates—zero velocity]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Radiogenic heating rate`

  Value: 0

  Default: 0e0

  Description: H0

  Possible values: [Double -1.79769e+308...1.79769e+308 (inclusive)]

- *Parameter name:* `Tangential velocity boundary indicators`

  Value: 1

  Default:

  Description: A comma separated list of integers denoting those boundaries on which the velocity is tangential and unrestrained, i.e., free-slip where no external forces act to prescribe a particular tangential velocity (although there is a force that requires the flow to be tangential).

  Possible values: [List list of ¡[Integer range 0...255 (inclusive)]¿ of length 0...4294967295 (inclusive)]

- *Parameter name:* `Zero velocity boundary indicators`

  Value: 0, 2, 3

  Default:

  Description: A comma separated list of integers denoting those boundaries on which the velocity is zero.

  Possible values: [List list of ¡[Integer range 0...255 (inclusive)]¿ of length 0...4294967295 (inclusive)]

5.40 Parameters in section `Postprocess`

- *Parameter name:* `List of postprocessors`

  Value: visualization, velocity statistics, temperature statistics, heat flux statistics

  Default: all

  Description: A comma separated list of postprocessor objects that should be run at the end of each time step. Some of these postprocessors will declare their own parameters which may, for example,

include that they will actually do something only every so many time steps or years. Alternatively, the text 'all' indicates that all available postprocessors should be run after each time step.

The following postprocessors are available:

'composition statistics': A postprocessor that computes some statistics about the compositional fields, if present in this simulation. In particular, it computes maximal and minimal values of each field, as well as the total mass contained in this field as defined by the integral $m_i(t) = \int_\Omega c_i(\mathbf{x},t)\,dx$.

'depth average': A postprocessor that computes depth averaged quantities and writes them out.

'DuretzEtAl error': A postprocessor that compares the solution of the benchmarks from the Duretz et al., G-Cubed, 2011, paper with the one computed by ASPECT and reports the error. Specifically, it can compute the errors for the SolCx, SolKz and inclusion benchmarks. The postprocessor inquires which material model is currently being used and adjusts which exact solution to use accordingly.

'heat flux statistics': A postprocessor that computes some statistics about the heat flux across boundaries.

'heat flux statistics for the table model': A postprocessor that computes some statistics about the heat flux across boundaries.

'velocity statistics for the table model': A postprocessor that computes some statistics about the velocity field.

'Tan Gurnis error': A postprocessor that compares the solution of the benchmarks from the Tan/Gurnis (2007) paper with the one computed by ASPECT by outputing data that is compared using a matlab script.

'temperature statistics': A postprocessor that computes some statistics about the temperature field.

'tracers': Postprocessor that propagates passive tracer particles based on the velocity field.

'velocity statistics': A postprocessor that computes some statistics about the velocity field.

'visualization': A postprocessor that takes the solution and writes it into files that can be read by a graphical visualization program. Additional run time parameters are read from the parameter subsection 'Visualization'.

Possible values: [MultipleSelection composition statistics—depth average—DuretzEtAl error—heat flux statistics—heat flux statistics for the table model—velocity statistics for the table model—Tan Gurnis error—temperature statistics—tracers—velocity statistics—visualization—all]

5.41 Parameters in section `Postprocess/Depth average`

- *Parameter name:* `Time between graphical output`

  Value: 1e8

  Default: 1e8

  Description: The time interval between each generation of graphical output files. A value of zero indicates that output should be generated in each time step. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.42 Parameters in section `Postprocess/Tracers`

- *Parameter name:* `Data output format`

  Value: none

  Default: none

Description: File format to output raw particle data in.

Possible values: [Selection none—ascii—vtu—hdf5]

- *Parameter name:* `Integration scheme`

  Value: rk2

  Default: rk2

  Description: Integration scheme to move particles.

  Possible values: [Selection euler—rk2—rk4—hybrid]

- *Parameter name:* `Number of tracers`

  Value: 1e3

  Default: 1e3

  Description: Total number of tracers to create (not per processor or per element).

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Time between data output`

  Value: 1e8

  Default: 1e8

  Description: The time interval between each generation of output files. A value of zero indicates that output should be generated every time step. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.43 Parameters in section `Postprocess/Visualization`

- *Parameter name:* `List of output variables`

  Value:

  Default:

  Description: A comma separated list of visualization objects that should be run whenever writing graphical output. By default, the graphical output files will always contain the primary variables velocity, pressure, and temperature. However, one frequently wants to also visualize derived quantities, such as the thermodynamic phase that corresponds to a given temperature-pressure value, or the corresponding seismic wave speeds. The visualization objects do exactly this: they compute such derived quantities and place them into the output file. The current parameter is the place where you decide which of these additional output variables you want to have in your output file.

  The following postprocessors are available:

  'density': A visualization output object that generates output for the density.

  'error indicator': A visualization output object that generates output showing the estimated error or other mesh refinement indicator as a spatially variable function with one value per cell.

  'friction heating': A visualization output object that generates output for the amount of friction heating often referred to as $\tau : \epsilon$. More concisely, in the incompressible case, the quantity that is output is defined as $\eta\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})$ where η is itself a function of temperature, pressure and strain rate. In the compressible case, the quantity that's computed is $\eta[\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr } \varepsilon(\mathbf{u}))\mathbf{I}] : [\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr } \varepsilon(\mathbf{u}))\mathbf{I}]$.

  'nonadiabatic pressure': A visualization output object that generates output for the non-adiabatic component of the pressure.

'nonadiabatic temperature': A visualization output object that generates output for the non-adiabatic component of the pressure.

'partition': A visualization output object that generates output for the parallel partition that every cell of the mesh is associated with.

'Vs anomaly': A visualization output object that generates output showing the anomaly in the seismic shear wave speed V_s as a spatially variable function with one value per cell. This anomaly is shown as a percentage change relative to the average value of V_s at the depth of this cell.

'Vp anomaly': A visualization output object that generates output showing the anomaly in the seismic compression wave speed V_p as a spatially variable function with one value per cell. This anomaly is shown as a percentage change relative to the average value of V_p at the depth of this cell.

'seismic vp': A visualization output object that generates output for the seismic P-wave speed.

'seismic vs': A visualization output object that generates output for the seismic S-wave speed.

'specific heat': A visualization output object that generates output for the specific heat C_p.

'strain rate': A visualization output object that generates output for the norm of the strain rate, i.e., for the quantity $\sqrt{\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})}$ in the incompressible case and $\sqrt{[\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr } \varepsilon(\mathbf{u}))\mathbf{I}] : [\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr } \varepsilon(\mathbf{u}))\mathbf{I}]}$ in the compressible case.

'thermal expansivity': A visualization output object that generates output for the thermal expansivity.

'thermodynamic phase': A visualization output object that generates output for the integer number of the phase that is thermodynamically stable at the temperature and pressure of the current point.

'viscosity': A visualization output object that generates output for the viscosity.

'viscosity ratio': A visualization output object that generates output for the ratio between dislocation viscosity and diffusion viscosity.

Possible values: [MultipleSelection density—error indicator—friction heating—nonadiabatic pressure—nonadiabatic temperature—partition—Vs anomaly—Vp anomaly—seismic vp—seismic vs—specific heat—strain rate—thermal expansivity—thermodynamic phase—viscosity—viscosity ratio—all]

- *Parameter name:* `Number of grouped files`

  Value: 0

  Default: 0

  Description: VTU file output supports grouping files from several CPUs into one file using MPI I/O when writing on a parallel filesystem. Select 0 for no grouping. This will disable parallel file output and instead write one file per processor in a background thread. A value of 1 will generate one big file containing the whole solution.

  Possible values: [Integer range 0...2147483647 (inclusive)]

- *Parameter name:* `Output format`

  Value: vtu

  Default: vtu

  Description: The file format to be used for graphical output.

  Possible values: [Selection none—dx—ucd—gnuplot—povray—eps—gmv—tecplot—tecplot_binary—vtk—vtu—hdf5—intermediate]

- *Parameter name:* `Time between graphical output`

  Value: 0

  Default: 1e8

Description: The time interval between each generation of graphical output files. A value of zero indicates that output should be generated in each time step. Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

Possible values: [Double 0...1.79769e+308 (inclusive)]

5.44 Parameters in section `Termination criteria`

- *Parameter name:* `Checkpoint on termination`

  Value: false

  Default: false

  Description: Whether to checkpoint the simulation right before termination.

  Possible values: [Bool]

- *Parameter name:* `Termination criteria`

  Value:

  Default:

  Description: A comma separated list of termination criteria that will determine when the simulation should end. The following termination criteria are available:

  'steady_rms_velocity': A criterion that terminates the simulation when the RMS of the velocity field stays within a certain range for a specified period of time.

  'user_request': Terminate the simulation gracefully when a file with a specified name appears in the output directory. This allows the user to gracefully exit the simulation at any time.

  Possible values: [MultipleSelection steady_rms_velocity—user_request—all]

5.45 Parameters in section `Termination criteria/Steady state velocity`

- *Parameter name:* `Maximum relative deviation`

  Value: 0.05

  Default: 0.05

  Description: The maximum relative deviation of the RMS in recent simulation time for the system to be considered in steady state and the simulation terminated.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

- *Parameter name:* `Time in steady state`

  Value: 1e7

  Default: 1e7

  Description: The minimum length of simulation time that the system should be in steady state before termination.Units: years if the 'Use years in output instead of seconds' parameter is set; seconds otherwise.

  Possible values: [Double 0...1.79769e+308 (inclusive)]

5.46 Parameters in section `Termination criteria/User request`

- *Parameter name:* `File name`

  Value: terminate_aspect

  Default: terminate_aspect

  Possible values: [FileName (Type: input)]

6 Cookbooks

In this section, let us present a number of "cookbooks" – examples of how to use ASPECT in typical or less typical ways. As discussed in Sections 4 and 5, ASPECT is driven by run-time parameter files, and so setting up a particular situation primarily comes down to creating a parameter file that has the right entries. Thus, the subsections below will discuss in detail what parameters to set and to what values. Note that parameter files need not specify *all* parameters – of which there is a bewildering number – but only those that are relevant to the particular situation we would like to model. All parameters not listed explicitly in the input file are simply left at their default value (the default values are also documented in Section 5).

Of course, there are situations where what you want to do is not covered by the models already implemented. Specifically, you may want to try a different geometry, a different material or gravity model, or different boundary conditions. In such cases, you will need to implement these extensions in the actual source code. Section 7 provides information on how to do that.

The remainder of this section shows a number of applications of ASPECT. They are grouped into three categories: Simple setups of examples that show thermal convection (Section 6.1), setups that try to model geophysical situations (Section 6.2) and setups that are used to benchmark ASPECT to ensure correctness or to test accuracy of our solvers (Section 6.3).

Note: The input files discussed in the following sections can generally be found in the `cookbooks/` directory of your ASPECT installation.

6.1 Simple setups

6.1.1 Convection in a box

In this first example, let us consider a simple situation: a 2d box of dimensions $[0,1]\times[0,1]$ that is heated from below, insulated at the left and right, and cooled from the top. We will also consider the simplest model, the incompressible Boussinesq approximation with constant coefficients $\eta, \rho_0, \mathbf{g}, C_p k$, for this testcase. Furthermore, we assume that the medium expands linearly with temperature. This leads to the following set of equations:

$$-\nabla\cdot[2\eta\varepsilon(\mathbf{u})]+\nabla p=\rho_0(1-\alpha(T-T_0))\mathbf{g} \qquad \text{in } \Omega, \tag{18}$$

$$\nabla\cdot\mathbf{u}=0 \qquad \text{in } \Omega, \tag{19}$$

$$\rho_0(1-\alpha(T-T_0))C_p\left(\frac{\partial T}{\partial t}+\mathbf{u}\cdot\nabla T\right)-\nabla\cdot k\nabla T=0 \qquad \text{in } \Omega. \tag{20}$$

It is well known that we can non-dimensionalize this set of equations by choosing introducing the Raleigh number $Ra=\frac{g\alpha}{\eta k}$. Formally, we can obtain the non-dimensionalized equations by using the above form and setting coefficients in the following way:

$$\rho_0=C_p=k=\alpha=\eta=1, \qquad T_0=0, \qquad g=Ra,$$

where $\mathbf{g}=-g\mathbf{e}_z$ is the gravity vector in negative z-direction. While this would be a valid description of the problem, it is not what one typically finds in the literature because there the density in the temperature equation is chosen as ρ_0 rather than $\rho(1-\alpha(T-T_0))$ as used by ASPECT. However, we can mimick this by choosing a very small value for α – small enough to ensure that for all reasonable temperatures, the density used here is equal to ρ_0 for all practical purposes –, and instead making g correspondingly larger. Consequently, in this cookbook we will use the following set of parameters:

$$\rho_0=C_p=T_0=k=\eta=1, \qquad T_0=0, \qquad \alpha=10^{-10}, \qquad g=10^{10}Ra.$$

We will see all of these values again in the input file discussed below. The problem is completed by stating the velocity boundary conditions: tangential flow along all four of the boundaries of the box.

This situation describes a well-known benchmark problems for which a lot is known and against which we can compare our results. For example, the following is well understood:

- For values of the Rayleigh number less than a critical number $Ra_c \approx 780$, thermal diffusion dominates convective heat transport and any movement in the fluid is damped exponentially. If the Rayleigh number is moderately larger than this threshold then a stable convection pattern forms that transports heat from the bottom to the top boundaries. The simulations we will set up operates in this regime. Specifically, we will choose $Ra = 10^4$.

  On the other hand, if the Rayleigh number becomes even larger, a serious of period doublings starts that makes the system become more and more unstable. We will investigate some of this behavior at the end of this section.

- For certain values of the Rayleigh number, very accurate values for the heat flux through the bottom and top boundaries are available in the literate. For example, Blankenbach *et al.* report a non-dimensional heat flux of 4.884409 ± 0.00001, see [BBC+89]. We will compare our results against this value below.

With this said, let us consider how to represent this situation in practice.

The input file. The verbal description of this problem can be translated into an ASPECT input file in the following way (see Section 5 for a description of all of the parameters that appear in the following input file, and the indices at the end of this manual if you want to find a particular parameter; you can find the input file to run this cookbook example in `cookbooks/convection-box.prm`):

```
# At the top, we define the number of space dimensions we would like to
# work in:
set Dimension                                = 2

# There are several global variables that have to do with what
# time system we want to work in and what the end time is. We
# also designate an output directory.
set Use years in output instead of seconds = false
set End time                                 = 0.5
set Output directory                         = output

# Then there are variables that describe the tolerance of
# the linear solver as well as how the pressure should
# be normalized. Here, we choose a zero average pressure
# at the surface of the domain (for the current geometry, the
# surface is defined as the top boundary).
set Linear solver tolerance                  = 1e-15
set Temperature solver tolerance             = 1e-15

set Pressure normalization                   = surface
set Surface pressure                         = 0


# Then come a number of sections that deal with the setup
# of the problem to solve. The first one deals with the
# geometry of the domain within which we want to solve.
# The sections that follow all have the same basic setup
# where we select the name of a particular model (here,
# the box geometry) and then, in a further subsection,
# set the parameters that are specific to this particular
# model.
subsection Geometry model
  set Model name = box

  subsection Box
    set X extent = 1
```

```
    set Y extent = 1
  end
end


# The next section deals with the initial conditions for the
# temperature (there are no initial conditions for the
# velocity variable since the velocity is assumed to always
# be in a static equilibrium with the temperature field).
# There are a number of models with the 'function' model
# a generic one that allows us to enter the actual initial
# conditions in the form of a formula that can contain
# constants. We choose a linear temperature profile that
# matches the boundary conditions defined below plus
# a small perturbation:
subsection Initial conditions
  set Model name = function

  subsection Function
    set Variable names      = x,z
    set Function constants  = p=0.01, L=1, pi=3.1415926536, k=1
    set Function expression = (1.0-z) - p*cos(k*pi*x/L)*sin(pi*z)
  end
end


# Then follows a section that describes the boundary conditions
# for the temperature. The model we choose is called 'box' and
# allows to set a constant temperature on each of the four sides
# of the box geometry. In our case, we choose something that is
# heated from below and cooled from above. (As will be seen
# in the next section, the actual temperature prescribed here
# at the left and right does not matter.)
subsection Boundary temperature model
  set Model name = box

  subsection Box
    set Bottom temperature = 1
    set Left temperature   = 0
    set Right temperature  = 0
    set Top temperature    = 0
  end
end


# We then also have to prescribe several other parts of the model
# such as which boundaries actually carry a prescribed boundary
# temperature (as described in the documentation of the 'box'
# geometry, boundaries 2 and 3 are the bottom and top boundaries)
# whereas all other parts of the boundary are insulated (i.e.,
# no heat flux through these boundaries; this is also often used
# to specify symmetry boundaries).
subsection Model settings
  set Fixed temperature boundary indicators   = 2,3

  # The next parameters then describe on which parts of the
  # boundary we prescribe a zero or nonzero velocity and
  # on which parts the flow is allowed to be tangential.
  # Here, all four sides of the box allow tangential
  # unrestricted flow but with a zero normal component:
  set Zero velocity boundary indicators       =
  set Prescribed velocity boundary indicators =
  set Tangential velocity boundary indicators = 0,1,2,3

  # The final part of this section describes whether we
```

```
  # want to include adiabatic heating (from a small
  # compressibility of the medium) or from shear friction,
  # as well as the rate of internal heating. We do not
  # want to use any of these options here:
  set Include adiabatic heating               = false
  set Include shear heating                   = false
  set Radiogenic heating rate                 = 0
end


# The following two sections describe first the
# direction (vertical) and magnitude of gravity and the
# material model (i.e., density, viscosity, etc). We have
# discussed the settings used here in the introduction to
# this cookbook in the manual already.
subsection Gravity model
  set Model name = vertical

  subsection Vertical
    set Magnitude = 1e14    # = Ra / Thermal expansion coefficient
  end
end


subsection Material model
  set Model name = simple # default:

  subsection Simple model
    set Reference density             = 1
    set Reference specific heat       = 1
    set Reference temperature         = 0
    set Thermal conductivity          = 1
    set Thermal expansion coefficient = 1e-10
    set Viscosity                     = 1
  end
end


# The settings above all pertain to the description of the
# continuous partial differential equations we want to solve.
# The following section deals with the discretization of
# this problem, namely the kind of mesh we want to compute
# on. We here use a globally refined mesh without
# adaptive mesh refinement.
subsection Mesh refinement
  set Initial global refinement                = 4
  set Initial adaptive refinement              = 0
  set Time steps between mesh refinement       = 0
end


# The final part is to specify what ASPECT should do with the
# solution once computed at the end of every time step. The
# process of evaluating the solution is called 'postprocessing'
# and we choose to compute velocity and temperature statistics,
# statistics about the heat flux through the boundaries of the
# domain, and to generate graphical output files for later
# visualization. These output files are created every time
# a time step crosses time points separated by 0.01. Given
# our start time (zero) and final time (0.5) this means that
# we will obtain 50 output files.
subsection Postprocess
  set List of postprocessors = velocity statistics, temperature statistics, ...
                                          ... heat flux statistics, visualization
```

```
  subsection Visualization
    set Time between graphical output = 0.01
  end
end
```

Running the program. When you run this program for the first time, you are probably still running ASPECT in debug mode (see Section 4.3) and you will get output like the following:

```
Number of active cells: 256 (on 5 levels)
Number of degrees of freedom: 3,556 (2,178+289+1,089)

*** Timestep 0:  t=0 seconds
   Solving temperature system... 0 iterations.
   Rebuilding Stokes preconditioner...
   Solving Stokes system... 30+5 iterations.

[... ...]

*** Timestep 1077:  t=0.499901 seconds
   Solving temperature system... 9 iterations.
   Solving Stokes system... 5 iterations.

   Postprocessing:
     RMS, max velocity:                43.1 m/s, 69.8 m/s
     Temperature min/avg/max:          0 K, 0.5 K, 1 K
     Heat fluxes through boundary parts: 0.02056 W, -0.02061 W, -4.931 W, 4.931 W



+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |       454s |            |
|                                             |            |            |
| Section                         | no. calls |  wall time | % of total |
+---------------------------------+-----------+------------+------------+
| Assemble Stokes system          |      1078 |      19.2s |       4.2% |
| Assemble temperature system     |      1078 |       329s |        72% |
| Build Stokes preconditioner     |         1 |    0.0995s |     0.022% |
| Build temperature preconditioner|      1078 |      5.84s |       1.3% |
| Solve Stokes system             |      1078 |      15.6s |       3.4% |
| Solve temperature system        |      1078 |      3.72s |      0.82% |
| Initialization                  |         2 |    0.0474s |      0.01% |
| Postprocessing                  |      1078 |      61.9s |        14% |
| Setup dof systems               |         1 |     0.221s |     0.049% |
+---------------------------------+-----------+------------+------------+
```

If you've read up on the difference between debug and optimized mode (and you should before you switch!) then consider disabling debug mode. If you run the program again, every number should look exactly the same (and it does, in fact, as I am writing this) except for the timing information printed every hundred time steps and at the end of the program:

```
+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |      48.3s |            |
|                                             |            |            |
| Section                         | no. calls |  wall time | % of total |
+---------------------------------+-----------+------------+------------+
| Assemble Stokes system          |      1078 |      1.68s |       3.5% |
| Assemble temperature system     |      1078 |      26.3s |        54% |
| Build Stokes preconditioner     |         1 |    0.0401s |     0.083% |
| Build temperature preconditioner|      1078 |      4.87s |        10% |
| Solve Stokes system             |      1078 |      6.76s |        14% |
| Solve temperature system        |      1078 |      1.76s |       3.7% |
| Initialization                  |         2 |    0.0241s |      0.05% |
| Postprocessing                  |      1078 |      4.99s |        10% |
```

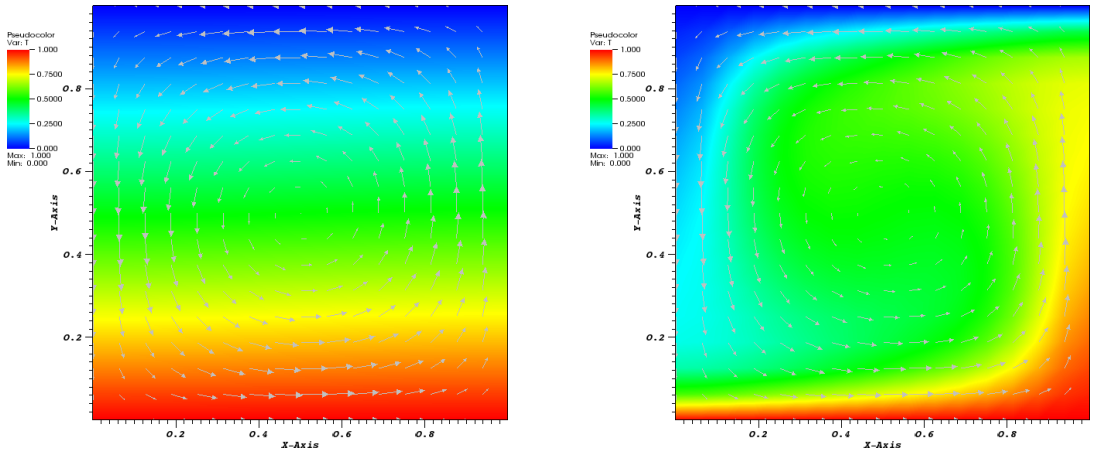


Figure 5: *Convection in a box: Initial temperature and velocity field (left) and final state (right).*

```
| Setup dof systems                    |          1 |     0.0394s |      0.082% |
+--------------------------------------+------------+-------------+-------------+
```

In other words, the program ran about 10 times faster than before. Not all operations became faster to the same degree: assembly, for example, is an area that traverses a lot of code both in ASPECT and in DEAL.II and so encounters a lot of verification code in debug mode. On the other hand, solving linear systems primarily requires lots of matrix vector operations. Overall, the fact that in this example, assembling linear systems and preconditioners takes so much time compared to actually solving them is primarily a reflection of how simple the problem is that we solve in this example. This can also be seen in the fact that the number of iterations necessary to solve the Stokes and temperature equations is so low. For more complex problems with nonconstant coefficients such as the viscosity, as well as in 3d, we have to spend much more work solving linear systems whereas the effort to assemble linear systems remains the same.

Visualizing results. Having run the program, we now want to visualize the numerical results we got. ASPECT can generate graphical output in formats understood by pretty much any visualization program (see the parameters described in Section 5.43) but we will here follow the discussion in Section 4.4 and use the default VTU output format to visualize using the Visit program.

In the parameter file we have specified that graphical output should be generated every 0.01 time units. Looking through these output files, we find that the flow and temperature fields quickly converge to a stationary state. Fig. 5 shows the initial and final states of this simulation.

There are many other things we can learn from the output files generated by ASPECT, specifically from the statistics file that contains information collected at every time step and that has been discussed in Section 4.4.2. In particular, in our input file, we have selected that we would like to compute velocity, temperature, and heat flux statistics. These statistics, among others, are listed in the statistics file whose head looks like this for the current input file:

```
# 1: Time step number
# 2: Time (seconds)
# 3: Number of mesh cells
# 4: Number of Stokes degrees of freedom
# 5: Number of temperature degrees of freedom
# 6: Iterations for temperature solver
# 7: Iterations for Stokes solver
# 8: Time step size (seconds)
# 9: RMS velocity (m/s)
# 10: Max. velocity (m/s)
# 11: Minimal temperature (K)
```

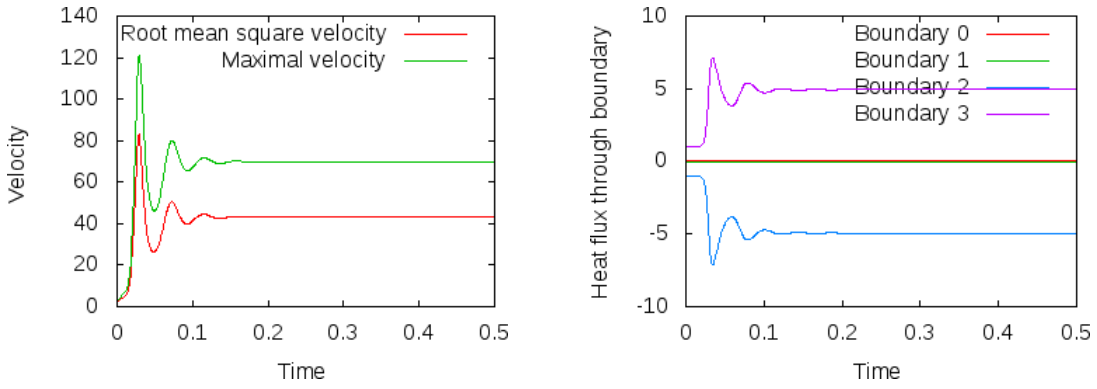


Figure 6: *Convection in a box: Root mean square and maximal velocity as a function of simulation time (left). Heat flux through the four boundaries of the box (right).*

```
# 12: Average temperature (K)
# 13: Maximal temperature (K)
# 14: Average nondimensional temperature (K)
# 15: Outward heat flux through boundary with indicator 0 (W)
# 16: Outward heat flux through boundary with indicator 1 (W)
# 17: Outward heat flux through boundary with indicator 2 (W)
# 18: Outward heat flux through boundary with indicator 3 (W)
# 19: Visualization file name
... lots of numbers arranged in columns ...
```

Fig. 6 shows the results of visualizing the data that can be found in columns 2 (the time) plotted against columns 9 and 10 (root mean square and maximal velocities). Plots of this kind can be generated with `Gnuplot` by typing (see Section 4.4.2 for a more thorough discussion):

```
plot "output/statistics" using 2:9 with lines
```

Fig. 6 shows clearly that the simulation enters a steady state after about $t \approx 0.1$ and then changes very little. This can also be observed using the graphical output files from which we have generated Fig. 5. One can look further into this data to find that the flux through the top and bottom boundaries is not exactly the same (up to the obvious difference in sign, given that at the bottom boundary heat flows into the domain and at the top boundary out of it) at the beginning of the simulation until the fluid has attained its equilibrium. However, after $t \approx 0.2$, the fluxes differ by only $5 \cdot 10^{-5}$, i.e., by less than 0.001% of their magnitude.[11] The flux we get at the last time step, 4.931, is less than 1% away from the value reported in [BBC+89] although we compute on a 16×16 mesh and the values reported by Blankenbach are extrapolated from meshes of size up to 72×72. This shows the accuracy that can be obtained using a higher order finite element. Secondly, the fluxes through the left and right boundary are not exactly zero but small. Of course, we have prescribed boundary conditions of the form $\frac{\partial T}{\partial \mathbf{n}} = 0$ along these boundaries, but this is subject to discretization errors. It is easy to verify that the heat flux through these two boundaries disappears as we refine the mesh further.

Furthermore, ASPECT automatically also collects statistics about many of its internal workings. Fig. 7 shows the number of iterations required to solve the Stokes and temperature linear systems in each time step. It is easy to see that these are more difficult to solve in the beginning when the solution still changes significant from time step to time step. However, after some time, the solution remains mostly the same and solvers then only need 9 or 10 iterations for the temperature equation and 4 or 5 iterations for the Stokes equations because the starting guess for the linear solver – the previous time step's solution – is already pretty good. If you look at any of the more complex cookbooks, you will find that one needs many more iterations to solve these equations.

[11] This difference is far smaller than the numerical error in the heat flux on the mesh this data is computed on.

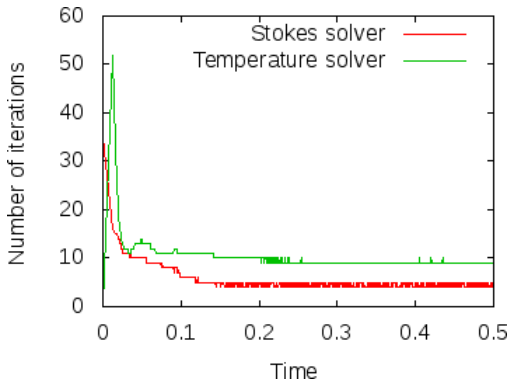


Figure 7: *Convection in a box: Number of linear iterations required to solve the Stokes and temperature equations in each time step.*

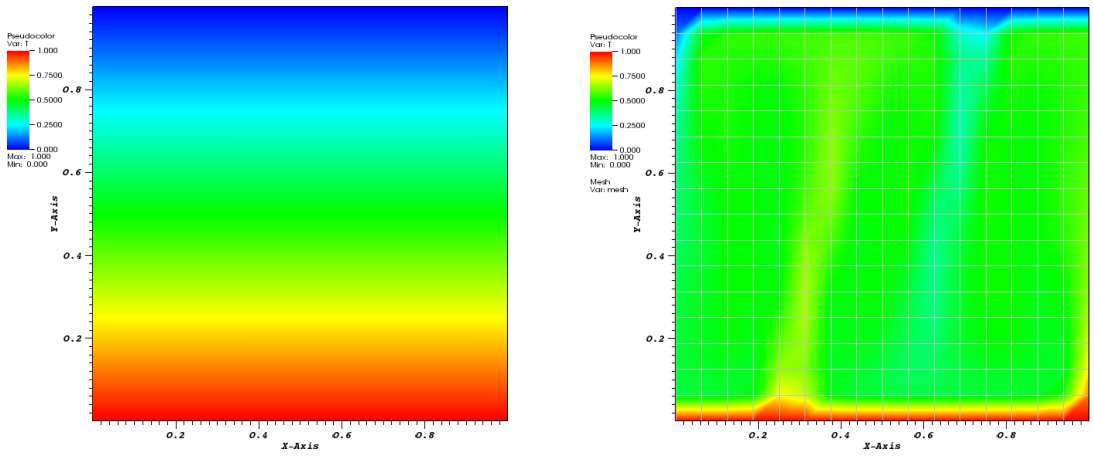


Figure 8: *Convection in a box: Temperature fields at the end of a simulation for $Ra = 10^2$ where thermal diffusion dominates (left) and $Ra = 10^6$ where convective heat transport dominates (right). The mesh on the right is clearly too coarse to resolve the structure of the solution.*

Play time 1: Different Rayleigh numbers. After showing you results for the input file as it can be found in `cookbooks/convection-box.prm`, let us end this section with a few ideas on how to play with it and what to explore. The first direction one could take this example is certainly to consider different Rayleigh numbers. As mentioned above, for the value $Ra = 10^4$ for which the results above have been produced, one gets a stable convection pattern. On the other hand, for values $Ra < Ra_c \approx 780$, any movement of the fluid dies down exponentially and we end up with a situation where the fluid doesn't move and heat is transported from the bottom to the top only through heat conduction. This can be explained by considering that the Rayleigh number in a box of unit extent is defined as $Ra = \frac{g\alpha}{\eta k}$. A small Rayleigh number means that the viscosity is too large (i.e., the buoyancy given by the product of the magnitude of gravity times the thermal expension coefficient is not strong enough to overcome friction forces within the fluid).

On the other hand, if the Rayleigh number is large (i.e., the viscosity is small or the buoyancy large) then the fluid develops an unsteady convection period. As we consider fluids with larger and larger Ra, this pattern goes through a sequence of period-doubling events until flow finally becomes chaotic. The structures of the flow pattern also become smaller and smaller.

We illustrate these situations in Fig.s 8 and 9. The first shows the temperature field at the end of a simulation for $Ra = 10^2$ (below Ra_c) and at $Ra = 10^6$. Obviously, for the right picture, the mesh is not fine

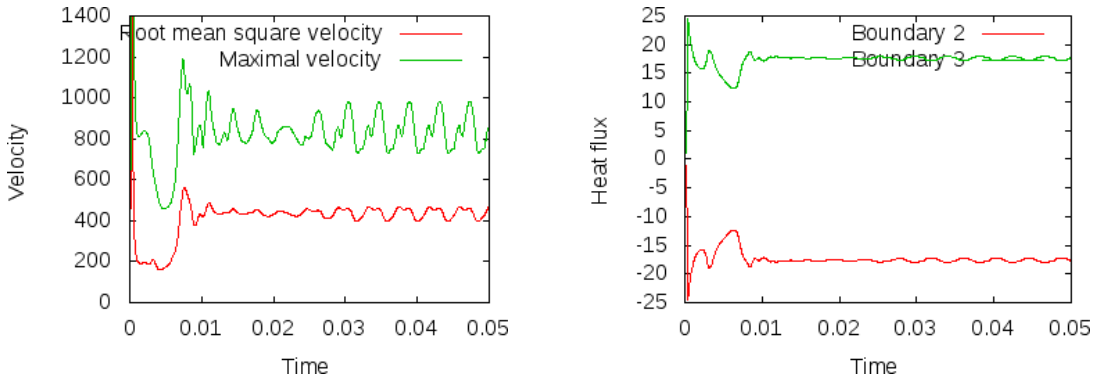


Figure 9: *Convection in a box: Velocities (left) and heat flux across the top and bottom boundaries (right) as a function of time at* $Ra = 10^6$.

enough to accurately resolve the features of the flow field and we would have to refine it more. The second of the figures shows the velocity and heatflux statistics for the computation with $Ra = 10^6$; it is obvious here that the flow no longer settles into a steady state but has a periodic behavior. This can also be seen by looking at movies of the solution.

To generate these results, remember that we have chosen $\alpha = 10^{-10}$ and $g = 10^{10}Ra$ in our input file. In other words, changing the input file to contain the parameter setting

```
subsection Gravity model
  subsection Vertical
    set Magnitude = 1e16    # = Ra / Thermal expansion coefficient
  end
end
```

will achieve the desired effect of computing with $Ra = 10^6$.

Play time 2: Thinking about finer meshes. In our computations for $Ra = 10^4$ we used a 16×16 mesh and obtained a value for the heat flux that differed from the generally accepted value from Blankenbach *et al.* [BBC+89] by less than 1%. However, it may be interesting to think about computing even more accurately. This is easily done by using a finer mesh, for example. In the parameter file above, we have chosen the mesh setting as follows:

```
subsection Mesh refinement
  set Initial global refinement                = 4
  set Initial adaptive refinement              = 0
  set Time steps between mesh refinement       = 0
end
```

We start out with a box geometry consisting of a single cell that is refined four times. Each time we split each cell into its 4 children, obtaining the 16×16 mesh already mentioned. The other settings indicate that we do not want to refine the mesh adaptively at all in the first time step, and a setting of zero for the last parameter means that we also never want to adapt the mesh again at a later time. Let us stick with the never-changing, globally refined mesh for now (we will come back to adaptive mesh refinement again at a later time) and only vary the initial global refinement. In particular, we could choose the parameter `Initial global refinement` to be 5, 6, or even larger. This will get us closer to the exact solution albeit at the expense of a significantly increased computational time.

A better strategy is to realize that for $Ra = 10^4$, the flow enters a steady state after settling in during the first part of the simulation (see, for example, the graphs in Fig. 6). Since we are not particularly interested in this initial transient process, there is really no reason to spend CPU time using a fine mesh and correspondingly small time steps during this part of the simulation (remember that each refinement results

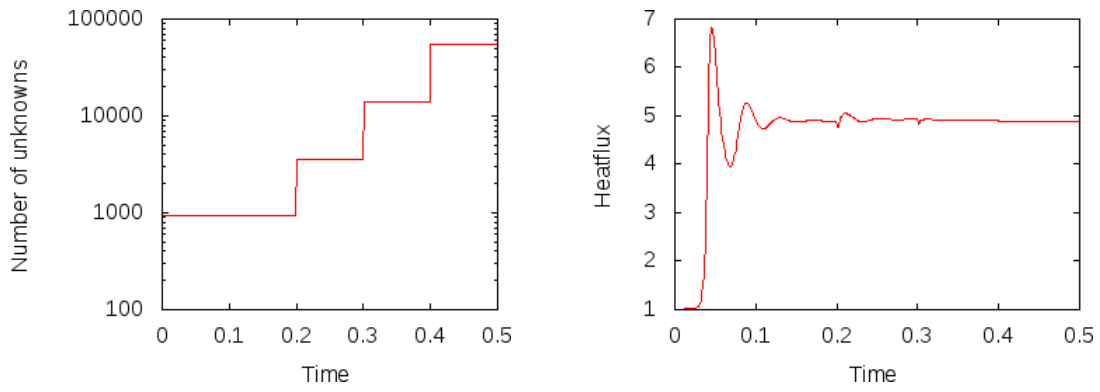


Figure 10: *Convection in a box: Refinement in stages. Total number of unknowns in each time step, including all velocity, pressure and temperature unknowns (left) and heat flux across the top boundary (right).*

in four times as many cells in 2d and a time step half as long, making reaching a particular time at least 8 times as expensive, assuming that all solvers in ASPECT scale perfectly with the number of cells). Rather, we can use a parameter in the ASPECT input file that let's us increase the mesh resolution at later times. To this end, let us use the following snippet for the input file:

```
subsection Mesh refinement
  set Initial global refinement                = 3
  set Initial adaptive refinement              = 0
  set Time steps between mesh refinement       = 0
  set Additional refinement times              = 0.2, 0.3, 0.4
  set Refinement fraction                      = 1.0
  set Coarsening fraction                      = 0.0
end
```

What this does is the following: We start with an 8×8 mesh (3 times globally refined) but then at times $t = 0.2, 0.3$ and 0.4 we refine the mesh using the default refinement indicator (which one this is is not important because of the next statement). Each time, we refine, we refine a fraction 1.0 of the cells, i.e., *all* cells and we coarsen a fraction of 0.0 of the cells, i.e. no cells at all. In effect, at these additional refinement times, we do another global refinement, bringing us to refinement levels 4, 5 and finally 6.

Fig. 10 shows the results. In the left panel, we see how the number of unknowns grows over time (note the logscale for the y-axis). The right panel displays the heat flux. The jumps in the number of cells is clearly visible in this picture as well. This may be surprising at first but remember that the mesh is clearly too coarse in the beginning to really resolve the flow and so we should expect that the solution changes significantly if the mesh is refined. This effect becomes smaller with every additional refinement and is barely visible at the last time this happens, indicating that the mesh before this refinement step may already have been fine enough to resolve the majority of the dynamics.

In any case, we can compare the heat fluxes we obtain at the end of these computations: With a globally four times refined mesh, we get a value of 4.931 (an error of approximately 1% against the accepted value from Blankenbach, 4.884409 ± 0.00001). With a globally five times refined mesh we get 4.914 (an error of 0.6%) and with the mesh generated using the procedure above we get 4.895 with the four digits printed on the screen[12] (corresponding to an error of 0.2%). In other words, our simple procedure of refining the mesh during the simulation run yields an accuracy of three times smaller than using the globally refined approach even though the compute time is not much larger than that necessary for the 5 times globally refined mesh.

[12]The statistics file gives this value to more digits: 4.89488768. However, these are clearly more digits than the result is accurate.

Play time 3: Changing the finite element in use. Another way to increase the accuracy of a finite element computation is to use a higher polynomial degree for the finite element shape functions. By default, ASPECT uses quadratic shape functions for the velocity and the temperature and linear ones for the pressure. However, this can be changed with a single number in the input file.

Before doing so, let us consider some aspects of such a change. First, looking at the pictures of the solution in Fig. 5, one could surmise that the quadratic elements should be able to resolve the velocity field reasonably well given that it is rather smooth. On the other hand, the temperature field has a boundary layer at the top and bottom. One could conjecture that the temperature polynomial degree is therefore the limiting factor and not the polynomial degree for the flow variables. We will test this conjecture below. Secondly, given the nature of the equations, increasing the polynomial degree of the flow variables increases the cost to solve these equations by a factor of $\frac{22}{9}$ in 2d (you can get this factor by counting the number of degrees of freedom uniquely associated with each cell) but leaves the time step size and the cost of solving the temperature system unchanged. On the other hand, increasing the polynomial degree of the temperature variable from 2 to 3 requires $\frac{9}{4}$ times as many degrees of freedom for the temperature and also requires us to reduce the size of the time step by a factor of $\frac{2}{3}$. Because solving the temperature system is not a dominant factor in each time step (see the timing results shown at the end of the screen output above), the reduction in time step is the only important factor. Overall, increasing the polynomial degree of the temperature variable turns out to be the cheaper of the two options.

Following these considerations, let us add the following section to the parameter file:

```
subsection Discretization
  set Stokes velocity polynomial degree       = 2
  set Temperature polynomial degree           = 3
end
```

This leaves the velocity and pressure shape functions at quadratic and linear polynomial degree but increases the polynomial degree of the temperature from quadratic to cubic. Using the original, four times globally refined mesh, we then get the following output:

```
Number of active cells: 256 (on 5 levels)
Number of degrees of freedom: 4,868 (2,178+289+2,401)

*** Timestep 0:  t=0 seconds
   Solving temperature system... 0 iterations.
   Rebuilding Stokes preconditioner...
   Solving Stokes system... 30+5 iterations.

[... ...]

*** Timestep 1619:  t=0.499807 seconds
   Solving temperature system... 8 iterations.
   Solving Stokes system... 5 iterations.

   Postprocessing:
     RMS, max velocity:                 42.9 m/s, 69.5 m/s
     Temperature min/avg/max:           0 K, 0.5 K, 1 K
     Heat fluxes through boundary parts: -0.004622 W, 0.004624 W, -4.878 W, 4.878 W


+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |       127s |            |
|                                             |            |            |
| Section                         | no. calls |  wall time | % of total |
+---------------------------------+-----------+------------+------------+
| Assemble Stokes system          |      1620 |      3.03s |       2.4% |
| Assemble temperature system     |      1620 |      75.7s |       60%  |
| Build Stokes preconditioner     |         1 |    0.0422s |     0.033% |
| Build temperature preconditioner|      1620 |      21.7s |       17%  |
| Solve Stokes system             |      1620 |      10.3s |       8.1% |
| Solve temperature system        |      1620 |       4.9s |       3.8% |
```

```
| Initialization                    |          2 |     0.0246s |      0.019% |
| Postprocessing                    |       1620 |       8.05s |       6.3% |
| Setup dof systems                 |          1 |     0.0438s |      0.034% |
+-----------------------------------+------------+-------------+-------------+
```

Note here that the heat flux through the top and bottom boundaries is now computed as 4.878, an error of 0.13%. This is 4 times more accurate than the once more globally refined mesh with the original quadratic elements, at a cost significantly smaller. Furthermore, we can of course combine this with the mesh that is gradually refined as simulation time progresses, and we then get a heat flux that is equal to 4.8843, only 0.002% away from the accepted value!

As a final remark, to test our hypothesis that it was indeed the temperature polynomial degree that was the limiting factor, we can increase the Stokes polynomial degree to 3 while leaving the temperature polynomial degree at 2. A quick computation shows that in that case we get a heat flux of 4.931 – exactly the same value as we got initially with the lower order Stokes element. In other words, at least for this testcase, it really was the temperature variable that limits the accuracy.

6.1.2 Convection in a box with prescribed, variable velocity boundary conditions

A similarly simple setup is to equip the model we had in the previous section with a different set of boundary conditions. There, we used slip boundary conditions, i.e., the fluid can flow tangentially along the four sides of our box but this tangential velocity is unspecified. On the other hand, in many situations, one would like to actually prescribe the tangential flow velocity as well. A typical application would be to use boundary conditions at the top that describe experimentally determined velocities of plates. This cookbook shows a simple version of something like this. To make it slightly more interesting, we choose a 2×1 domain in 2d.

Like for many other things, ASPECT has a set of plugins for prescribed velocity boundary values (see Sections 5.6 and 7.2.5). These plugins allow one to write sophisticated models for the boundary velocity on parts or all of the boundary, but there is also one simple implementation that just takes a formula for the components of the velocity.

To illustrate this, let us consider the `cookbooks/platelike-boundary.prm` input file. It essentially extends the input file considered in the previous example. The part of this file that we are particularly interested in in the current context is the selection of the kind of boundary conditions on the four sides of the box geometry, which we do using a section like this:

```
subsection Model settings
  set Fixed temperature boundary indicators   = 2, 3
  set Zero velocity boundary indicators       =
  set Tangential velocity boundary indicators = 0, 1, 2
  set Prescribed velocity boundary indicators = 3: function
end
```

Following the convention for numbering boundaries described in the previous section, this means that we prescribe a fixed temperature at the bottom and top sides of the box (boundary numbers two and three). We use tangential flow at boundaries zero, one and two (left, right and bottom). Finally, the last entry above is a comma separated list (here with only a single element) of pairs consisting of the number of a boundary and the name of the prescribed velocity boundary model to be used on this boundary. Here, we use the `function` boundary model, which allows us to provide a function-like notation for the components of the velocity vector at the boundary.

The second part we need is that we actually describe the function that sets the velocity. We do this as follows:

```
subsection Boundary velocity model
  subsection Function
    set Variable names      = x,z,t
    set Function constants  = pi=3.1415926
    set Function expression = if(x>1+sin(0.5*pi*t), 1, -1); 0
  end
end
```

The first of these gives names to the components of the position vector (here, we are in 2d and we use x and z as spatial variable names) and the time. We could have left this entry at its default, `x,y,t`, but since we often think in terms of "depth" as the vertical direction, let us use `z` for the second coordinate. In the second parameter we define symbolic constants that can be used in the formula for the velocity that is specified in the last parameter. This formula needs to have as many components as there are space dimensions, separated by semicolons. As stated, this means that we prescribe the (horizontal) x-velocity and set the vertical velocity to zero. The horizontal component is here either 1 or -1, depending on whether we are to the right or the left of the point $1+\sin(\pi t/2)$ that is moving back and forth with time once every four time units. The `if` statement understood by the parser we use for these formulas has the syntax `if(condition, value-if-true, value-if-false)`.

Note: While you can enter most any expression into the parser for these velocity boundary conditions, not all make sense. In particular, if you use an incompressible medium like we do here, then you need to make sure that either the flow you prescribe is indeed tangential, or that at least the flow into and out of the boundary this function applies to is balanced so that in sum the amount of material in the domain stays constant.
It is in general not possible for ASPECT to verify that a given input is sensible. However, you will quickly find out if it isn't: The linear solver for the Stokes equations will simply not converge. For example, if your function expression in the input file above read

```
if(x>1+sin(0.5*pi*t), 1, -1); 1
```

then at the time of writing this you would get the following error message:

```
*** Timestep 0:  t=0 seconds
 Solving temperature system...  0 iterations.
 Rebuilding Stokes preconditioner...
 Solving Stokes system...

 ...some timing output ...


 -----------------------------------------------------
 Exception on processing:
 Iterative method reported convergence failure in step 9539 with residual 6.0552
 Aborting!
 -----------------------------------------------------
```

The reason is, of course, that there is no incompressible (divergence free) flow field that allows for a constant vertical outflow component along the top boundary without corresponding inflow anywhere else.

The remainder of the setup is described in the following, complete input file:

```
############### Global parameters

set Dimension                                = 2
set Start time                               = 0
set End time                                 = 20
set Use years in output instead of seconds = false
set Output directory                         = output


############### Parameters describing the model
# Let us here choose again a box domain of size 2x1
# where we fix the temperature at the bottom and top,
# allow free slip along the bottom, left and right,
# and prescribe the velocity along the top using the
# 'function' description.
```

```
subsection Geometry model
  set Model name = box

  subsection Box
    set X extent = 2
    set Y extent = 1
  end
end


subsection Model settings
  set Fixed temperature boundary indicators   = 2, 3
  set Zero velocity boundary indicators       =
  set Tangential velocity boundary indicators = 0, 1, 2
  set Prescribed velocity boundary indicators = 3: function
end


# We then set the temperature to one at the bottom and zero
# at the top:
subsection Boundary temperature model
  set Model name = box

  subsection Box
    set Bottom temperature = 1
    set Top temperature    = 0
  end
end


# The velocity along the top boundary models a spreading
# center that is moving left and right:
subsection Boundary velocity model
  subsection Function
    set Variable names      = x,z,t
    set Function constants  = pi=3.1415926
    set Function expression = if(x>1+sin(0.5*pi*t), 1, -1); 0
  end
end


# We then choose a vertical gravity model and describe the
# initial temperature with a vertical gradient. The default
# strength for gravity is one. The material model is the
# same as before.
subsection Gravity model
  set Model name = vertical
end


subsection Initial conditions
  set Model name = function

  subsection Function
    set Variable names      = x,z
    set Function expression = (1-z)
  end
end


subsection Material model
  set Model name = simple

  subsection Simple model
```

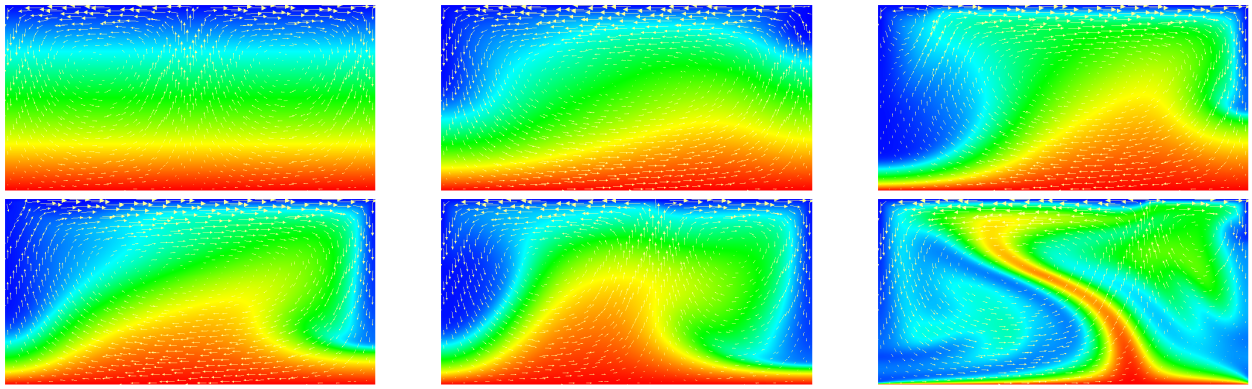


Figure 11: Variable velocity boundary conditions: Temperature and velocity fields at the initial time (top left) and at various other points in time during the simulation.

```
    set Thermal conductivity          = 1e-6
    set Thermal expansion coefficient = 1e-4
    set Viscosity                     = 1
  end
end


# The final part of this input file describes how many times the
# mesh is refined and what to do with the solution once computed
subsection Mesh refinement
  set Initial adaptive refinement        = 0
  set Initial global refinement          = 5
  set Time steps between mesh refinement = 0
end


subsection Postprocess
  set List of postprocessors = visualization, temperature statistics, heat flux statistics

  subsection Visualization
    set Time between graphical output = 0.1
  end
end
```

This model description yields a setup with a Rayleigh number of 200 (taking into account that the domain has size 2). It would, thus, be dominated by heat conduction rather than convection if the prescribed velocity boundary conditions did not provide a stirring action. Visualizing the results of this simulation[13] yields images like the ones shown in Fig. 11.

6.1.3 Using passive and active compositional fields

One frequently wants to track where material goes, either because one simply wants to see where stuff ends up (e.g., to determine if a particular model yields mixing between the lower and upper mantle) or because the material model in fact depends not only pressure, temperature and location but also on the mass fractions of certain chemical or other species. We will refer to the first case as *passive* and the latter as *active* to indicate the role of the additional quantities whose distribution we want to track. We refer to the whole process as

[13] In fact, the pictures are generated using a twice more refined mesh to provide adequate resolution. We keep the default setting of five global refinements in the parameter file as documented above to keep compute time reasonable when using the default settings.

compositional since we consider quantities that have the flavor of something that denotes the composition of the material at any given point.

There are basically two ways to achieve this: one can advect a set of particles ("tracers") along with the velocity field, or one can advect along a field. In the first case, where the closest particle came from indicates the value of the concentration at any given position. In the latter case, the concentration(s) at any given position is simply given by the value of the field(s) at this location.

ASPECT implements both strategies, at least to a certain degree. In this cookbook, we will follow the route of advected fields.

The passive case. We will consider the exact same situation as in the previous section but we will ask where the material that started in the bottom 20% of the domain ends up, as well as the material that started in the top 20%. For the moment, let us assume that there is no material between the materials at the bottom, the top, and the middle. The way to describe this situation is to simply add the following block of definitions to the parameter file (you can find the full parameter file in `cookbooks/compositional-passive.prm`:

```
# This is the new part: We declare that there will
# be two compositional fields that will be
# advected along. Their initial conditions are given by
# a function that is one for the lowermost 0.2 height
# units of the domain and zero otherwise in the first case,
# and one in the top most 0.2 height units in the latter.
subsection Compositional fields
  set Number of fields = 2
end

subsection Compositional initial conditions
  set Model name = function

  subsection Function
    set Variable names      = x,y
    set Function expression = if(y<0.2, 1, 0) ; if(y>0.8, 1, 0)
  end
end
```

Running this simulation yields results such as the ones shown in Fig. 12 where we show the values of the functions $c_1(\mathbf{x},t)$ and $c_2(\mathbf{x},t)$ at various times in the simulation. Because these fields were one only inside the lowermost and uppermost parts of the domain, zero everywhere else, and because they have simply been advected along with the flow field, the places where they are larger than one half indicate where material has been transported to so far.[14]

Fig. 12 shows one aspect of compositional fields that occasionally makes them difficult to use for very long time computations. The simulation shown here runs for 20 time units, where every cycle of the spreading center at the top moving left and right takes 4 time units, for a total of 5 such cycles. While this is certainly no short-term simulation, it is obviously visible in the figure that the interface between the materials has diffused over time. Fig. 13 shows a zoom into the center of the domain at the final time of the simulation. The figure only shows values that are larger than 0.5, and it looks like the transition from red or blue to the edge of the shown region is no wider than 3 cells. This means that the computation is not overly diffusive but it is nevertheless true that this method has difficulty following long and thin filaments.[15] This is an area in which ASPECT may see improvements in the future.

[14] Of course, this interpretation suggests that we could have achieved the same goal by encoding everything into a single function – that would, for example, have had initial values one, zero and minus one in the three parts of the domain we are interested in.

[15] We note that this is no different for tracers where the position of tracers has to be integrated over time and is subject to numerical error. In simulations, their location is therefore not the exact one but also subject to a diffusive process resulting from numerical inaccuracies. Furthermore, in long thin filaments, the number of tracers per cell often becomes too small and new tracers have to be inserted; their properties are then interpolated from the surrounding tracers, a process that also incurs a smoothing penalty.

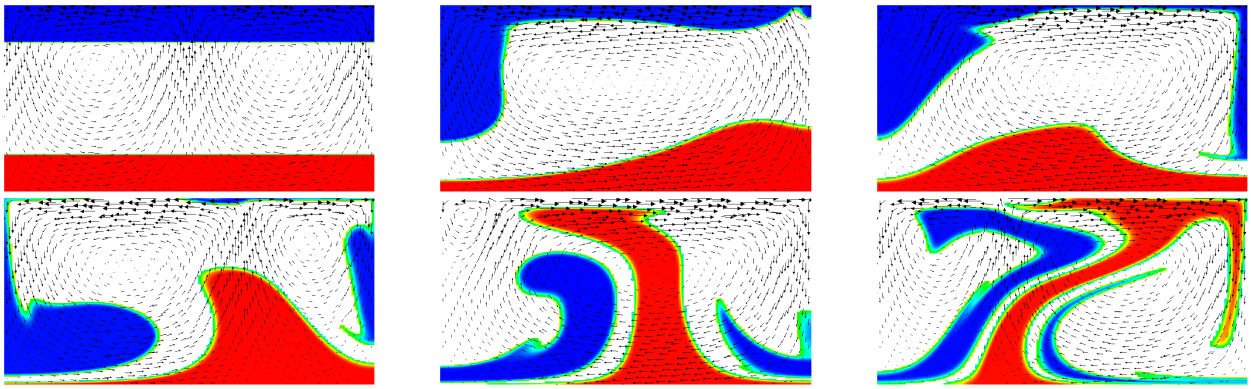


Figure 12: Passive compositional fields: The figures show, at different times in the simulation, the velocity field along with those locations where the first compositional field is larger than 0.5 (in red, indicating the locations where material from the bottom of the domain has gone) as well as where the second compositional field is larger than 0.5 (in blue, indicating material from the top of the domain. The results were obtained with two more global refinement steps compared to the `cookbooks/compositional-passive.prm` input file.

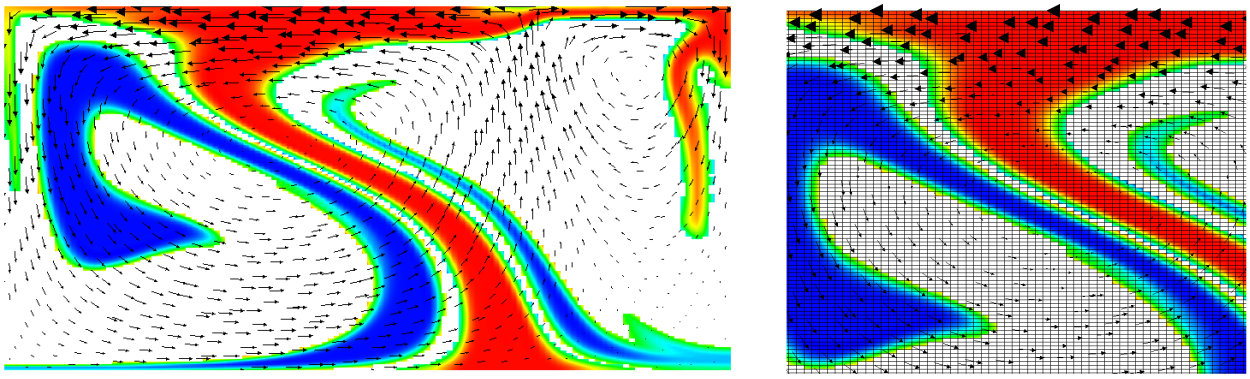


Figure 13: Passive compositional fields: A later image of the simulation corresponding to the sequence shown in Fig. 12 (left) and zoom-in on the center, also showing the mesh (right).

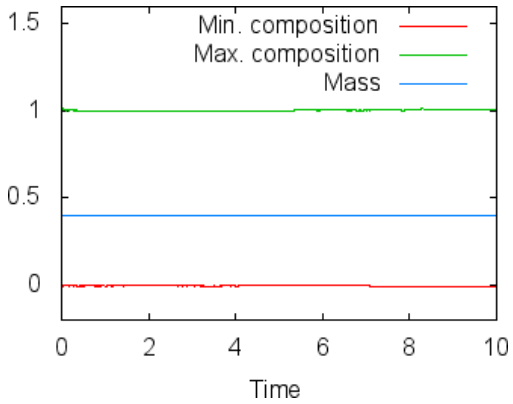


Figure 14: Passive compositional fields: Minimum and maximum of the first compositional variable over time, as well as the mass $m_1(t) = \int_\Omega c_1(\mathbf{x},t)$ stored in this variable.

A different way of looking at the quality of compositional fields as opposed to tracers is to ask whether they conserve mass. In the current context, the mass contained in the ith compositional field is $m_i(t) = \int_\Omega c_i(\mathbf{x},t)$. This can easily be achieve in the following way, by adding the `composition statistics` postprocessor:

```
subsection Postprocess
  set List of postprocessors = visualization, temperature statistics, composition statistics
end
```

While the scheme we use to advect the compositional fields is not strictly conservative, it is almost perfectly so in practice. For example, in the computations shown in this section (using two additional global mesh refinements over the settings in the parameter file `cookbooks/compositional-passive.prm`), Fig. 14 shows the maximal and minimal values of the first compositional fields over time, along with the mass $m_1(t)$ (these are all tabulated in columns of the statistics file, see Sections 4.1 and 4.4.2). While the maximum and minimum fluctuate slightly due to the instability of the finite element method in resolving discontinuous functions, the mass appears stable at a value of 0.403646 (the exact value, namely the area that was initially filled by each material, is 0.4; the difference is a result of the fact that we can't exactly represent the step function on our mesh with the finite element space). In fact, the maximal difference in this value between time steps 1 and 500 is only $1.1 \cdot 10^{-6}$. In other words, these numbers show that the compositional field approach is almost exactly mass conservative.

The active case. The next step, of course, is to make the flow actually depend on the composition. After all, compositional fields are not only intended to indicate where material come from, but also to indicate the properties of this material. In general, the way to achieve this is to write material models where the density, viscosity, and other parameters depend on the composition, taking into account what the compositional fields actually denote (e.g., if they simply indicate the origin of material, or the concentration of things like olivine, perovskite, ...). The construction of material models is discussed in much greater detail in Section 7.2.1; we do not want to revisit this issue here and instead choose – once again – the simplest material model that is implemented in ASPECT: the `simple` model.

The place where we are going to hook in a compositional dependence is the density. In the `simple` model, the density is fundamentally described by a material that expands linearly with the temperature; for small density variations, this corresponds to a density model of the form $\rho(T) = \rho_0(1-\alpha(T-T_0))$. This is, by virtue of its simplicity, the most often considered density model. But the `simple` model also has a hook to make the density depend on the first compositional field $c_1(\mathbf{x},t)$, yielding a dependence of the form $\rho(T) = \rho_0(1-\alpha(T-T_0)) + \gamma c_1$. Here, let us choose $\rho_0 = 1, \alpha = 0.01, T_0 = 0, \gamma = 100$. The rest of our model setup will be as in the passive case above. Because the temperature will be between zero and one, the temperature induced density variations will be restricted to 0.01, whereas the density variation by origin of the material is 100. This should make sure that dense material remains at the bottom despite the fact that it is hotter than the surrounding material.[16]

This setup of the problem can be described using an input file that is almost completely unchanged from the passive case. The only difference is the use of the following section (the complete input file can be found in `cookbooks/compositional-active.prm`:

```
subsection Material model
  set Model name = simple

  subsection Simple model
    set Thermal conductivity                = 1e-6
    set Thermal expansion coefficient       = 0.01
    set Viscosity                           = 1
    set Reference density                   = 1
    set Reference temperature               = 0
```

[16] The actual values do not matter as much here. They are chosen in such a way that the system – previously driven primarily by the velocity boundary conditions at the top – now also feels the impact of the density variations. To have an effect, the buoyancy induced by the density difference between materials must be strong enough to balance or at least approach the forces exerted by whatever is driving the velocity at the top.

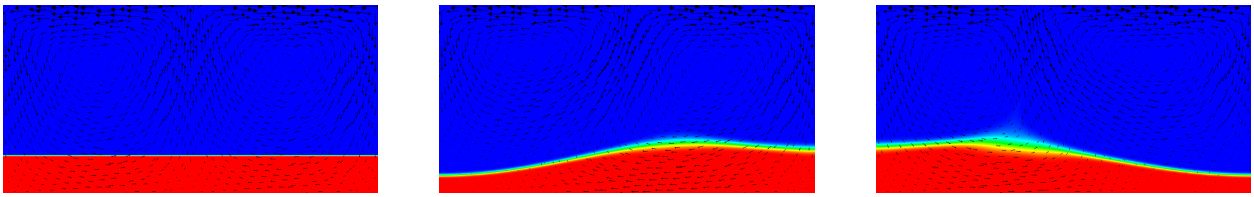


Figure 15: Active compositional fields: Compositional field 1 at the time $t = 0, 10, 20$. Compared to the results shown in Fig. 12 it is clear that the heavy material stays at the bottom of the domain now. The effect of the density on the velocity field is also clearly visible by noting that at all three times the spreading center at the top boundary is in exactly the same position; this would result in exactly the same velocity field if the density and temperature were constant.

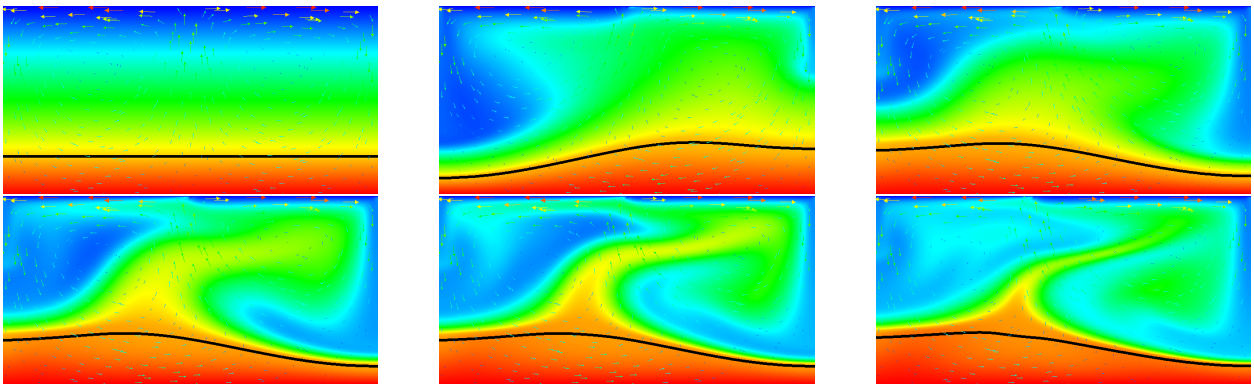


Figure 16: Active compositional fields: Temperature fields at $t = 0, 2, 4, 8, 12, 20$. The black line is the isocontour line $c_1(\vec{x}, t) = 0.5$ delineating the position of the dense material at the bottom.

```
    set Density differential for compositional field 1 = 0.1
  end
end
```

To debug the model, we will also want to visualize the density in our graphical output files. This is done using the following addition to the postprocessing section, using the `density` visualization plugin:

```
subsection Postprocess
  set List of postprocessors = visualization, temperature statistics, composition statistics

  subsection Visualization
    set List of output variables = density
    set Time between graphical output = 0.1
  end
end
```

Results of this model are visualized in Fig.s 15 and 16. What is visible is that over the course of the simulation, the material that starts at the bottom of the domain remains there. This can only happen if the circulation is significantly affected by the high density material once the interface starts to become non-horizontal, and this is indeed visible in the velocity vectors. As a second consequence, if the material at the bottom does not move away, then there needs to be a different way for the heat provided at the bottom to get through the bottom layer: either there must be a secondary convection system in the bottom layer, or heat is simply conducted. The pictures in the figure seem to suggest that the latter is the case.

It is easy, using the outline above, to play with the various factors that drive this system, namely:

- The magnitude of the velocity prescribed at the top.

- The magnitude of the velocities induced by thermal buoyancy, as resulting from the magnitude of gravity and the thermal expansion coefficient.
- The magnitude of the velocities induced by compositional variability, as described by the coefficient γ and the magnitude of gravity.

Using the coefficients involved in these considerations, it is trivially possible to map out the parameter space to find which of these effects is dominant. As mentioned in discussing the values in the input file, what is important is the *relative* size of these parameters, not the fact that currently the density in the material at the bottom is 100 times larger than in the rest of the domain, an effect that from a physical perspective clearly makes no sense at all.

6.1.4 Using tracer particles

To be written

6.2 Geophysical setups

To be written

Include something that uses the GPlates interface

6.3 Benchmarks

Benchmarks are used to verify that a solver solves the problem correctly, i.e., to *verify* correctness of a code.[17] Over the past decades, the geodynamics community has come up with a large number of benchmarks. Depending on the goals of their original inventors, they describe stationary problems in which only the solution of the flow problem is of interest (but the flow may be compressible or incompressible, with constant or variable viscosity, etc), or they may actually model time-dependent processes. Some of them have solutions that are analytically known and can be compared with, while for others, there are only sets of numbers that are approximately known. We have implemented a number of them in ASPECT to convince ourselves (and our users) that ASPECT indeed works as intended and advertised. Some of these benchmarks are discussed below. Numerical results for these benchmarks are also presented in [KHB12] in much more detail than shown here.

6.3.1 The SolCx Stokes benchmark

The SolCx benchmark is intended to test the accuracy of the solution to a problem that has a large jump in the viscosity along a line through the domain. Such situations are common in geophysics: for example, the viscosity in a cold, subducting slab is much larger than in the surrounding, relatively hot mantle material.

The SolCx benchmark computes the Stokes flow field of a fluid driven by spatial density variations, subject to a spatially variable viscosity. Specifically, the domain is $\Omega = [0,1]^2$, gravity is $\mathbf{g} = (0,-1)^T$ and the density is given by $\rho(\mathbf{x}) = \sin(\pi x_1)\cos(\pi x_2)$; this can be considered a density perturbation to a constant background density. The viscosity is

$$\eta(\mathbf{x}) = \begin{cases} 1 & \text{for } x_1 \leq 0.5, \\ 10^6 & \text{for } x_1 > 0.5. \end{cases}$$

This strongly discontinuous viscosity field yields an almost stagnant flow in the right half of the domain and consequently a singularity in the pressure along the interface. Boundary conditions are free slip on all of $\partial\Omega$. The temperature plays no role in this benchmark. The prescribed density field and the resulting velocity field are shown in Fig. 17.

The SolCx benchmark was previously used in [DMGT11, Section 4.1.1] (references to earlier uses of the benchmark are available there) and its analytic solution is given in [Zho96]. ASPECT contains an implementation of this analytic solution taken from the Underworld package (see [MQL+07] and `http:`

[17] Verification is the first half of the *verification and validation* (V&V) procedure: *verification* intends to ensure that the mathematical model is solved correctly, while *validation* intends to ensure that the mathematical model is correct. Obviously, much of the aim of computational geodynamics is to validate the models that we have.

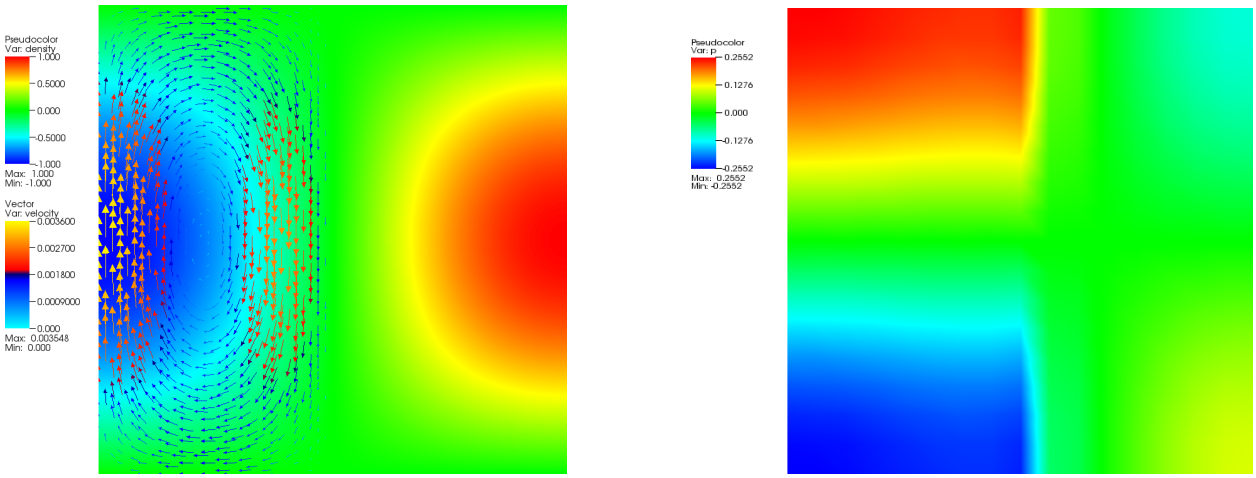


Figure 17: SolCx Stokes benchmark. Left: The density perturbation field and overlaid to it some velocity vectors. The viscosity is very large in the right hand, leading to a stagnant flow in this region. Right: The pressure on a relatively coarse mesh, showing the internal layer along the line where the viscosity jumps.

//www.underworldproject.org/, and correcting for the mismatch in sign between the implementation and the description in [DMGT11]).

To run this benchmark, the following input file will do:

```
################ Global parameters

set Dimension                              = 2

set Start time                             = 0
set End time                               = 0

set Output directory                       = output

set Pressure normalization                 = volume


################ Parameters describing the model

subsection Geometry model
  set Model name = box

  subsection Box
    set X extent = 1
    set Y extent = 1
  end
end


subsection Model settings
  set Prescribed velocity boundary indicators =
  set Tangential velocity boundary indicators = 0,1,2,3
  set Zero velocity boundary indicators       =
end


subsection Material model
  set Model name = SolCx
```

```
  subsection SolCx
    set Viscosity jump = 1e6
  end
end


subsection Gravity model
  set Model name = vertical
end


############### Parameters describing the temperature field

subsection Boundary temperature model
  set Model name = box
end


subsection Initial conditions
  set Model name = perturbed box
end



############### Parameters describing the discretization

subsection Discretization
  set Stokes velocity polynomial degree       = 2
  set Use locally conservative discretization = false
end


subsection Mesh refinement
  set Initial adaptive refinement             = 0
  set Initial global refinement               = 4
end


############### Parameters describing the what to do with the solution

subsection Postprocess
  set List of postprocessors = DuretzEtAl error, visualization
end
```

Since this is the first cookbook in the benchmarking section, let us go through the different parts of this file in more detail:

- The first part consists of parameter setting for overall parameters. Specifically, we set the dimension in which this benchmark runs to two and choose an output directory. Since we are not interested in a time dependent solution, we set the end time equal to the start time, which results in only a single time step being computed.

  The last parameter of this section, `Pressure normalization`, is set in such a way that the pressure is chosen so that its *domain* average is zero, rather than the pressure along the surface, see Section 2.5.

- The next part of the input file describes the setup of the benchmark. Specifically, we have to say how the geometry should look like (a box of size 1×1) and what the velocity boundary conditions shall be (tangential flow all around – the box geometry defines four boundary indicators for the left, right, bottom and top boundaries, see also Section 5.15). This is followed by subsections choosing the material model (where we choose a particular model implemented in ASPECT that describes the spatially variable density and viscosity fields, along with the size of the viscosity jump) and finally the chosen gravity model (a gravity field that is the constant vector $(0,-1)^T$, see Section 5.18).

- The part that follows this describes the boundary and initial values for the temperature. While we are not interested in the evolution of the temperature field in this benchmark, we nevertheless need to set something. The values given here are the minimal set of inputs.

- The second-to-last part sets discretization parameters. Specifically, it determines what kind of Stokes element to choose (see Section 5.13 and the extensive discussion in [KHB12]). We do not adaptively refine the mesh but only do four global refinement steps at the very beginning. This is obviously a parameter worth playing with.

- The final section on postprocessors determines what to do with the solution once computed. Here, we do two things: we ask ASPECT to compute the error in the solution using the setup described in the Duretz et al. paper [DMGT11], and we request that output files for later visualization are generated and placed in the output directory. The functions that compute the error automatically query which kind of material model had been chosen, i.e., they can know whether we are solving the SolCx benchmark or one of the other benchmarks discussed in the following subsections.

Upon running ASPECT with this input file, you will get output of the following kind (obviously with different timings, and details of the output may also change as development of the code continues):

```
aspect/cookbooks> ../lib/aspect sol_cx.prm
Number of active cells: 256 (on 5 levels)
Number of degrees of freedom: 3,556 (2,178+289+1,089)

*** Timestep 0:  t=0 years
   Solving temperature system... 0 iterations.
   Rebuilding Stokes preconditioner...
   Solving Stokes system... 30+3 iterations.

   Postprocessing:
     Errors u_L1, p_L1, u_L2, p_L2: 1.125997e-06, 2.994143e-03, 1.670009e-06, 9.778441e-03
     Writing graphical output:      output/solution-00000


+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |      1.51s |            |
|                                             |            |            |
| Section                         | no. calls |  wall time | % of total |
+---------------------------------+-----------+------------+------------+
| Assemble Stokes system          |         1 |     0.114s |       7.6% |
| Assemble temperature system     |         1 |     0.284s |        19% |
| Build Stokes preconditioner     |         1 |    0.0935s |       6.2% |
| Build temperature preconditioner|         1 |    0.0043s |      0.29% |
| Solve Stokes system             |         1 |    0.0717s |       4.8% |
| Solve temperature system        |         1 |  0.000753s |      0.05% |
| Postprocessing                  |         1 |     0.627s |        42% |
| Setup dof systems               |         1 |      0.19s |        13% |
+---------------------------------+-----------+------------+------------+
```

One can then visualize the solution in a number of different ways (see Section 4.4), yielding pictures like those shown in Fig. 17. One can also analyze the error as shown in various different ways, for example as a function of the mesh refinement level, the element chosen, etc.; we have done so extensively in [KHB12].

6.3.2 The SolKz Stokes benchmark

The SolKz benchmark is another variation on the same theme as the SolCx benchmark above: it solves a Stokes problem with a spatially variable viscosity but this time the viscosity is not a discontinuous function but grows exponentially with the vertical coordinate so that it's overall variation is again 10^6. The forcing is again chosen by imposing a spatially variable density variation. For details, refer again to [DMGT11].

The following input file, only a small variation of the one in the previous section, solves this benchmark:

```
############### Global parameters

set Dimension                                = 2

set Start time                               = 0
set End time                                 = 0

set Output directory                         = output

set Pressure normalization                   = volume


############### Parameters describing the model

subsection Geometry model
  set Model name = box

  subsection Box
    set X extent = 1
    set Y extent = 1
  end
end


subsection Model settings
  set Prescribed velocity boundary indicators =
  set Tangential velocity boundary indicators = 0,1,2,3
  set Zero velocity boundary indicators       =
end


subsection Material model
  set Model name = SolKz
end


subsection Gravity model
  set Model name = vertical
end


############### Parameters describing the temperature field

subsection Boundary temperature model
  set Model name = box
end


subsection Initial conditions
  set Model name = perturbed box
end



############### Parameters describing the discretization

subsection Discretization
  set Stokes velocity polynomial degree       = 2
  set Use locally conservative discretization = false
end


subsection Mesh refinement
  set Initial adaptive refinement             = 0
```

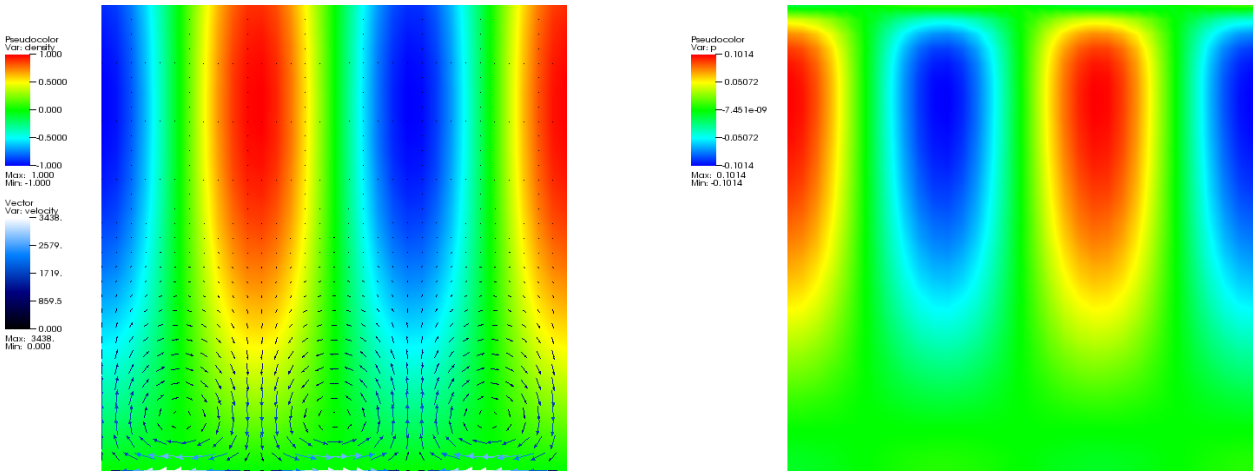


Figure 18: SolKz Stokes benchmark. Left: The density perturbation field and overlaid to it some velocity vectors. The viscosity grows exponentially in the vertical direction, leading to small velocities at the top despite the large density variations. Right: The pressure.

```
  set Initial global refinement                = 4
end


############### Parameters describing the what to do with the solution

subsection Postprocess
  set List of postprocessors = DuretzEtAl error, visualization
end
```

The output when running ASPECT on this parameter file looks similar to the one shown for the SolCx case. The solution when computed with one more level of global refinement is visualized in Fig. 18.

6.3.3 The "inclusion" Stokes benchmark

The "inclusion" benchmark again solves a problem with a discontinuous viscosity, but this time the viscosity is chosen in such a way that the discontinuity is along a circle. This ensures that, unlike in the SolCx benchmark discussed above, the discontinuity in the viscosity never aligns to cell boundaries, leading to much larger difficulties in obtaining an accurate representation of the pressure. Specifically, the almost discontinuous pressure along this interface leads to oscillations in the numerical solution. This can be seen in the visualizations shown in Fig. 19. As before, for details we refer to [DMGT11]. The analytic solution against which we compare is given in [SP03]. An extensive discussion of convergence properties is given in [KHB12].

As before, the benchmark can be run with a small variation of the input files already discussed above:

Revisit this once we have the machinery in place to choose nonzero boundary conditions in a more elegant way.

```
############### Global parameters

set Dimension                              = 2

set Start time                             = 0
set End time                               = 0

set Output directory                       = output

set Pressure normalization                 = volume
```

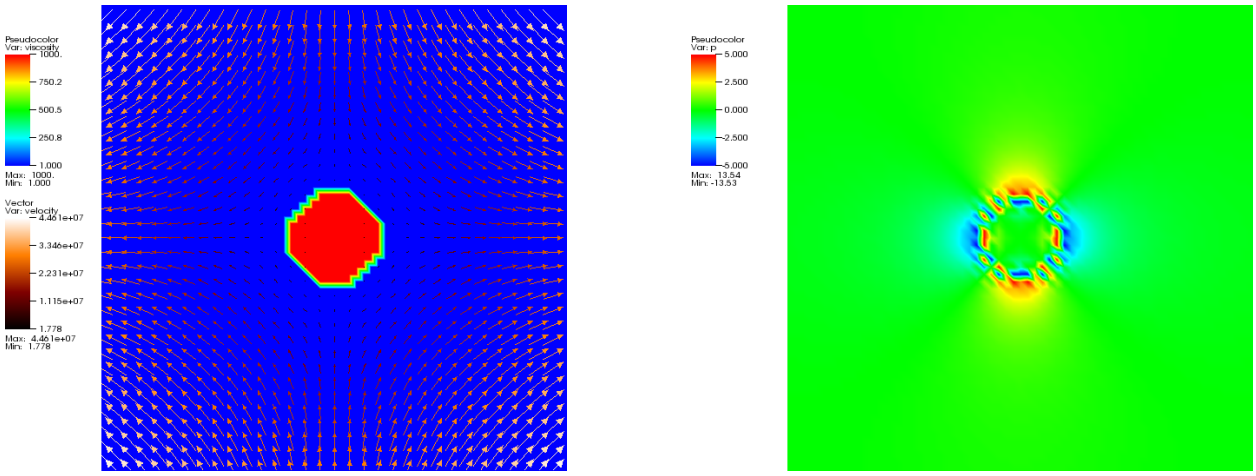


Figure 19: Inclusion Stokes benchmark. Left: The viscosity field when interpolated onto the mesh (internally, the "exact" viscosity field – large inside a circle, small outside – is used), and overlaid to it some velocity vectors. Right: The pressure with its oscillations along the interface. The oscillations become more localized as the mesh is refined.

```
############### Parameters describing the model

subsection Geometry model
  set Model name = box

  subsection Box
    set X extent = 2
    set Y extent = 2
  end
end


subsection Model settings
  set Prescribed velocity boundary indicators = 0,1,2,3
  set Tangential velocity boundary indicators =
  set Zero velocity boundary indicators       =
end


subsection Material model
  set Model name = Inclusion

  subsection Inclusion
    set Viscosity jump = 1e3
  end
end


subsection Gravity model
  set Model name = vertical
end


############### Parameters describing the temperature field
```

```
subsection Boundary temperature model
  set Model name = box
end


subsection Initial conditions
  set Model name = perturbed box
end



############### Parameters describing the discretization

subsection Discretization
  set Stokes velocity polynomial degree       = 2
  set Use locally conservative discretization = false
end


subsection Mesh refinement
  set Initial adaptive refinement             = 0
  set Initial global refinement               = 6
end


############### Parameters describing the what to do with the solution

subsection Postprocess
  set List of postprocessors = DuretzEtAl error, visualization
end
```

6.3.4 The "Stokes' law" benchmark

This section was contributed by Juliane Dannberg.

Stokes' law was derived by George Gabriel Stokes in 1851 and describes the frictional force a sphere with a density different than the surrounding fluid experiences in a laminar flowing viscous medium. A setup for testing this law is a sphere with the radius r falling in a highly viscous fluid with lower density. Due to its higher density the sphere is accelerated by the gravitational force. While the frictional force increases with the velocity of the falling particle, the buoyancy force remains constant. Thus, after some time the forces will be balanced and the settling velocity of the sphere v_s will remain constant:

$$\underbrace{6\pi\,\eta\,r\,v_s}_{\text{frictional force}} = \underbrace{4/3\pi\,r^3\,\Delta\rho\,g}_{\text{buoyancy force}}, \tag{21}$$

where η is the dynamic viscosity of the fluid, $\Delta\rho$ is the density difference between sphere and fluid and g the gravitational acceleration. The resulting settling velocity is then given by

$$v_s = \frac{2}{9}\frac{\Delta\rho\,r^2\,g}{\eta}. \tag{22}$$

Because we do not take into account inertia in our numerical computation, the falling particle will reach the constant settling velocity right after the first timestep.

For the setup of this benchmark, we chose the following parameters:

$$\begin{aligned} r &= 200\,\text{km} \\ \Delta\rho &= 100\,\text{kg/m}^3 \\ \eta &= 10^{22}\,\text{Pa s} \\ g &= 9.81\,\text{m/s}^2. \end{aligned}$$

With these values, the exact value of sinking velocity is $v_s = 8.72 \cdot 10^{-10}\,\text{m/s}$.

To run this benchmark, we need to set up an input file that describes the situation. In principle, what we need to do is to describe a spherical object with a density that is larger than the surrounding material. There are multiple ways of doing this. For example, we could simply set the initial temperature of the material in the sphere to a lower value, yielding a higher density with any of the common material models. Or, we could use ASPECT's facilities to advect along what are called "compositional fields" and make the density dependent on these fields.

We will go with the second approach and tell ASPECT to advect a single compositional field. The initial conditions for this field will be zero outside the sphere and one inside. We then need to also tell the material model to increase the density by $\Delta\rho = 100 kg\,m^{-3}$ times the concentration of the compositional field. This can be done, like everything else, from the input file.

All of this setup is then described by the following input file. (You can find the input file to run this cookbook example in `cookbooks/stokes.prm`. For your first runs you will probably want to reduce the number of mesh refinement steps to make things run more quickly.)

```
################ Global parameters
# We use a 3d setup. Since we are only interested
# in a steady state solution, we set the end time
# equal to the start time to force a single time
# step before the program terminates.

set Dimension                                = 3

set Start time                               = 0
set End time                                 = 0
set Use years in output instead of seconds = false

set Output directory                         = output


################ Parameters describing the model
# The setup is a 3d box with edge length 2890000 in which
# all 6 sides have free slip boundary conditions. Because
# the temperature plays no role in this model we need not
# bother to describe temperature boundary conditions or
# the material parameters that pertain to the temperature.


subsection Geometry model
  set Model name = box

  subsection Box
    set X extent  = 2890000
    set Y extent  = 2890000
    set Z extent  = 2890000
  end
end


subsection Model settings
  set Tangential velocity boundary indicators = 0,1,2,3,4,5
end


subsection Material model
  set Model name = simple

  subsection Simple model
    set Reference density             = 3300
    set Viscosity                     = 1e22
  end
end
```

```
subsection Gravity model
  set Model name = vertical

  subsection Vertical
    set Magnitude = 9.81
  end
end


############### Parameters describing the temperature field
# As above, there is no need to set anything for the
# temperature boundary conditions.

subsection Boundary temperature model
  set Model name = box
end

subsection Initial conditions
  set Model name = function

  subsection Function
    set Function expression = 0
  end
end

############### Parameters describing the compositional field
# This, however, is the more important part: We need to describe
# the compositional field and its influence on the density
# function. The following blocks say that we want to
# advect a single compositional field and that we give it an
# initial value that is zero outside a sphere of radius
# r=200000m and centered at the point (p,p,p) with
# p=1445000 (which is half the diameter of the box) and one inside.
# The last block re-opens the material model and sets the
# density differential per unit change in compositional field to
# 100.

subsection Compositional fields
  set Number of fields = 1
end

subsection Compositional initial conditions
  set Model name = function

  subsection Function
    set Variable names      = x,y,z
    set Function constants  = r=200000,p=1445000
    set Function expression = if(sqrt((x-p)*(x-p)+(y-p)*(y-p)+(z-p)*(z-p)) > r, 0, 1)
  end
end

subsection Material model
  subsection Simple model
    set Density differential for compositional field 1 = 100
  end
end




############### Parameters describing the discretization
# The following parameters describe how often we want to refine
# the mesh globally and adaptively, what fraction of cells should
```

```
# be refined in each adaptive refinement step, and what refinement
# indicator to use when refining the mesh adaptively.

subsection Mesh refinement
  set Initial adaptive refinement        = 4
  set Initial global refinement          = 4
  set Refinement fraction                = 0.2
  set Strategy                           = velocity
end


############### Parameters describing the what to do with the solution
# The final section allows us to choose which postprocessors to
# run at the end of each time step. We select to generate graphical
# output that will consist of the primary variables (velocity, pressure,
# temperature and the compositional fields) as well as the density and
# viscosity. We also select to compute some statistics about the
# velocity field.

subsection Postprocess
  set List of postprocessors = visualization, velocity statistics

  subsection Visualization
    set List of output variables = density, viscosity
  end
end
```

Usig this input file, let us try to evaluate the results of the current computations for the settling velocity of the sphere. You can visualize the output in different ways, one of it being ParaView and shown in Fig. 20 (an alternative is to use Visit as described in Section 4.4; 3d images of this simulation using Visit are shown in Fig. 21). Here, Paraview has the advantage that you can calculate the average velocity of the sphere using the following filters:

1. Threshold (Scalars: C_1, Lower Threshold 0.5, Upper Threshold 1),
2. Integrate Variables,
3. Cell Data to Point Data,
4. Calculator (use the formula sqrt(velocity_xˆ2+ velocity_yˆ2+velocity_zˆ2)/Volume).

If you then look at the Calculator object in the Spreadsheet View, you can see the average sinking velocity of the sphere in the column "Result" and compare it to the theoretical value $v_s = 8.72 \cdot 10^{-10}$ m/s. In this case, the numerical result is $8.865 \cdot 10^{-10}$ m/s when you add a few more refinement steps to actually resolve the 3d flow field adequately. The "velocity statistics" postprocessor we have selected above also provides us with a maximal velocity that is on the same order of magnitude. The difference between the analytical and the numerical values can be explained by different at least the following three points: (i) In our case the sphere is viscous and not rigid as assumed in Stokes' initial model, leading to a velocity field that varies inside the sphere rather than being constant. (ii) Stokes' law is derived using an infinite domain but we have a finite box instead. (iii) The mesh may not yet fine enough to provide a fully converges solution. Nevertheless, the fact that we get a result that is accurate to less than 2% is a good indication that ASPECT implements the equations correctly.

7 Extending Aspect

ASPECT is designed to be an extensible code. In particular, the program uses a plugin architecture in which it is trivial to replace or extend certain components of the program:

- the material description,

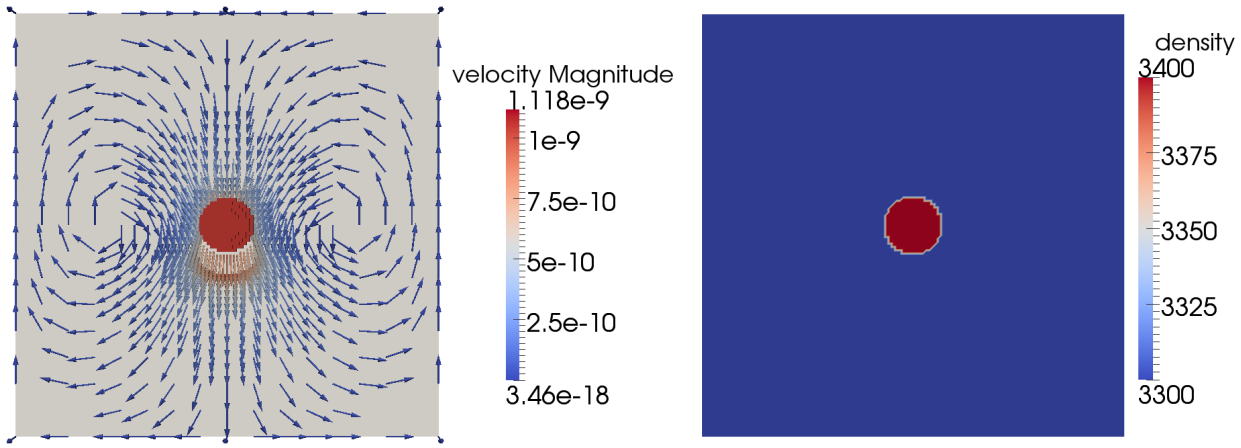


Figure 20: Stokes benchmark. Both figures show only a 2D slice of the three-dimensional model. Left: The compositional field and overlaid to it some velocity vectors. The composition is 1 inside a sphere with the radius of 200 km and 0 outside of this sphere. As the velocity vectors show, the sphere sinks in the viscous medium. Right: The density distribution of the model. The compositional density contrast of 100 kg/m^3 leads to a higher density inside of the sphere.

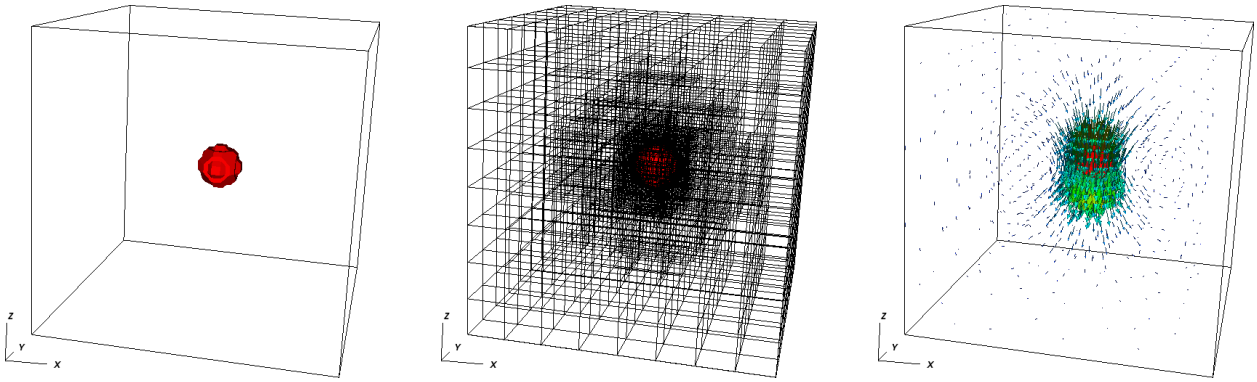


Figure 21: Stokes benchmark. Three-dimensional views of the compositional field (left), the adaptively refined mesh (center) and the resulting velocity field (right).

- the geometry,
- the gravity description,
- the initial conditions,
- the boundary conditions,
- the functions that postprocess the solution, i.e., that can compute derived quantities such as heat fluxes over part of the boundary, mean velocities, etc.,
- the functions that generate derived quantities that can be put into graphical output files for visualization such as fields that depict the strength of the friction heating term, spatially dependent actual viscosities, and so on,
- the computation of refinement indicators,
- the determination of how long a computation should run.

We will discuss the way this is achieved in Sections 7.1 and 7.2. Changing the core functionality, i.e., the basic equations (1)–(3), and how they are solved is arguably more involved. We will discuss this in Section 7.3.

In either of these two cases, you will need to extend the source code of the program. Since ASPECT is written in C++ using the DEAL.II library, you will have to be proficient in C++. You will also likely have to familiarize yourself with this library for which there is an extensive amount of documentation:

- The manual at http://www.dealii.org/developer/doxygen/deal.II/index.html that describes in detail what every class, function and variable in DEAL.II does.
- A collection of modules at http://www.dealii.org/developer/doxygen/deal.II/modules.html that give an overview of whole groups of classes and functions and how they work together to achieve their goal.
- The DEAL.II tutorial at http://www.dealii.org/developer/doxygen/tutorial/index.html that provides a step-by-step introduction to the library using a sequence of several dozen programs that introduce gradually more complex topics. In particular, you will learn DEAL.II's way of *dimension independent programming* that allows you to write the program once, test it in 2d, and run the exact same code in 3d without having to debug it a second time.
- The step-31 and step-32 tutorial programs at http://www.dealii.org/developer/doxygen/deal.II/step_31.html and http://www.dealii.org/developer/doxygen/deal.II/step_32.html from which ASPECT directly descends.
- The DEAL.II Frequently Asked Questions at http://dealii.sourceforge.net/index.php/Deal.II_Questions_and_Answers that also have extensive sections on developing code with DEAL.II as well as on debugging. It also answers a number of questions we frequently get about the use of C++ in DEAL.II.
- Several other parts of the DEAL.II website at http://www.dealii.org/ also have information that may be relevant if you dive deeper into developing code. If you have questions, the mailing lists at http://www.dealii.org/mail.html are also of general help.
- A general overview of DEAL.II is also provided in the paper [BHK07].

As a general note, by default ASPECT utilizes a DEAL.II feature called *debug mode*, see also the introduction to this topic in Section 4.3. If you develop code, you will definitely want this feature to be on, as it will capture the vast majority of bugs you will invariably introduce in your code.

When you write new functionality and run the code for the first time, you will almost invariably first have to deal with a number of these assertions that point out problems in your code. While this may be annoying at first, remember that these are actual bugs in your code that have to be fixed anyway and that are much easier to find if the program aborts than if you have to go by their more indirect results such as wrong answers. The Frequently Asked Questions at http://dealii.sourceforge.net/index.php/Deal.II_Questions_and_Answers contain a section on how to debug DEAL.II programs.

The downside of debug mode, as mentioned before, is that it makes the program much slower. Consequently, once you are confident that your program actually does what it is intended to do – **but no earlier!** –, you may want to switch to optimized mode that links ASPECT with a version of the DEAL.II libraries that uses compiler optimizations and that does not contain the `assert` statements discussed above. This switch can be facilitated by editing the top of the ASPECT `Makefile` and recompiling the program.

In addition to these general comments, ASPECT is itself extensively documented. You can find documentation on all classes, functions and namespaces starting from the `doc/doxygen/index.html` page.

7.1 The idea of plugins and the `SimulatorAccess` and `Introspection` classes

The most common modification you will probably want to do to ASPECT are to switch to a different material model (i.e., have different values of functional dependencies for the coefficients $\eta, \rho, C_p, \ldots$ discussed in Section 2.2); change the geometry; change the direction and magnitude of the gravity vector $\mathbf{g}$; or change the initial and boundary conditions.

To make this as simple as possible, all of these parts of the program (and some more) have been separated into modules that can be replaced quickly and where it is simple to add a new implementation and make it available to the rest of the program and the input parameter file. The way this is achieved is through the following two steps:

- The core of ASPECT really only communicates with material models, geometry descriptions, etc., through a simple and very basic interface. These interfaces are declared in the `include/aspect/material_model/interface.h`, `include/aspect/geometry_model/interface.h`, etc., header files. These classes are always called `Interface`, are located in namespaces that identify their purpose, and their documentation can be found from the general class overview in `doc/doxygen/classes.html`.

  To show an example of a rather minimal case, here is the declaration of the aspect::GravityModel::Interface class (documentation comments have been removed):

```
class Interface
{
  public:
    virtual ~Interface();

    virtual
    Tensor<1,dim>
    gravity_vector (const Point<dim> &position) const = 0;

    static void declare_parameters (ParameterHandler &prm);

    virtual void parse_parameters (ParameterHandler &prm);
};
```

  If you want to implement a new model for gravity, you just need to write a class that derives from this base class and implements the `gravity_vector` function. If your model wants to read parameters from the input file, you also need to have functions called `declare_parameters` and `parse_parameters` in

your class with the same signatures as the ones above. On the other hand, if the new model does not need any run-time parameters, you do not need to overload these functions.[18]

Each of the categories above that allow plugins have several implementations of their respective interfaces that you can use to get an idea of how to implement a new model.

- At the end of the file where you implement your new model, you need to have a call to the macro `ASPECT_REGISTER_GRAVITY_MODEL` (or the equivalent for the other kinds of plugins). For example, let us say that you had implemented a gravity model that takes actual gravimetric readings from the GRACE satellites into account, and had put everything that is necessary into a class `aspect::GravityModel::GRACE`. Then you need a statement like this at the bottom of the file:

```
ASPECT_REGISTER_GRAVITY_MODEL
(GRACE,
 "grace",
 "A gravity model derived from GRACE "
 "data. Run-time parameters are read from the parameter "
 "file in subsection 'Radial constant'.");
```

  Here, the first argument to the macro is the name of the class. The second is the name by which this model can be selected in the parameter file. And the third one is a documentation string that describes the purpose of the class (see, for example, Section 5.18 for an example of how existing models describe themselves).

  This little piece of code ensures several things: (i) That the parameters this class declares are known when reading the parameter file. (ii) That you can select this model (by the name "grace") via the run-time parameter `Gravity model/Model name`. (iii) That ASPECT can create an object of this kind when selected in the parameter file.

  Note that you need not announce the existence of this class in any other part of the code: Everything should just work automatically.[19] This has the advantage that things are neatly separated: You do not need to understand the core of ASPECT to be able to add a new gravity model that can then be selected in an input file. In fact, this is true for all of the plugins we have: by and large, they just receive some data from the simulator and do something with it (e.g., postprocessors), or they just provide information (e.g., initial meshes, gravity models), but they writing either does not imply that you have even fundamental understanding of what the core of the program does.

The procedure for the other areas where plugins are supported works essentially the same, with the obvious change in namespace for the interface class and macro name.

In the following, we will discuss the requirements for individual plugins. Before doing so, however, let us discuss ways in which plugins can query other information, in particular about the current state of the simulation. To this end, let us not consider those plugins that by and large just provide information without any context of the simulation, such as gravity models, prescribed boundary velocities, or initial temperatures. Rather, let us consider things like postprocessors that can compute things like boundary heat fluxes. Taking this as an example (see Section 7.2.7), you are required to write a function with the following interface

```
template <int dim>
class MyPostprocessor : public aspect::Postprocess::Interface
{
```

[18] At first glance one may think that only the `parse_parameters` function can be overloaded since `declare_parameters` is not virtual. However, while the latter is called by the class that manages plugins through pointers to the interface class, the former function is called essentially at the time of registering a plugin, from code that knows the actual type and name of the class you are implementing. Thus, it can call the function – if it exists in your class, or the default implementation in the base class if it doesn't – even without it being declared as virtual.

[19] The existing implementations of models of the gravity and other interfaces declare the class in a header file and define the member functions in a `.cc` file. This is done so that these classes show up in our doxygen-generated documentation, but it is not necessary: you can put your entire class declaration and implementation into a single file as long as you call the macro discussed above on it. This single file is all you need to touch to add a new model.

```
  public:
    virtual
    std::pair<std::string,std::string>
    execute (TableHandler &statistics);

  // ... more things ...
```

The idea is that in the implementation of the `execute` function you would compute whatever you are interested in (e.g., heat fluxes) and return this information in the statistics object that then gets written to a file (see Sections 4.1 and 4.4.2). A postprocessor may also generate other files if it so likes – e.g., graphical output, a file that stores the locations of tracers, etc. To do so, obviously you need access to the current solution. This is stored in a vector somewhere in the core of ASPECT. However, this vector is, by itself, not sufficient: you also need to know the finite element space it is associated with, and for that the triangulation it is defined on. Furthermore, you may need to know what the current simulation time is. A variety of other pieces of information enters computations in these kinds of plugins.

All of this information is of course part of the core of ASPECT, as part of the aspect::Simulator class. However, this is a rather heavy class: it's got dozens of member variables and functions, and it is the one that does all of the numerical heavy lifting. Furthermore, to access data in this class would require that you need to learn about the internals, the data structures, and the design of this class. It would be poor design if plugins had to access information from this core class directly. Rather, the way this works is that those plugin classes that wish to access information about the state of the simulation inherit from the aspect::SimulatorAccess class. This class has an interface that looks like this:

```
template <int dim>
class SimulatorAccess
{
protected:
  double        get_time () const;

  std::string   get_output_directory () const;

  const LinearAlgebra::BlockVector &
  get_solution () const;

  const DoFHandler<dim> &
  get_dof_handler () const;

  // ... many more things ...
```

This way, SimulatorAccess makes information available to plugins without the need for them to understand details of the core of ASPECT. Rather, if the core changes, the SimulatorAccess class can still provide exactly the same interface. Thus, it insulates plugins from having to know the core. Equally importantly, since SimulatorAccess only offers its information in a read-only way it insulates the core from plugins since they can not interfere in the workings of the core except through the interface they themselves provide to the core.

Using this class, if a plugin class `MyPostprocess` is then not only derived from the corresponding `Interface` class but *also* from the SimulatorAccess class, then you can write a member function of the following kind (a non-sensical but instructive example; see Section 7.2.7 for more details on what postprocessors do and how they are implemented):[20]

```
template <int dim>
std::pair<std::string,std::string>
MyPostprocessor<dim>::execute (TableHandler &statistics)
{
  // compute the mean value of vector component 'dim' of the solution
```

[20] For complicated, technical reasons, in the code below we need to access elements of the SimulatorAccess class using the notation `this->get_solution()`, etc. This is due to the fact that both the current class and the base class are templates. A long description of why it is necessary to use `this->` can be found in the DEAL.II Frequently Asked Questions.

```
    // (which here is the pressure block) using a deal.II function:
    const double
      average_pressure = VectorTools::compute_mean_value (this->get_mapping(),
                                                          this->get_dof_handler(),
                                                          QGauss<dim>(2),
                                                          this->get_solution(),
                                                          dim);
    statistics.add_value ("Average_pressure", average_pressure);

    // return that there is nothing to print to screen (a useful
    // plugin would produce something more elaborate here):
    return std::pair<std::string,std::string>();
  }
```

The second piece of information that plugins can use is called "introspection". In the code snippet above, we had to use that the pressure variable is at position `dim`. This kind of *implicit knowledge* is usually bad style: it is error prone because one can easily forget where each component is located; and it is an obstacle to the extensibility of a code if this kind of knowledge is scattered all across the code base.

Introspection is a way out of this dilemma. Using the `SimulatorAccess::introspection()` function returns a reference to an object (of type aspect::Introspection) that plugins can use to learn about these sort of conventions. For example, `this->introspection().component_mask.pressure` returns a component mask (a deal.II concept that describes a list of booleans for each component in a finite element that are true if a component is part of a variable we would like to select and false otherwise) that describes which component of the finite element corresponds to the pressure. The variable, `dim`, we need above to indicate that we want the pressure component can be accessed as `this->introspection().component_indices.pressure`. While this is certainly not shorter than just writing `dim`, it may in fact be easier to remember. It is most definitely less prone to errors and makes it simpler to extend the code in the future because we don't litter the sources with "magic constants" like the one above.

This aspect::Introspection class has a significant number of variables that can be used in this way, i.e., they provide symbolic names for things one frequently has to do and that would otherwise require implicit knowledge of things such as the order of variables, etc.

7.2 Materials, geometries, gravitation and other plugin types

7.2.1 Material models

Need to update this given the current state of the plugin

The material model is responsible for describing the various coefficients in the equations that ASPECT solves. To implement a new material model, you need to overload the aspect::MaterialModel::Interface class and use the `ASPECT_REGISTER_MATERIAL_MODEL` macro to register your new class. The implementation of the new class should be in namespace `aspect::MaterialModel`.

Specifically, your new class needs to implement the basic interface:

```
template <int dim>
class aspect::MaterialModel::Interface
{
  public:
    // Physical parameters used in the basic equations
    virtual double viscosity (const double                   temperature,
                              const double                   pressure,
                              const SymmetricTensor<2,dim> &strain_rate,
                              const Point<dim>             &position) const = 0;

    virtual double density (const double       temperature,
                            const double       pressure,
                            const Point<dim> &position) const = 0;

    virtual double compressibility (const double temperature,
                                    const double pressure,
                                    const Point<dim> &position) const = 0;
```

```
virtual double specific_heat (const double      temperature,
                              const double      pressure,
                              const Point<dim> &position) const = 0;

virtual double thermal_expansion_coefficient (const double      temperature,
                                              const double      pressure,
                                              const Point<dim> &position) const;

virtual double thermal_conductivity (const double temperature,
                                     const double pressure,
                                     const Point<dim> &position) const
                                     = 0;

// Qualitative properties one can ask a material model
virtual bool
viscosity_depends_on (const NonlinearDependence::Dependence dependence) const = 0;

virtual bool
density_depends_on (const NonlinearDependence::Dependence dependence) const = 0;

virtual bool
compressibility_depends_on (const NonlinearDependence::Dependence dependence) const = 0;

virtual bool
specific_heat_depends_on (const NonlinearDependence::Dependence dependence) const = 0;

virtual bool
thermal_conductivity_depends_on (const NonlinearDependence::Dependence dependence) const = 0;

virtual bool is_compressible () const = 0;

// Partial derivatives of physical parameters
virtual double
viscosity_derivative (const double               temperature,
                      const double               pressure,
                      const Point<dim>          &position,
                      const NonlinearDependence::Dependence dependence) const;

virtual double
density_derivative (const double               temperature,
                    const double               pressure,
                    const Point<dim>          &position,
                    const NonlinearDependence::Dependence dependence) const;

virtual double
compressibility_derivative (const double               temperature,
                            const double               pressure,
                            const Point<dim>          &position,
                            const NonlinearDependence::Dependence dependence) const;

virtual double
specific_heat_derivative (const double               temperature,
                          const double               pressure,
                          const Point<dim>          &position,
                          const NonlinearDependence::Dependence dependence) const;

virtual double
thermal_conductivity_derivative (const double               temperature,
                                 const double               pressure,
                                 const Point<dim>          &position,
                                 const NonlinearDependence::Dependence dependence) const;

// Reference quantities
virtual double reference_viscosity () const = 0;
```

```
    virtual double reference_density () const = 0;

    virtual double reference_thermal_expansion_coefficient () const = 0;

    // Auxiliary material properties used for postprocessing
    virtual
    double
    seismic_Vp (const double      temperature,
                const double      pressure) const;

    virtual
    double
    seismic_Vs (const double      temperature,
                const double      pressure) const;
    virtual
    unsigned int
    thermodynamic_phase (const double      temperature,
                         const double      pressure) const;

    // Functions used in dealing with run-time parameters
    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

Here, the first set of functions refer to the coefficients η, C_p, k, ρ in equations (1)–(3), each as a function of temperature, pressure, position and, in the case of the viscosity, the strain rate. Implementations of these methods may of course choose to ignore dependencies on any of these arguments. The second set of functions describes the nonlinear dependence of the various coefficients on pressure, temperature, or strain rate, and the next block then provides the numerical values of these dependencies. This information will be used in future versions of ASPECT to implement a fully nonlinear solution scheme based on, for example, a Newton iteration. The remaining functions are used in postprocessing as well as handling run-time parameters. The exact meaning of these member functions is documented in the aspect::MaterialModel::Interface class documentation. Note that some of the functions listed above have a default implementation, as discussed on the documentation page just mentioned.

The function `is_compressible` returns whether we should consider the material as compressible or not, see Section 2.8.1 on the Boussinesq model. As discussed there, incompressibility as described by this function does not necessarily imply that the density is constant; rather, it may still depend on temperature or pressure. In the current context, compressibility simply means whether we should solve the contuity equation as $\nabla \cdot (\rho \mathbf{u}) = 0$ (compressible Stokes) or as $\nabla \cdot \mathbf{u} = 0$ (incompressible Stokes).

The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.2 Geometry models

The geometry model is responsible for describing the domain in which we want to solve the equations. A domain is described in DEAL.II by a coarse mesh and, if necessary, an object that characterizes the boundary. Together, these two suffice to reconstruct any domain by adaptively refining the coarse mesh and placing new nodes generated by refining cells onto the surface described by the boundary object. The geometry model is also responsible to describe to the rest of the code which parts of the boundary represent Dirichlet-type (fixed temperature) or Neumann-type (no heat flux) boundaries for the temperature, and where the velocity is considered zero or tangential to the boundary. This information is encoded in functions that return which boundary indicators represent these types of boundaries; in DEAL.II, a boundary indicator is a number attached to each piece of the boundary that can be used to represent the type of boundary a piece

belongs to.

To implement a new geometry model, you need to overload the aspect::GeometryModel::Interface class and use the `ASPECT_REGISTER_GEOMETRY_MODEL` macro to register your new class. The implementation of the new class should be in namespace `aspect::GeometryModel`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::GeometryModel::Interface
{
  public:
    virtual
    void
    create_coarse_mesh (parallel::distributed::Triangulation<dim> &coarse_grid) const = 0;

    virtual
    double
    length_scale () const = 0;

    virtual
    double depth(const Point<dim> &position) const = 0;

    virtual
    Point<dim> representative_point(const double depth) const = 0;

    virtual
    double maximal_depth() const = 0;

    virtual
    std::set<types::boundary_id_t>
    get_used_boundary_indicators () const = 0;

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The kind of information these functions need to provide is extensively discussed in the documentation of this interface class at aspect::GeometryModel::Interface. The purpose of the last two functions has been discussed in the general overview of plugins above.

The `create_coarse_mesh` function does not only create the actual mesh (i.e., the locations of the vertices of the coarse mesh and how they connect to cells) but it must also set the boundary indicators for all parts of the boundary of the mesh. The DEAL.II glossary describes the purpose of boundary indicators as follows:

> In a `Triangulation` object, every part of the boundary is associated with a unique number (of type `types::boundary_id`) that is used to identify which boundary geometry object is responsible to generate new points when the mesh is refined. By convention, this boundary indicator is also often used to determine what kinds of boundary conditions are to be applied to a particular part of a boundary. The boundary is composed of the faces of the cells and, in 3d, the edges of these faces.
>
> By default, all boundary indicators of a mesh are zero, unless you are reading from a mesh file that specifically sets them to something different, or unless you use one of the mesh generation functions in namespace `GridGenerator` that have a 'colorize' option. A typical piece of code that sets the boundary indicator on part of the boundary to something else would look like this, here setting the boundary indicator to 42 for all faces located at $x = -1$:

```
  for (typename Triangulation<dim>::active_cell_iterator
```

```
        cell = triangulation.begin_active();
      cell != triangulation.end();
      ++cell)
    for (unsigned int f=0; f<GeometryInfo<dim>::faces_per_cell; ++f)
      if (cell->face(f)->at_boundary())
        if (cell->face(f)->center()[0] == -1)
          cell->face(f)->set_boundary_indicator (42);
```

This calls functions `TriaAccessor::set_boundary_indicator`. In 3d, it may also be appropriate to call `TriaAccessor::set_all_boundary_indicators` instead on each of the selected faces. To query the boundary indicator of a particular face or edge, use `TriaAccessor::boundary_indicator`.

The code above only sets the boundary indicators of a particular part of the boundary, but it does not by itself change the way the Triangulation class treats this boundary for the purposes of mesh refinement. For this, you need to call `Triangulation::set_boundary` to associate a boundary object with a particular boundary indicator. This allows the Triangulation object to use a different method of finding new points on faces and edges to be refined; the default is to use a `StraightBoundary` object for all faces and edges. The results section of step-49 has a worked example that shows all of this in action.

The second use of boundary indicators is to describe not only which geometry object to use on a particular boundary but to select a part of the boundary for particular boundary conditions. *[...]*

Note: Boundary indicators are inherited from mother faces and edges to their children upon mesh refinement. Some more information about boundary indicators is also presented in a section of the documentation of the Triangulation class.

Two comments are in order here. First, if a coarse triangulation's faces already accurately represent where you want to pose which boundary condition (for example to set temperature values or determine which are no-flow and which are tangential flow boundary conditions), then it is sufficient to set these boundary indicators only once at the beginning of the program since they will be inherited upon mesh refinement to the child faces. Here, *at the beginning of the program* is equivalent to inside the `create_coarse_mesh())` function of the geometry module shown above that generates the coarse mesh.

Secondly, however, if you can only accurately determine which boundary indicator should hold where on a refined mesh – for example because the coarse mesh is the cube $[0,L]^3$ and you want to have a fixed velocity boundary describing an extending slab only for those faces for which $z > L - L_{\text{slab}}$ – then you need a way to set the boundary indicator for all boundary faces either to the value representing the slab or the fluid underneath *after every mesh refinement step*. By doing so, child faces can obtain boundary indicators different from that of their parents. DEAL.II triangulations support this kind of operations using a so-called *post-refinement signal*. In essence, what this means is that you can provide a function that will be called by the triangulation immediately after every mesh refinement step.

The way to do this is by writing a function that sets boundary indicators and that will be called by the `Triangulation` class. The triangulation does not provide a pointer to itself to the function being called, nor any other information, so the trick is to get this information into the function. C++ provides a nice mechanism for this that is best explained using an example:

```
#include <deal.II/base/std_cxx1x/bind.h>

template <int dim>
void set_boundary_indicators (parallel::distributed::Triangulation<dim> &triangulation)
{
  ... set boundary indicators on the triangulation object ...
}

template <int dim>
void
MyGeometry<dim>::
```

```
create_coarse_mesh (parallel::distributed::Triangulation<dim> &coarse_grid) const
{
  ... create the coarse mesh ...

  coarse_grid.signals.post_refinement.connect
    (std_cxx1x::bind (&set_boundary_indicators<dim>,
                      std_cxx1x::ref(coarse_grid)));

}
```

What the call to `std_cxx1x::bind` does is to produce an object that can be called like a function with no arguments. It does so by taking the address of a function that does, in fact, take an argument but permanently fix this one argument to a reference to the coarse grid triangulation. After each refinement step, the triangulation will then call the object so created which will in turn call `set_boundary_indicators<dim>` with the reference to the coarse grid as argument.

This approach can be generalized. In the example above, we have used a global function that will be called. However, sometimes it is necessary that this function is in fact a member function of the class that generates the mesh, for example because it needs to access run-time parameters. This can be achieved as follows: assuming the `set_boundary_indicators()` function has been declared as a (non-static, but possibly private) member function of the `MyGeometry` class, then the following will work:

```
#include <deal.II/base/std_cxx1x/bind.h>

template <int dim>
void
MyGeometry<dim>::
set_boundary_indicators (parallel::distributed::Triangulation<dim> &triangulation) const
{
  ... set boundary indicators on the triangulation object ...
}

template <int dim>
void
MyGeometry<dim>::
create_coarse_mesh (parallel::distributed::Triangulation<dim> &coarse_grid) const
{
  ... create the coarse mesh ...

  coarse_grid.signals.post_refinement.connect
    (std_cxx1x::bind (&MyGeometry<dim>::set_boundary_indicators,
                      std_cxx1x::cref(*this),
                      std_cxx1x::ref(coarse_grid)));
}
```

Here, like any other member function, `set_boundary_indicators` implicitly takes a pointer or reference to the object it belongs to as first argument. `std::bind` again creates an object that can be called like a global function with no arguments, and this object in turn calls `set_boundary_indicators` with a pointer to the current object and a reference to the triangulation to work on. Note that because the `create_coarse_mesh` function is declared as `const`, it is necessary that the `set_boundary_indicators` function is also declared `const`.

Note: For reasons that have to do with the way the `parallel::distributed::Triangulation` is implemented, functions that have been attached to the post-refinement signal of the triangulation are called more than once, sometimes several times, every time the triangulation is actually refined.

7.2.3 Gravity models

The gravity model is responsible for describing the magnitude and direction of the gravity vector at each point inside the domain. To implement a new gravity model, you need to overload the aspect::GravityModel::Interface

class and use the `ASPECT_REGISTER_GRAVITY_MODEL` macro to register your new class. The implementation of the new class should be in namespace `aspect::GravityModel`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::GravityModel::Interface
{
  public:
    virtual
    Tensor<1,dim>
    gravity_vector (const Point<dim> &position) const = 0;

    virtual
    void
    update ();

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The kind of information these functions need to provide is discussed in the documentation of this interface class at aspect::GravityModel::Interface. The first needs to return a gravity vector at a given position, whereas the second is called at the beginning of each time step, for example to allow a model to update itself based on the current time or the solution of the previous time step. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.4 Initial conditions

The initial conditions model is responsible for describing the initial temperature distribution throughout the domain. It essentially has to provide a function that for each point can return the initial temperature. Note that the model (1)–(3) does not require initial values for the pressure or velocity. However, if coefficients are nonlinear, one can significantly reduce the number of initial nonlinear iterations if a good guess for them is available; consequently, ASPECT initializes the pressure with the adiabatically computed hydrostatic pressure, and a zero velocity. Neither of these two has to be provided by the objects considered in this section.

To implement a new initial conditions model, you need to overload the aspect::InitialConditions::Interface class and use the `ASPECT_REGISTER_INITIAL_CONDITIONS` macro to register your new class. The implementation of the new class should be in namespace `aspect::InitialConditions`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::InitialConditions::Interface
{
  public:
    void
    initialize (const GeometryModel::Interface<dim>        &geometry_model,
                const BoundaryTemperature::Interface<dim> &boundary_temperature,
                const AdiabaticConditions<dim>             &adiabatic_conditions);

    virtual
    double
    initial_temperature (const Point<dim> &position) const = 0;

    static
    void
```

```
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The meaning of the first class should be clear. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.5 Prescribed velocity boundary conditions

Most of the time, one chooses relatively simple boundary values for the velocity: either a zero boundary velocity, a tangential flow model in which the tangential velocity is unspecified but the normal velocity is zero at the boundary, or one in which all components of the velocity are unspecified (i.e., for example, an outflow or inflow condition where the total stress in the fluid is assumed to be zero). However, sometimes we want to choose a velocity model in which the velocity on the boundary equals some prescribed value. A typical example is one in which plate velocities are known, for example their current values or historical reconstructions. In that case, one needs a model in which one needs to be able to evaluate the velocity at individual points at the boundary. This can be implemented via plugins.

To implement a new boundary velocity model, you need to overload the aspect::VelocityBoundaryConditions::Interface class and use the `ASPECT_REGISTER_VELOCITY_BOUNDARY_CONDITIONS` macro to register your new class. The implementation of the new class should be in namespace `aspect::VelocityBoundaryConditions`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::VelocityBoundaryConditions::Interface
{
  public:
    virtual
    Tensor<1,dim>
    boundary_velocity (const Point<dim> &position) const = 0;

    virtual
    void
    initialize (const GeometryModel::Interface<dim> &geometry_model);

    virtual
    void
    set_current_time (const double time);

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The first of these functions needs to provide the velocity at the given point. The next two are other member functions that can (but need not) be overloaded if a model wants to do initialization steps at the beginning of the program or at the beginning of each time step. Examples are models that need to call an external program to obtain plate velocities for the current time, or from historical records, in which case it is far cheaper to do so only once at the beginning of the time step than for every boundary point separately.

The remaining functions are obvious, and are also discussed in the documentation of this interface class at aspect::VelocityBoundaryConditions::Interface. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.6 Temperature boundary conditions

The boundary conditions are responsible for describing the temperature values at those parts of the boundary at which the temperature is fixed (see Section 7.2.2 for how it is determined which parts of the boundary this applies to).

To implement a new boundary conditions model, you need to overload the aspect::BoundaryTemperature::Interface class and use the `ASPECT_REGISTER_BOUNDARY_TEMPERATURE_MODEL` macro to register your new class. The implementation of the new class should be in namespace `aspect::BoundaryTemperature`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::BoundaryTemperature::Interface
{
  public:
    virtual
    double
    temperature (const GeometryModel::Interface<dim> &geometry_model,
                 const unsigned int                   boundary_indicator,
                 const Point<dim>                    &location) const = 0;

    virtual
    double minimal_temperature () const = 0;

    virtual
    double maximal_temperature () const = 0;

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The first of these functions needs to provide the fixed temperature at the given point. The geometry model and the boundary indicator of the particular piece of boundary on which the point is located is also given as a hint in determining where this point may be located; this may, for example, be used to determine if a point is on the inner or outer boundary of a spherical shell. The remaining functions are obvious, and are also discussed in the documentation of this interface class at aspect::BoundaryTemperature::Interface. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.7 Postprocessors: Evaluating the solution after each time step

Postprocessors are arguably the most complex and powerful of the plugins available in ASPECT since they do not only passively provide any information but can actually compute quantities derived from the solution. They are executed once at the end of each time step and, unlike all the other plugins discussed above, there can be an arbitrary number of active postprocessors in the same program (for the plugins discussed in previous sections it was clear that there is always exactly one material model, geometry model, etc.).

Motivation. The original motivation for postprocessors is that the goal of a simulation is of course not the simulation itself, but that we want to do something with the solution. Examples for already existing postprocessors are:

- Generating output in file formats that are understood by visualization programs. This is facilitated by the aspect::Postprocess::Visualization class and a separate class of visualization postprocessors, see Section 7.2.8.

- Computing statistics about the velocity field (e.g., computing minimal, maximal, and average velocities), temperature field (minimal, maximal, and average temperatures), or about the heat fluxes across boundaries of the domain. This is provided by the aspect::Postprocess::VelocityStatistics, aspect::Postprocess::TemperatureStatistics, aspect::Postprocess::HeatFluxStatistics classes, respectively.

Since writing this text, there may have been other additions as well.

However, postprocessors can be more powerful than this. For example, while the ones listed above are by and large stateless, i.e., they do not carry information from one invocation at one timestep to the next invocation,[21] there is nothing that prohibits postprocessors from doing so. For example, the following ideas would fit nicely into the postprocessor framework:

- *Passive tracers:* If one would like to follow the trajectory of material as it is advected along with the flow field, one technique is to use tracer particles. To implement this, one would start with an initial population of particles distributed in a certain way, for example close to the core-mantle boundary. At the end of each time step, one would then need to move them forward with the flow field by one time increment. As long as these particles do not affect the flow field (i.e., they do not carry any information that feeds into material properties; in other words, they are *passive*), their location could well be stored in a postprocessor object and then be output in periodic intervals for visualization. In fact, such a passive tracer postprocessor is already available.

- *Surface or crustal processes:* Another possibility would be to keep track of surface or crustal processes induced by mantle flow. An example would be to keep track of the thermal history of a piece of crust by updating it every time step with the heat flux from the mantle below. One could also imagine integrating changes in the surface topography by considering the surface divergence of the surface velocity computed in the previous time step: if the surface divergence is positive, the topography is lowered, eventually forming a trench; if the divergence is negative, a mountain belt eventually forms.

In all of these cases, the essential limitation is that postprocessors are *passive*, i.e., that they do not affect the simulation but only observe it.

The statistics file. Postprocessors fall into two categories: ones that produce lots of output every time they run (e.g., the visualization postprocessor), and ones that only produce one, two, or in any case a small and fixed number of often numerical results (e.g., the postprocessors computing velocity, temperature, or heat flux statistics). While the former are on their own in implementing how they want to store their data to disk, there is a mechanism in place that allows the latter class of postprocessors to store their data into a central file that is updated at the end of each time step, after all postprocessors are run.

To this end, the function that executes each of the postprocessors is given a reference to a `dealii::TableHandler` object that allows to store data in named columns, with one row for each time step. This table is then stored in the `statistics` file in the directory designated for output in the input parameter file. It allows for easy visualization of trends over all time steps. To see how to put data into this statistics object, take a look at the existing postprocessor objects.

Note that the data deposited into the statistics object need not be numeric in type, though it often is. An example of text-based entries in this table is the visualization class that stores the name of the graphical output file written in a particular time step.

Implementing a postprocessor. Ultimately, implementing a new postprocessor is no different than any of the other plugins. Specifically, you'll have to write a class that overloads the aspect::Postprocess::Interface base class and use the `ASPECT_REGISTER_POSTPROCESSOR` macro to register your new class. The implementation of the new class should be in namespace `aspect::Postprocess`.

In reality, however, implementing new postprocessors is often more difficult. Primarily, this difficulty results from two facts:

[21] This is not entirely true. The visualization plugin keeps track of how many output files it has already generated, so that they can be numbered consecutively.

- Postprocessors are not self-contained (only providing information) but in fact need to access the solution of the model at each time step. That is, of course, the purpose of postprocessors, but it requires that the writer of a plugin has a certain amount of knowledge of how the solution is computed by the main `Simulator` class, and how it is represented in data structures. To alleviate this somewhat, and to insulate the two worlds from each other, postprocessors do not directly access the data structures of the simulator class. Rather, in addition to deriving from the aspect::Postprocess::Interface base class, postprocessors also derive from the SimulatorAccess class that has a number of member functions postprocessors can call to obtain read-only access to some of the information stored in the main class of ASPECT. See the documentation of this class to see what kind of information is available to postprocessors. See also Section 7.1 for more information about the `SimulatorAccess` class.

- Writing a new postprocessor typically requires a fair amount of knowledge how to leverage the DEAL.II library to extract information from the solution. The existing postprocessors are certainly good examples to start from in trying to understand how to do this.

Given these comments, the interface a postprocessor class has to implement is rather basic:

```
template <int dim>
class aspect::Postprocess::Interface
{
  public:
    virtual
    std::pair<std::string,std::string>
    execute (TableHandler &statistics) = 0;

    virtual
    void
    save (std::map<std::string, std::string> &status_strings) const;

    virtual
    void
    load (const std::map<std::string, std::string> &status_strings);

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The purpose of these functions is described in detail in the documentation of the aspect::Postprocess::Interface class. While the first one is responsible for evaluating the solution at the end of a time step, the `save/load` functions are used in checkpointing the program and restarting it at a previously saved point during the simulation. The first of these functions therefore needs to store the status of the object as a string under a unique key in the database described by the argument, while the latter function restores the same state as before by looking up the status string under the same key. The default implementation of these functions is to do nothing; postprocessors that do have non-static member variables that contain a state need to overload these functions.

There are numerous postprocessors already implemented. If you want to implement a new one, it would be helpful to look at the existing ones to see how they implement their functionality.

7.2.8 Visualization postprocessors

As mentioned in the previous section, one of the postprocessors that are already implemented in ASPECT is the aspect::Postprocess::Visualization class that takes the solution and outputs it as a collection of files that can then be visualized graphically, see Section 4.4. The question is which variables to output: the

solution of the basic equations we solve here is characterized by the velocity, pressure and temperature; on the other hand, we are frequently interested in derived, spatially and temporally variable quantities such as the viscosity for the actual pressure, temperature and strain rate at a given location, or seismic wave speeds.

ASPECT already implements a good number of such derived quantities that one may want to visualize. On the other hand, always outputting *all* of them would yield very large output files, and would furthermore not scale very well as the list continues to grow. Consequently, as with the postprocessors described in the previous section, what *can* be computed is implemented in a number of plugins and what *is* computed is selected in the input parameter file (see Section 5.43).

Defining visualization postprocessors works in much the same way as for the other plugins discussed in this section. Specifically, an implementation of such a plugin needs to be a class that derives from interface classes, should by convention be in namespace `aspect::Postprocess::VisualizationPostprocessors`, and is registered using a macro, here called `ASPECT_REGISTER_VISUALIZATION_POSTPROCESSOR`. Like the postprocessor plugins, visualization postprocessors can derive from class aspect::Postprocess::SimulatorAccess if they need to know specifics of the simulation such as access to the material models and to get access to the introspection facility outlined in Section 7.1. A typical example is the plugin that produces the viscosity as a spatially variable field by evaluating the viscosity function of the material model using the pressure, temperature and location of each visualization point (implemented in the `aspect::Postprocess::VisualizationPostprocessors::Viscosity` class). On the other hand, a hypothetical plugin that simply outputs the norm of the strain rate $\sqrt{\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})}$ would not need access to anything but the solution vector (which the plugin's main function is given as an argument) and consequently is not derived from the aspect::Postprocess::SimulatorAccess class.[22]

Visualization plugins can come in two flavors:

- *Plugins that compute things from the solution in a pointwise way:* The classes in this group are derived not only from the respective interface class (and possibly the SimulatorAccess class) but also from the deal.II class `DataPostprocessor` or any of the classes like `DataPostprocessorScalar` or `DataPostprocessorVector`. These classes can be thought of as filters: DataOut will call a function in them for every cell and this function will transform the values or gradients of the solution and other information such as the location of quadrature points into the desired quantity to output. A typical case would be if the quantity $g(x)$ you want to output can be written as a function $g(x) = G(u(x), \nabla u(x), x, ...)$ in a pointwise sense where $u(x)$ is the value of the solution vector (i.e., the velocities, pressure, temperature, etc) at an evaluation point. In the context of this program an example would be to output the density of the medium as a spatially variable function since this is a quantity that for realistic media depends pointwise on the values of the solution.

  To sum this, slightly confusing multiple inheritance up, visualization postprocessors do the following:

  - If necessary, they derive from aspect::Postprocess::SimulatorAccess.
  - They derive from aspect::Postprocess::VisualizationPostprocessors::Interface. The functions of this interface class are all already implemented as doing nothing in the base class but can be overriden in a plugin. Specifically, the following functions exist:

```
class Interface
{
  public:
    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
```

[22] The actual plugin `aspect::Postprocess::VisualizationPostprocessors::StrainRate` only computes $\sqrt{\varepsilon(\mathbf{u}) : \varepsilon(\mathbf{u})}$ in the incompressible case. In the compressible case, it computes $\sqrt{[\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr}\ \varepsilon(\mathbf{u}))\mathbf{I}] : [\varepsilon(\mathbf{u}) - \frac{1}{3}(\text{tr}\ \varepsilon(\mathbf{u}))\mathbf{I}]}$ instead. To test whether the model is compressible or not, the plugin needs access to the material model object, which the class gains by deriving from aspect::Postprocess::SimulatorAccess and then calling `this->get_material_model().is_compressible()`.

```
    virtual
    void save (std::map<std::string, std::string> &status_strings) const;

    virtual
    void load (const std::map<std::string, std::string> &status_strings);
};
```

– They derive from either the `dealii::DataPostprocessor` class, or the simpler to use `dealii::DataPostprocessor` or `dealii::DataPostprocessorVector` classes. For example, to derive from the second of these classes, the following interface functions has to be implemented:

```
class dealii::DataPostprocessorScalar
{
  public:
    virtual
    void
    compute_derived_quantities_vector
      (const std::vector<Vector<double> >               &uh,
       const std::vector<std::vector<Tensor<1,dim> > > &duh,
       const std::vector<std::vector<Tensor<2,dim> > > &dduh,
       const std::vector<Point<dim> >                  &normals,
       const std::vector<Point<dim> >                  &evaluation_points,
       std::vector<Vector<double> >                    &computed_quantities) const;
};
```

What this function does is described in detail in the deal.II documentation. In addition, one has to write a suitable constructor to call `dealii::DataPostprocessorScalar::DataPostprocessorScalar`.

- *Plugins that compute things from the solution in a cellwise way:* The second possibility is for a class to not derive from `dealii::DataPostprocessor` but instead from the aspect::Postprocess::VisualizationPostprocessors::Ce class. In this case, a visualization postprocessor would generate and return a vector that consists of one element per cell. The intent of this option is to output quantities that are not pointwise functions of the solution but instead can only be computed as integrals or other functionals on a per-cell basis. A typical case would be error estimators that do depend on the solution but not in a pointwise sense; rather, they yield one value per cell of the mesh. See the documentation of the `CellDataVectorCreator` class for more information.

If all of this sounds confusing, we recommend consulting the implementation of the various visualization plugins that already exist in the ASPECT sources, and using them as a template.

7.2.9 Mesh refinement criteria

Despite research since the mid-1980s, it isn't completely clear how to refine meshes for complex situations like the ones modeled by ASPECT. The basic problem is that mesh refinement criteria either can refine based on some variable such as the temperature, the pressure, the velocity, or a compositional field, but that oftentimes this by itself is not quite what one wants. For example, we know that Earth has discontinuities, e.g., at 440km and 610km depth. In these places, densities and other material properties suddenly change. Their resolution in computation models is important as we know that they affect convection patterns. At the same time, there is only a small effect on the primary variables in a computation – maybe a jump in the second or third derivative, for example, but not a discontinuity that would be clear to see. As a consequence, automatic refinement criteria do not always refine these interfaces as well as necessary.

To alleviate this, ASPECT has plugins for mesh refinement. Through the parameters in Section 5.38, one can select when to refine but also which refinement criteria should be used and how they should be combined if multiple refinement criteria are selected. Furthermore, through the usual plugin mechanism, one can extend the list of available mesh refinement criteria (see the parameter "Strategy" in Section 5.38). Each such plugin is responsible for producing a vector of values (one per active cell on the current processor,

though only those values for cells that the current processor owns are used) with an indicator of how badly this cell needs to be refined: large values mean that the cell should be refined, small values that the cell may be coarsened away.

To implement a new mesh refinement criterion, you need to overload the aspect::MeshRefinement::Interface class and use the `ASPECT_REGISTER_MESH_REFINEMENT_CRITERION` macro to register your new class. The implementation of the new class should be in namespace `aspect::MeshRefinement`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::MeshRefinement::Interface
{
  public:
    virtual
    void
    execute (Vector<float> &error_indicators) const = 0;

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
    void
    parse_parameters (ParameterHandler &prm);
};
```

The first of these functions computes the set of refinement criteria (one per cell) and returns it in the given argument. Typical examples can be found in the existing implementations in the `source/mesh_refinement` directory. As usual, your termination criterion implementation will likely need to be derived from the `SimulatorAccess` to get access to the current state of the simulation.

The remaining functions are obvious, and are also discussed in the documentation of this interface class at aspect::MeshRefinement::Interface. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.2.10 Criteria for terminating a simulation

ASPECT allows for different ways of terminating a simulation. For example, the simulation may have reached a final time specified in the input file. However, it also allows for ways to terminate a simulation when it has reached a steady state (or, rather, some criterion determines that it is close enough to steady state), or by an external action such as placing a specially named file in the output directory. With the exception of the end time, the criteria determining termination of a simulation are all implemented in plugins. The parameters describing these criteria are listed in Section 5.44.

To implement a termination criterion, you need to overload the aspect::TerminationCriteria::Interface class and use the `ASPECT_REGISTER_TERMINATION_CRITERION` macro to register your new class. The implementation of the new class should be in namespace `aspect::TerminationCriteria`.

Specifically, your new class needs to implement the following basic interface:

```
template <int dim>
class aspect::TerminationCriteria::Interface
{
  public:
    virtual
    bool
    execute () const = 0;

    static
    void
    declare_parameters (ParameterHandler &prm);

    virtual
```

```
        void
        parse_parameters (ParameterHandler &prm);
    };
```

The first of these functions returns a value that indicates whether the simulation should be terminated. Typical examples can be found in the existing implementations in the `source/termination_criteria` directory. As usual, your termination criterion implementation will likely need to be derived from the `SimulatorAccess` to get access to the current state of the simulation.

The remaining functions are obvious, and are also discussed in the documentation of this interface class at aspect::TerminationCriteria::Interface. The purpose of the last two functions has been discussed in the general overview of plugins above.

7.3 Extending the basic solver

The core functionality of the code, i.e., that part of the code that implements the time stepping, assembles matrices, solves linear and nonlinear systems, etc., is in the `aspect::Simulator` class (see the doxygen documentation of this class). Since the implementation of this class has more than 3,000 lines of code, it is split into several files that are all located in the `source/simulator` directory. Specifically, functionality is split into the following files:

- `source/simulator/core.cc`: This file contains the functions that drive the overall algorithm (in particular `Simulator::run`) through the main time stepping loop and the functions immediately called by `Simulator::run`.
- `source/simulator/assembly.cc`: This is where all the functions are located that are related to assembling linear systems.
- `source/simulator/solver.cc`: This file provides everything that has to do with solving and preconditioning the linear systems.
- `source/simulator/initial_conditions.cc`: The functions in this file deal with setting initial conditions for all variables.
- `source/simulator/checkpoint_restart.cc`: The location of functionality related to saving the current state of the program to a set of files and restoring it from these files again.
- `source/simulator/helper_functions.cc`: This file contains a set of functions that do the odd thing in support of the rest of the simulator class.
- `source/simulator/parameters.cc`: This is where we define and read run-time parameters that pertain to the top-level functionality of the program.

Obviously, if you want to extend this core functionality, it is useful to first understand the numerical methods this class implements. To this end, take a look at the paper that describes these methods, see [KHB12]. Further, there are two predecessor programs whose extensive documentation is at a much higher level than the one typically found inside ASPECT itself, since they are meant to teach the basic components of convection simulators as part of the DEAL.II tutorial:

- The step-31 program at `http://www.dealii.org/developer/doxygen/deal.II/step_31.html`: This program is the first version of a convection solver. It does not run in parallel, but it introduces many of the concepts relating to the time discretization, the linear solvers, etc.
- The step-32 program at `http://www.dealii.org/developer/doxygen/deal.II/step_32.html`: This is a parallel version of the step-31 program that already solves on a spherical shell geometry. The focus of the documentation in this program is on the techniques necessary to make the program run in parallel, as well as some of the consequences of making things run with realistic geometries, material models, etc.

Neither of these two programs is nearly as modular as ASPECT, but that was also not the goal in creating them. They will, however, serve as good introductions to the general approach for solving thermal convection problems.

Note: Neither this manual, nor the documentation in ASPECT makes much of an attempt at teaching how to use the DEAL.II library upon which ASPECT is built. Nevertheless, you will likely have to know at least the basics of DEAL.II to successfully work on the ASPECT code. We refer to the resources listed at the beginning of this section as well as references [BHK07, BHK12].

8 Future plans for Aspect

We have a number of near-term plans for ASPECT that we hope to implement soon:

- *Iterating out the nonlinearity:* In the current version of ASPECT, we use the velocity, pressure and temperature of the previous time step to evaluate the coefficients that appear in the flow equations (1)–(2); and the velocity and pressure of the current time step as well as the previous time step's temperature to evaluate the coefficients in the temperature equation (3). This is an appropriate strategy if the model is not too nonlinear; however, it introduces inaccuracies and limits the size of the time step if coefficients strongly depend on the solution variables.

  To avoid this, one can iterate out the equations using either a fixed point or Newton scheme. Both approaches ensure that at the end of a time step, the values of coefficients and solution variables are consistent. On the other hand, one may have to solve the linear systems that describe a time step more than once, increasing the computational effort.

  We have started implementing such methods using a testbase code, based on earlier experiments by Jennifer Worthen [Wor12]. We hope to implement this feature in ASPECT early in 2012.

- *Faster 3d computations:* Whichever way you look at it, 3d computations are expensive. In parallel computations, the Stokes solve currently takes upward of 90% of the overall wallclock time, suggesting an obvious target for improvements based on better algorithms as well as from profiling the code to find hot spots. In particular, playing with better solver and/or preconditioner options would seem to be a useful goal.

- *Particle-based methods:* It is often useful to employ particle tracers to visualize where material is being transported. While conceptually simple, their implementation is made difficult in parallel computations if particles cross the boundary between parts of the regions owned by individual processors, as well as during re-partitioning the mesh between processors following mesh refinement. Eric Heien is working on an implementation of such passive tracers.

- *More realistic material models:* The number of material models available in ASPECT is currently relatively small. Obviously, how realistic a simulation is depends on how realistic a material model is. We hope to obtain descriptions of more realistic material descriptions over time, either given analytically or based on table-lookup of material properties.

- *Incorporating latent heat effects:* Real materials undergo phase transitions at certain pressures and temperatures, and these phase transitions release or take up energy (i.e., heat). The terms that need to be added to the temperature equation (3) are not very difficult but one needs a description of the latent heat based on the Clapeyron slope as a function of temperature and pressure [CY85, STO01], which we currently don't have. If someone contributes such a description we'll be happy to add the relevant terms into the model.

- *Melting:* An important part of mantle behavior is melting. Melting not only affects the properties of the material such as density or viscosity, but it also leads to chemical segregation and, in fact, to

the flow of two different fluids (the melt and the rock matrix) relative to each other. Modeling this additional process would yield significant insight.

- *Converting output into seismic velocities:* The predictions of mantle convection codes are often difficult to verify experimentally. On the other hand, simulations can be used to predict a seismic signature of the earth mantle – for example the location of transition zones that can be observed using seismic imaging. To facilitate such comparisons, it is of interest to output not only the primary solution variables but also convert them into the primary quantity visible in seismic imaging: compressive and shear wave velocities. Implementing this should be relatively straightforward if given a formula or table that expresses velocities in terms of the variables computed by ASPECT.

To end this section, let us repeat something already stated in the introduction:

Note: ASPECT is a community project. As such, we encourage contributions from the community to improve this code over time. Obvious candidates for such contributions are implementations of new plugins as discussed in Section 7.2 since they are typically self-contained and do not require much knowledge of the details of the remaining code. Obviously, however, we also encourage contributions to the core functionality in any form!

9 Finding answers to more questions

If you have questions that go beyond this manual, there are a number of resouces:

- For questions on the source code of Aspect, portability, installation, etc., use the ASPECTdevelopment mailing list at aspect-devel@geodynamics.org. Information about this mailing list is provided at http://geodynamics.org/cgi-bin/mailman/listinfo/aspect-devel. This mailing list is where the Aspect developers all hang out.
- Aspect is primarily based on the deal.II library (the dependency on Trilinos and p4est is primarily through deal.II, and not directly visible in the Aspect source code). If you have particular questions about deal.II, contact the mailing lists described at http://www.dealii.org/mail.html.
- In case of more general questions about mantle convection, you can contact the CIG mantle convection mailing lists at cig-mc@geodynamics.org. Information about this mailing list is provided at http://geodynamics.org/cgi-bin/mailman/listinfo/cig-MC.
- If you have specific questions about Aspect that are not suitable for public and archived mailing lists, you can contact the primary developers:
  - Wolfgang Bangerth: bangerth@math.tamu.edu.
  - Timo Heister: heister@math.tamu.edu.

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Index of run-time parameter entries

The following is a listing of all run-time parameters that can be set in the input parameter file. They are all described in Section 5 and the listed page numbers are where their detailed documentation can be found. A listing of all parameters sorted by the section name in which they are declared is given in the index on page 120 below.

Index of run-time parameters with section names

The following is a listing of all run-time parameters, sorted by the section in which they appear. To find entries sorted by their name, rather than their section, see the index on page 118 above.