COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)
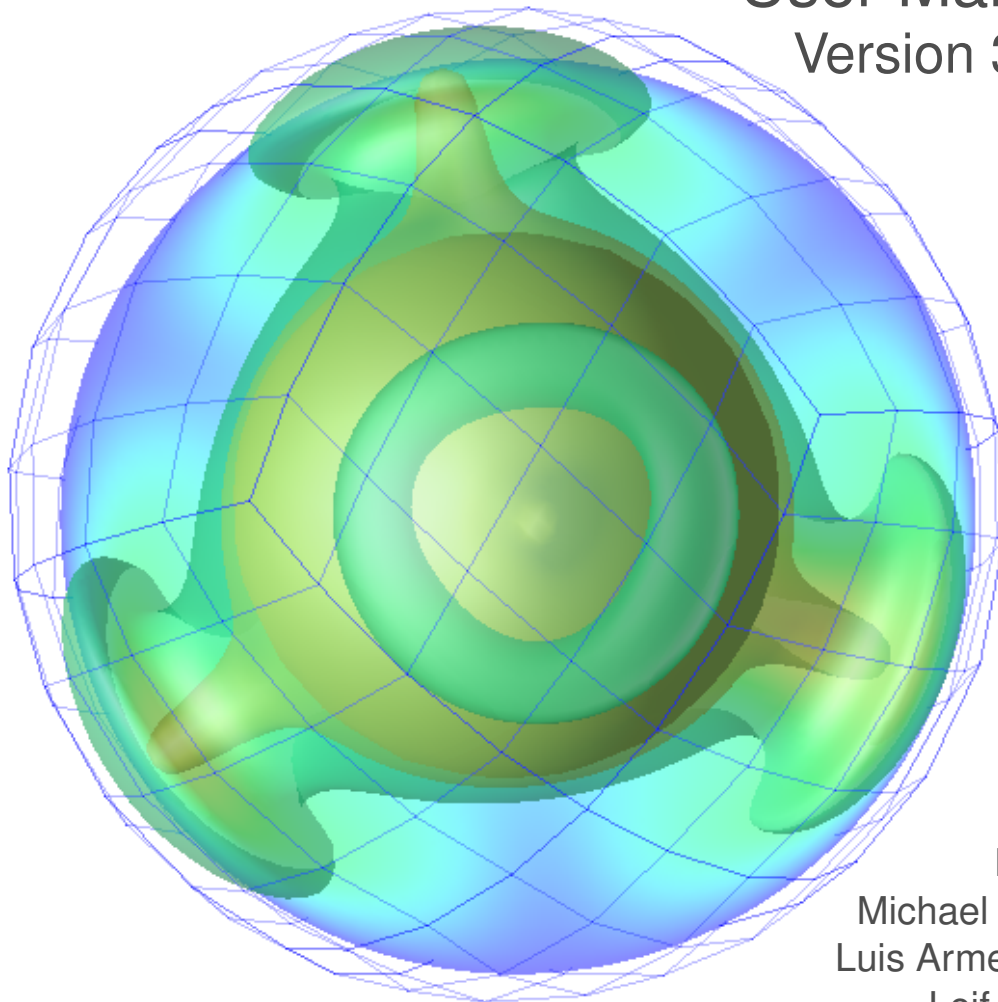
CitcomS

User Manual
Version 3.2.0

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CitcomS User Manual

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Preface

Preface

About This Document

This document is organized into three parts. Part I consists of traditional book front matter, including this preface. Part II begins with an introduction to Pyre and the Pyre-compatible version of CitcomS and their capabilities and proceeds to the details of implementation, including several "cookbooks" of short tutorials. Part III provides appendices and references.

The style of this publication is based on the Apple Publications Style Guide (`developer.apple.com/documentation/UserExperience/Conceptual/APStyleGuide/AppleStyleGuide2003.pdf`), as recommended by Python.org (`www.python.org`). The documentation was produced using LATEX, specifically the `pdflatex` tool from the TeXLive distribution (`www.tug.org/texlive`).

Errors and bug fixes in this manual should be directed to the CIG Mantle Convection Mailing List (`cig-mc@geodynamics.org`).

Who Will Use This Document

This documentation is aimed at two categories of users: scientists who prefer to use prepackaged and specialized analysis tools, and experienced computational Earth scientists. Of the latter, there are likely to be two classes of users: those who just run models, and those who modify the source code. Users who modify the source are likely to have familiarity with scripting, software installation, and programming, but are not necessarily professional programmers.

The manual was written for the usage of CitcomS on a variety of different platforms. CitcomS has run on shared memory computers (Sun, Hewlett-Packard, SGI, and IBM), commercial distributed memory machines (Intel and Cray/SGI), clusters (including machines on the NSF TeraGrid), Linux PCs and Mac OS X desktops.

Citation

Computational Infrastructure for Geodynamics (CIG) is making this source code available to you in the hope that the software will enhance your research in geophysics. The underlying C code for the finite element package and the Python bindings for the framework were donated to CIG in July of 2005. A number of individuals have contributed a significant portion of their careers toward the development of CitcomS and Pyre. It is essential that you recognize these individuals in the normal scientific practice by citing the appropriate peer reviewed papers and making appropriate acknowledgements.

The CitcomS development team asks that you cite both of the following:

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

- Tan, E., E. Choi, P. Thoutireddy, M. Gurnis, and M. Aivazis (2006), GeoFramework: Coupling multiple models of mantle convection within a computational framework, *Geochem., Geophys., Geosyst. 7,* Q06001, doi:10.1029/2005GC001155.

Additionally, if you are using tracers in CitcomS, please cite the following:

- McNamara, A.K., and S. Zhong (2004), Thermochemical structures within a spherical mantle: Superplumes or Piles?, *J. Geophys. Res.*, 109, B07402, doi:10.1029/2003JB002847.

The developers also request that in your oral presentations and in your paper acknowledgements that you indicate your use of this code, the authors of the code, and CIG (`geodynamics.org`).

Support

Pyre development is funded by the U.S. Dept. of Energy's Advanced Simulation and Computing program (`www.sandia.gov/NNSA/ASC`) and the National Science Foundation's (`www.nsf.gov`) Information Technology Research (ITR) program (grant #0205653). Continued support of CitcomS is based upon work supported by the National Science Foundation under Grant No. EAR-0406751. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

Conventions

Throughout this documentation, any mention of "username" is meant to indicate the user, meaning you should substitute your account name in its place.

Part II

Chapters

Chapter 1

Introduction

CitcomS is a finite element code designed to solve thermal convection problems relevant to earth's mantle released under the GNU General Public License (see Appendix D on page 125). Written in C, the code runs on a variety of parallel processing computers, including shared and distributed memory platforms. In an effort to increase the functionality of CitcomS to include greater control during simulations on large parallel systems, the software has been reengineered from previous versions of CitcomS to work with a Python-based modeling framework called Pyre. With Pyre, CitcomS can be dynamically coupled with other CitcomS simulations or with other codes such as SNAC, which solves crustal and lithospheric problems.

1.1 About CitcomS

CitcomS is a finite element code written in C that solves for thermo-chemical convection within a spherical shell. It can solve for problems within either a full or a restricted spherical domain. Although the code is capable of solving many different kinds of convection problems using the flexibility of finite elements, there are aspects of CitcomS which make it well-suited for solving problems in which the plate tectonic history is incorporated. Variable viscosity, including temperature-, pressure-, position-, composition-, and stress-dependent viscosity are all possible.

The fundamental basis for the numerical solution of any time-dependent convection problem is the sequential solution of an equation of motion and an energy equation. Convection problems are initially valued with boundary conditions, including all of the problems which are solved with CitcomS. The normal sequence of steps for the solution of convection problems starts with an initial temperature field. First, the momentum equation is solved. The solution of this equation gives us the velocity from which we then solve the advection-diffusion equation, giving us a new temperature. CitcomS uses this interleaved strategy. It is possible to run convection backward in time so as to guess an initial condition for a normal forward running initial and boundary value problem. However, users should be aware that even specialists in mantle convection modeling are just now starting to explore methods in this area and, as such, this is an emerging area of research.

This code uses an iterative solution scheme to solve for the velocity and pressure and, as such, a converged solution cannot be guaranteed. Nested inside the iterative scheme, the code uses either a conjugate gradient solver or a full multi-grid solver to solve the discretized matrix equations.

1.2 History

Citcom (for **C**alifornia **I**nstitute of **T**echnology **Co**nvection in the **M**antle) was originally written in the early 1990s by Louis Moresi. Although the code for three-dimensional problems was incorporated from its inception, early versions of the software only solved for time-dependent convection problems within two-dimensional Cartesian domains. Moresi's original code turned out to be incredibly modular and easily extensible. Consequently, the fundamental finite element infrastructure which Louis wrote is still in place and forms the basis for much of the code contained in the present release.

In the mid-1990s Moresi wrote versions of the code that solved the equations within three-dimensional Cartesian domains. Then Shijie Zhong successfully parallelized Citcom using message passing routines on a limited release Intel

supercomputer. Zhong then created a spherical version of the code which he named CitcomS. Lijie Han then created a regional version of CitcomS as well as an alternate version of message passing for an arbitrarily large number of processors. Clint Conrad created the first Beowulf implementations of the code using the MPI library, then Conrad and Eh Tan re-coded the message passing of the fully spherical version so that problems run on arbitrarily large numbers of processors could also be solved. A plethora of different versions of Citcom exist both on computers at the California Institute of Technology and around the world.

Consequently, by 2002, there were so many different versions of the code that some rationalization was in order. The software was migrated into a version control system and Eh Tan and Eun-seo Choi created a version of CitcomS that generates either a fully spherical or regional model. CitcomS was released to the community through the former GeoFramework project as version 1.0 and 1.1.

By 2004, in order to increase the functionality of CitcomS, the developers began to reengineer the code into an object-oriented environment specifically so it could work with a Python-based modeling framework called Pyre. This release of the software is essentially the product of those reengineering efforts. Eh Tan was the principal developer of CitcomS, with considerable help from Eun-seo Choi, Puru Thoutireddy, and Michael Aivazis.

CitcomS is one component of a larger collection of software encompassed by the former GeoFramework project, a collaboration between the Center for Advanced Computing Research (CACR) (`www.cacr.caltech.edu`) and the Seismological Laboratory (`www.gps.caltech.edu/seismo`), both at Caltech, and the Victorian Partnership for Advanced Computing (`www.vpac.org`) in Australia. The GeoFramework project developed a suite of tools to model multi-scale deformation for Earth science problems. This effort was motivated by the need to understand interactions between the long-term evolution of plate tectonics and shorter term processes such as the evolution of faults during and between earthquakes. During 2005 and 2006 much of the remaining software developed by GeoFramework was released under a GPL license and made available from CIG (`geodynamics.org`).

The second major release of CitcomS (2.0) incorporated the software framework Pyre, free surface modeling methods, and stress boundary conditions on the top and bottom surfaces. In the summer of 2005, as part of the 2.0.1 release, CIG replaced the old build procedure with the GNU Build System. A subsequent release, version 2.0.2, could compile and run on 64-bit systems.

The release of CitcomS 2.1 incorporated new features and functionality, the most important being the use of HDF5 (a parallel version of the Hierarchical Data Format). The HDF5 format allows you to deal with the massive data output created for production runs (see Chapter 4 on page 45). This version accepted `.cfg` files on input, which are easier to create and read. Other improvements included the incorporation of geoid calculations that had been left out of earlier releases, as well as new scripts to allow results to be visualized with MayaVi2 (`svn.enthought.com/enthought/wiki/MayaVi`) in addition to Generic Mapping Tools (GMT) (`gmt.soest.hawaii.edu`) and OpenDX (`www.opendx.org`). Instructions were provided on using this version as a preinstalled package on some of the NSF TeraGrid sites.

The release of CitcomS 2.2 incorporated the ability of tracing particles in the flow. The tracer code was developed by Allen McNamara and Shijie Zhong in 2004 and donated to CIG in early 2007. The tracer code has a wide range of applications in the mantle convection. It can be used in tracing the trajectory of passive particles, in delineating the top boundary of subducted slabs to define the low viscosity wedges, or in tracking the evolution of the chemical composition field.

The release of CitcomS 3.0 contains many new features, including two implementations of compressible convection, one by Wei Leng and Shijie Zhong and the other by Eh Tan; the ability to resume computation from previous checkpoints; multi-component chemical convection; a fixed non-Newtonian solver; an exchanger package for solver coupling; removing the rigid body rotation component from the velocity by Shijie Zhong; and an option to disable monitoring of maximum temperature. In addition, a rheology option for pseudo-plasiticity, composition dependent viscosity and heat generation, compressed ASCII output, and an easier way for mesh refinement for the radial coordinate were added by Thorsten Becker.

Additional changes that are not backward compatible include (1) the viscosity field at element level is not smoothed (this might slow down the convergence but will represent the viscosity field more accurately); (2) the Lenardic filter on temperature is disabled by default; (3) the rigid body rotation component is removed from the velocity by default; (4) use of a better pseudo-random number generator to generate the initial tracer; (5) the type of input parameter `coor` is changed from a boolean to an integer; (6) setting `restart=on` will resume the computation from the checkpoint files and will not need the tracer files (the old way of reading initial temperature from velo files can be achieved by `tic_method=-1`); and (7) the input parameter `reset_initial_composition` becomes obsolete. Among the seven backward-incompatible changes, the first four will affect the results.

The release of CitcomS 3.1 added the ability to convert temperature and composition to seismic velocities. The seismic velocities output can be uploaded to the CIG Seismology Web Portal for SPECFEM3D simulation to generate synthetic seismograms. Other enhancements include adding a self-gravitational effect on geoid and adding the Consistent-Boundary-Flux (CBF) method to compute dynamic topography, contributed by Shijie Zhong. Also, GMT/NetCDF grd input was added for surface velocity boundary conditions, initial temperature, material dependence and local Rayleigh number in surface layers, contributed by Thorsten Becker. Mike Gurnis contributed added capability to read in time- and geographic-dependent, top surface temperature boundary conditions. Finally, this version allows multi-component chemical viscosity.

Some of the aforementioned features are backward-incompatible, including:

1. The global mesh is changed. The coordinates of all nodes are slightly shifted laterally. The change is not visually discernible, but does affect the solution compared to previous versions.

2. The convergence criterion of the Stokes solver is changed. A single parameter "accuracy" is used to control the accuracy of the continuity and momentum equations. The default value of "accuracy" was 10^{-6} and is now 10^{-4}.

3. The input parameter "mantle_temp" is moved from the [CitcomS.solver.param] to the [CitcomS.solver.ic] section.

This release of CitcomS 3.2 adds numerous changes since 3.1.1 which was released in 2009. These include improved implementations of internal stress, radial layer dependent viscosity, and velocity boundary conditions. Improvements have also been made in solver convergence controls, VTK output and several bug fixes. Finally, the Pyre configuration option has been turned off by default, though it can be enabled during configuration. Other enhancements include:

• If Python 2.7 is detected, Pyre is disabled due to conflicts.

• Trial implementation of anisotropic viscosity.

• Added support of multigrid solver in Exchanger.

• Improved handling of grd-read velocity and traction boundary conditions.

• Changed default parameters for z_410, z_lmantle, z_lith to more Earth-like parameters.

• Added test implementation of steady state strain-rate weakening via PDEPV psrw=on parameter.

• Added Murnaghan's integrated linear EoS.

• Added augmented Lagrangian component of stiffness matrix in cbf topo.

• Performance optimizations for CUDA code. Contributed by Leif Strand.

• Fixed several bugs in the code and manual, including:

  – Fixed a bug in pseudo free surface, reported by Robert Moucha.
  – Correctly handle orphan tracers.
  – Added Pyre binding for write_q_files, z_layer, r_grid_layers, rr, nr, others.
  – Replaced fixed accuracy setting. Bug reported by Rob Moucha.
  – Fixed temperature perturbation bug for multiple processors.

1.3 About Pyre

Pyre is an object-oriented environment capable of specifying and launching numerical simulations on multiple platforms, including Beowulf class parallel computers and grid computing systems. Pyre allows the binding of multiple components such as solid and fluid models used in Earth science simulations, and different meshers. The Pyre framework enables the elegant setup, modification and launching of massively parallel three-dimensional solver applications.

The Pyre framework incorporates features aimed at enabling the scientific non-expert to perform tasks easily without hindering the expert. Target features for end users allow complete and intuitive simulation specification, reasonable defaults, consistency checks of input, good diagnostics, easy access to remote facilities, and status monitoring. Target features for developers include easy access to user input, a shorter development cycle, and good debugging support.

1.4   Pyre and CitcomS

Pyre provides a simulation framework that includes solver integration and coupling, uniform access to facilities, and integrated visualization. The framework offers a way to add new solvers to CitcomS and to fine-tune CitcomS simulations.

   Developers have created Pyre classes for CitcomS to facilitate simulation setup. However, they are not independent classes in a strict sense. They still share the same underlying data structure and their functionality is not divided clearly. CitcomS was not designed to be object-oriented and to make it so would require significant investment of effort with little return. However, the lack of object-oriented features does not hinder the coupling of CitcomS with other solvers.

1.5   Governing Equations

With CitcomS, the mantle is treated as an anelastic, compressible, viscous spherical shell under Truncated Anelastic Liquid Approximation. With these assumptions, thermal convection is governed by the equations for conservation of mass, momentum, and energy:

$$(\rho u_i)_{,i} = 0 \tag{1.1}$$

$$-P_{,i} + \left(\eta(u_{i,j} + u_{j,i} - \frac{2}{3}u_{k,k}\delta_{ij}) \right)_{,i} - \delta\rho g \delta_{ir} = 0 \tag{1.2}$$

$$\rho c_P \left(T_{,t} + u_i T_{,i} \right) = \rho c_P \kappa T_{,ii} - \rho \alpha g u_r T + \Phi + \rho \left(Q_{L,t} + u_i Q_{L,i} \right) + \rho H \tag{1.3}$$

where ρ is the density, u is the velocity, P is the dynamic pressure, η is the viscosity, δ_{ij} is the Kroneker delta tensor, $\delta\rho$ is the density anomaly, g is the gravitational acceleration, T is the temperature, c_P is the heat capacity, κ is the thermal diffusivity, α is the thermal expansivity, Φ is the viscous dissipation, Q_L is the latent heat due to phase transitions, and H is the heat production rate. The expression $X_{,y}$ represents the derivative of X with respect to y, where i and j are spatial indices, r is the radial direction, and t is time. With phase transitions and temperature and composition variations, the density anomalies are:

$$\delta\rho = -\alpha\bar{\rho}(T - \bar{T}_a) + \delta\rho_{ph}\Gamma + \delta\rho_{ch}C \tag{1.4}$$

where $\bar{\rho}$ is the radial profile of density, $\bar{T}_a$ is the radial profile of adiabatic temperature, $\delta\rho_{ph}$ is the density jump across a phase change, $\delta\rho_{ch}$ is the density difference between the compositions, Γ is the phase function, and C is the composition. The phase function is defined as:

$$\pi = \bar{\rho}g(1 - r - d_{ph}) - \gamma_{ph}(T - T_{ph}) \tag{1.5}$$

$$\Gamma = \frac{1}{2} \left(1 + \tanh\left(\frac{\pi}{\bar{\rho}g w_{ph}} \right) \right) \tag{1.6}$$

where π is the reduced pressure, d_{ph} and T_{ph} are the ambient depth and temperature of a phase change, γ_{ph} is the Clapeyron slope of a phase change, and w_{ph} is the width of a phase transition.

   These equations lead to the following normalization in which primed quantities are nondimensional:

$$\rho = \rho_0 \rho^{'} \tag{1.7}$$

$$\alpha = \alpha_0 \alpha^{'} \tag{1.8}$$

$$g = g_0 g^{'} \tag{1.9}$$

$$\kappa = \kappa_0 \kappa^{'} \tag{1.10}$$

$$\eta = \eta_0 \eta^{'} \tag{1.11}$$

$$c_P = c_{P0} c_P^{'} \tag{1.12}$$

$$x_i = R_0 x_i^{'} \tag{1.13}$$

$$u_i = \frac{\kappa_0}{R_0} u_i^{'} \tag{1.14}$$

$$T_0 = \Delta T T_0^{'} \tag{1.15}$$

$$T = \Delta T (T^{'} + T_0^{'}) \tag{1.16}$$

$$t = \frac{R_0^2}{\kappa_0} t^{'} \tag{1.17}$$

$$H = \frac{\kappa_0}{R_0^2} c_{P0} \Delta T H^{'} \tag{1.18}$$

$$P = \frac{\eta_0 \kappa_0}{R_0^2} P^{'} \tag{1.19}$$

$$d_{ph} = R_0 d_{ph}^{'} \tag{1.20}$$

$$\gamma_{ph} = \frac{\rho_0 g_0 R_0}{\Delta T} \gamma_{ph}^{'} \tag{1.21}$$

where ρ_0 is the reference density, α_0 is the reference thermal expansivity, g_0 is the reference gravity, κ_0 is the reference thermal diffusivity, η_0 is a reference viscosity, c_{P0} is the reference heat capacity, R_0 is the radius of the Earth, T_0 is the temperature at the surface, and ΔT is the temperature drop from the core-mantle boundary (CMB) to the surface. Dropping the primes, the equations become:

$$u_{i,i} + \frac{1}{\bar\rho}\frac{d\bar\rho}{dr}u_r = 0 \tag{1.22}$$

$$-P_{,i} + \left(\eta(u_{i,j} + u_{j,i} - \frac{2}{3}u_{k,k}\delta_{ij})\right)_{,i} + (Ra\bar\rho\alpha T - Ra_b\Gamma - Ra_cC)g\delta_{ir} = 0 \tag{1.23}$$

$$\begin{aligned}\bar\rho c_P\left(T_{,t} + u_iT_{,i}\right)\left(1 + 2\Gamma\left(1-\Gamma\right)\frac{\gamma_{ph}^2}{d_{ph}}\frac{Ra_b}{Ra}Di\left(T+T_0\right)\right) = \bar\rho c_P\kappa T_{,ii} \\ -\bar\rho\alpha g u_r Di\left(T+T_0\right)\left(1 + 2\Gamma\left(1-\Gamma\right)\frac{\gamma_{ph}}{d_{ph}}\frac{Ra_b}{Ra}\right) + \frac{Di}{Ra}\Phi + \bar\rho H\end{aligned} \tag{1.24}$$

where Ra, the thermal Rayleigh number, is defined as:

$$Ra = \frac{\rho_0 g_0\alpha_0\Delta T R_0^3}{\eta_0\kappa_0} \tag{1.25}$$

This is not the usual definition of the Raleigh number that is based on layer thickness; it is based on the radius of the Earth R_0. So for mantle convection problems where R_0 is slightly more than twice the layer thickness, our Ra is about a factor of 10 larger than by the usual definition. The phase-change Rayleigh number, Ra_b, the chemical Rayleigh number, Ra_c, the internal heating Rayleigh number, Ra_H, and the dissipation number Di, are defined as:

$$Ra_b = Ra\frac{\delta\rho_{ph}}{\rho_0\alpha_0\Delta T} \tag{1.26}$$

$$Ra_c = Ra\frac{\delta\rho_{ch}}{\rho_0\alpha_0\Delta T} \tag{1.27}$$

$$Ra_H = RaH\frac{R_0^3 - R_{CMB}^3}{3R_0^3} \tag{1.28}$$

$$Di = \frac{\alpha_0 g_0 R_0}{c_{P0}} \tag{1.29}$$

1.6   Numerical Methods

The governing equations are solved with the finite element method [9]. CitcomS employs an Uzawa algorithm to solve the momentum equation coupled with the incompressibility constraints [4, 10]. The energy equation is solved with a Steamline-Upwind Petrov-Galerkin method [11]. Brick elements are used, such as eight velocity nodes with trilinear shape functions and one constant pressure node for each element. The use of brick elements in 3D (or rectangular elements in 2D) is important for accurately determining the pressure, which controls the dynamic topography, in incompressible Stokes flow [9]. The discrete form of Equations 1.22 and 1.23 may be written in the following matrix form [6]:

$$\left(\mathbf{B}^T + \mathbf{C}\right)u = 0 \tag{1.30}$$

$$\mathbf{A}u + \mathbf{B}p = f \tag{1.31}$$

where $\mathbf{A}$ is the "stiffness" matrix, u is a vector of unknown velocities, $\mathbf{B}$ is the discrete gradient operator, $\mathbf{C}$ is the second term in Equation 1.22, p is a vector of unknown pressures, and f is a vector composed of the body and boundary forces acting on the fluid. The individual entries of $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ and f are obtained using a standard finite element formulation; see [6] for the explicit entries.

In the incompressible case, $\mathbf{C}$ is zero. Equation 1.31 can be transformed by premultiplying by $\mathbf{B}^T\mathbf{A}^{-1}$ and using Equation 1.30 to eliminate the velocity unknowns:

$$\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}p = \mathbf{B}^T\mathbf{A}^{-1}f \tag{1.32}$$

This equation is solved using the Uzawa algorithm, an established method for solving the minimization of a dual function [12], which simultaneously yields the velocity field. A conjugate gradient scheme [10, 13] is used for this iteration and forms the basis for the technique used in CitcomS.

In the compressible case, there are two different strategies to solve Equations 1.30 and 1.31. The first strategy is to add another layer of iterations when solving Equation 1.32. The right-hand-side vector is updated by the velocity solution of the previous iteration. This equation can be solved using the same conjugate gradient scheme as the incompressible case.

$$\mathbf{B}^T\mathbf{A}^{-1}\mathbf{B}p^{(i)} = \mathbf{B}^T\mathbf{A}^{-1}f - \mathbf{C}u^{(i-1)} \tag{1.33}$$

The second strategy is to transform Equation 1.31 by premultiplying by $\left(\mathbf{B}^T + \mathbf{C}\right)\mathbf{A}^{-1}$ and using Equation 1.30 to eliminate the velocity unknowns:

$$\left(\mathbf{B}^T + \mathbf{C}\right)\mathbf{A}^{-1}\mathbf{B}p = \left(\mathbf{B}^T + \mathbf{C}\right)\mathbf{A}^{-1}f \tag{1.34}$$

This equation is solved using a bi-conjugate gradient stabilized scheme.

1.7 Meshes and Geometry

There are two forms of meshes and geometries for CitcomS. By default CitcomS will produce a mesh within a regional geometry that is bound by lines of constant latitude and longitude. There is an option to generate a global mesh of a spherical shell.

For a regional mesh, CitcomS uses meshes that are regular, although considerable flexibility exists for grid refinement in the regional models. There is an option for mesh refinement in which the mesh is refined as a function of latitude, longitude, or radius. Such refinement is suitable for higher resolutions near boundary layers or within the center of the map domain, but is incapable of increasing the resolution near a curvilinear feature, as a plate boundary, unless that plate boundary is orientated north-south or east-west.

In regional meshes, *theta* (or x) is the colatitude measured from the north pole, *fi* (or y) is the east longitude, and z is the radius. *theta* and *fi* are in units of radians. Figure 1.1 shows the organization of the mesh in a regional problem. The numbering of the nodes is z-direction first, then x-direction, then y-direction. This numbering convention is used for the input and output data.
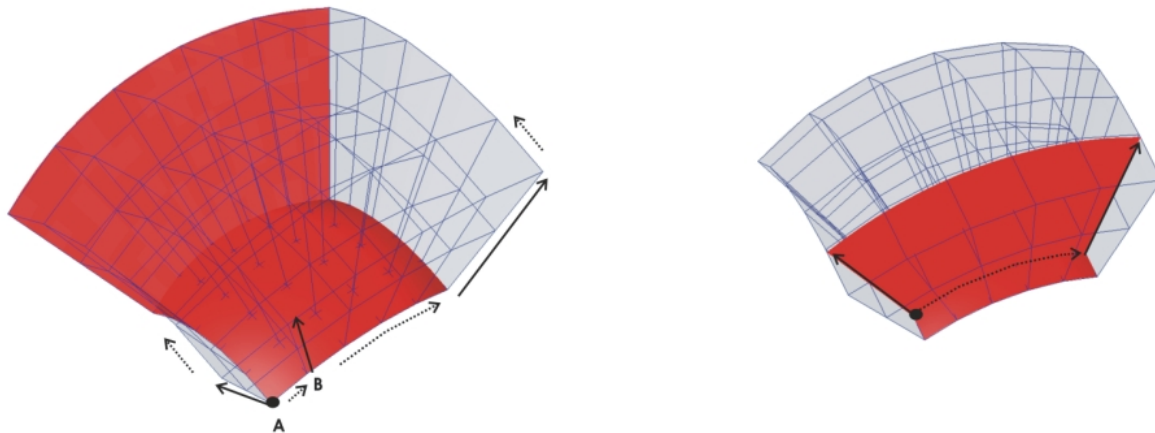
Figure 1.1: Global Node Numbering. Left: Global node numbering starts at the base of arrow A (theta_min, fi_min, radius_inner), and advances from 1 at the base to *nodez* at the tip. Upon reaching the tip, numbering continues from the base of arrow B (*nodez*+1) to its tip (2 *nodez*), and so on for all nodes on the plane fi = fi_min. Right: After completing each theta radius plane, the fi index is incremented and numbering commences from (theta_min, radius_inner) as on the left.

For a global mesh, CitcomS is also capable of generating a mesh for an entire spherical shell in which elements in map view are approximately equal in area. In the full spherical mode, CitcomS has 12 caps numbered 0 to 11 (Figure 1.2).
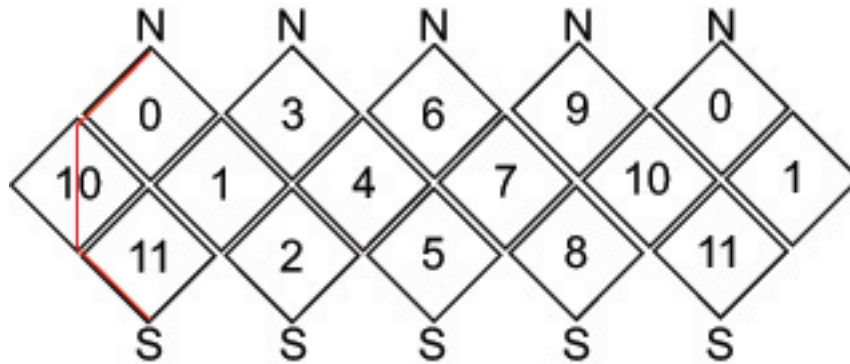
Figure 1.2: Topological connectivity of the 12 caps. N is the north pole and S is the south pole. The red line marks the 0 degree meridian.

The caps are approximately square in map view so that the edges of the square are oriented diagonally with respect to latitude and longitude. The four corners of the domain are connected by great circles (Figure 1.3). One would normally associate at least one processor with one cap. However, CitcomS can further decompose the domain such that additional processors are used to divide caps uniformly along the two edges of the caps (Figure 1.3) as well as in radius.
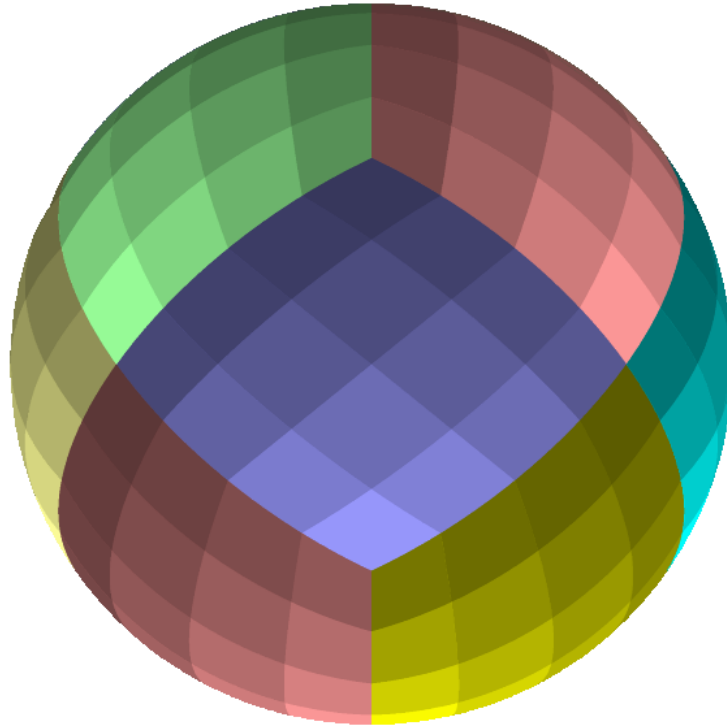
Figure 1.3: Orthographic projection of processors from a full CitcomS mesh in which there are 16 processors in map view for each cap. The CitcomS cap is shown as distinct colors while the processor domains within the caps are indicated by the intensity of the color. This example was produced for a run with 2 processors in radius such that the total number of processors was $12 \times 16 \times 2 = 384$.

Chapter 2

Installation and Getting Help

2.1 Introduction

CitcomS has been tested on Linux, Mac OS X, Sun Solaris and several NSF TeraGrid platforms. You should have no trouble installing CitcomS on most Unix-like systems.

Most users will install CitcomS from the released source package. The following sections will lead you through the installation process. Advanced users and software developers may be interested in downloading the latest CitcomS source code directly from the CIG source code repository, instead of using the prepared source package; see Section 2.13 later in this chapter.

2.2 Getting Help

For help, send e-mail to the CIG Mantle Convection Mailing List (`cig-mc@geodynamics.org`). You can subscribe to the Mailing List and view archived discussion at the Geodynamics Mail Lists web page (`geodynamics.org/cig/lists`).

2.3 System Requirements

Installation of CitcomS requires the following:

- A C compiler

- An MPI library

- If using Pyre: between Python 2.4 to 2.6, including header files (Python.h), and the pythia package (see below).

You can install all the dependencies in one command on most Linux machines. On Debian, Ubuntu or similar distributions, use this command (as `root`):

```
$ apt-get install build-essential python-dev \
          openmpi-dev openmpi-bin
```

On Red Hat, Fedora, CentOS, OpenSuSE or similar distributions, use this command (as `root`):

```
$ yum install make automake gcc gcc-c++ kernel-devel \
      python python-devel openmpi openmpi-libs openmpi-devel
```

On Mac OS X, Python is installed by default. You will need to install a C compiler and MPI library (see sections below).

MPI installations are typically configured for a particular compiler, and provide a special wrapper command to invoke the right compiler. Therefore, the choice of MPI implementation often determines which C compiler to use.

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> **Note:** Users familiar with older versions of CitcomS may prefer to install only the legacy CitcomS tools,
> `CitcomSFull` and `CitcomSRegional`, and forgo use of Python and the Pyre framework. By default
> in CitcomS 3.2.0 this is how CitcomS is configured. This process requires only a C compiler and an MPI
> library. For more information, see Section 2.12 later in this chapter.

If you are going to use solver coupling, you will also need a decent C++ compiler (e.g., g++ 3.2 or newer) and the
Exchanger package; see Section 2.7. Optionally, CitcomS can be configured to use a parallel HDF5 library; see
Section 2.8 on page 32.

2.3.1   C Compiler

On Unix or Linux systems, there is a high likelihood that a usable C compiler is already installed. To check, type `cc`
at the shell prompt:

```
$ cc
cc: no input files
$
```

On Linux, if the `cc` command is not found, install GCC using the package manager for your distribution.
    The Mac OS X version of GCC is included in a software development suite called Xcode. Xcode is available as a
free download at the Apple Developer Connection (`developer.apple.com`).

> Warning: If you are using an Intel compiler on an Itanium CPU, do not use the `-O3` optimization flag as
> reports indicate that this optimization level will generate incorrect codes. For any compiler, you should
> always be careful about the correctness of the compiled codes when using an `-O3` or higher optimization
> level.

2.3.2   MPI Library

CitcomS requires a library which implements the MPI standard (either version 1 or 2). Several free, open-source
implementations of MPI are available.
    A popular choice is MPICH (`www-unix.mcs.anl.gov/mpi/mpich`). Other choices include LAM/MPI
(`www.lam-mpi.org`) and Open MPI (`www.open-mpi.org`). Installing MPI from source involves walking
through the standard GNU build procedure (`configure && make && make install`) while logged in as
`root`.
    Linux users may have a prebuilt MPI package available for their distribution. On Mac OS X, the Fink package man-
ager offers a prepackaged version of LAM/MPI (`www.lam-mpi.org`); so if you have Fink (`fink.sourceforge.
net`) installed, simply enter the following command from a Terminal window to install LAM/MPI:

```
$ fink install lammpi lammpi-dev
```

2.3.2.1   MPI C Compiler Command

Once you have an MPI library installed, make sure its C complier command is on your PATH. Unfortunately, the name
of this command varies from one MPI implementation to the next. The CitcomS configuration script searches for the
following MPI C command names:

```
mpicc hcc mpcc mpcc_r mpxlc cmpicc
```

2.3.3   Python (Optional)

Your system may already have a suitable Python interpreter installed. To check, type the `python` command:

```
$ python -V
Python 2.5.2
```

Mac OS X 10.3 and later ships with a suitable version of Python preinstalled. If you're using an older version of Mac OS X, or for more information in general, see Python on the Mac (`www.python.org/download/mac`) at the Python web site.

On Linux, simply install the binary system package available for your distribution. Be sure to select the Python development package (typically called `python-dev`) in addition to the core Python package – even if you don't plan on doing any Python software development. The development package contains the Python header files (Python.h), which are necessary for building CitcomS.

If you are working on a cluster and `python` is too old, try poking around a little. Sometimes multiple versions of Python are installed on the same system:

```
$ python -V
Python 2.2.3
$ which python
/usr/bin/python
$ ls /usr/bin/python*
/usr/bin/python /usr/bin/python2 /usr/bin/python2.2
/usr/bin/python24 /usr/bin/python2.4
$
```

In the above scenario, it is useful to create an alias to the newer Python:

```
$ cd ~/bin
$ ln -s /usr/bin/python2.4 python
$ export PATH=$HOME/bin:$PATH
$ cd
$ hash -r
$ which python
~/bin/python
$ python -V
Python 2.4.1
$
```

If absolutely necessary, one can easily build Python from source using a C compiler. You can download Python from the Python website (`www.python.org`). Please note that Pyre in CitcomS does not work with Python 2.7 or higher.

2.3.4 Pythia (Optional)

The current version of pythia package can be downloaded from the CIG Pythia page.

2.4 Downloading and Unpacking Source

To obtain CitcomS, go to the Geodynamics Software Packages web page (`geodynamics.org/cig/software/packages/mc/citcoms`), download the source archive and unpack it using the `tar` command:

```
$ tar xzf CitcomS-3.2.0.tar.gz
```

If you don't have GNU Tar, try the following command instead:

```
$ gunzip -c CitcomS-3.2.0.tar.gz | tar xf -
```

2.5 Installation Procedure

After unpacking the source, use the following procedure to install CitcomS:

1. Navigate (i.e., `cd`) to the directory containing the CitcomS source.

   ```
   $ cd CitcomS-3.2.0
   ```

2. Type `./configure` to configure the package for your system.

   ```
   $ ./configure
   ```

3. Type `make` to build the package.

   ```
   $ make
   ```

If you are content to run CitcomS from the build directory, then you are done. Upon successful completion, the `make` command creates a script called `citcoms` in the `bin` subdirectory; this is the script you will use to run CitcomS. You may wish to add the `bin` directory to your `PATH`.

For more details about `configure`, see Section 2.6 below.

2.5.1   Installing to a Secondary Location (Optional)

Optionally, after building CitcomS, you can install it in a secondary location using the `make install` command. This is not necessary for using CitcomS and is not recommended for most situations. It is documented only for the sake of completeness.

By default, CitcomS is configured to install under `/usr/local`, which is not writable by normal users. To install as an ordinary user, give `make install` the `prefix` option, specifying a directory to which you have write access:

```
$ make install prefix=$HOME/cig
```

The above command will install CitcomS under `$HOME/cig`. Afterwards, you may wish to add `PREFIX/bin` (`$HOME/cig/bin`, in this example) to your `PATH`.

After running `make install`, you may (if desired) run `make clean` in the build directory to save disk space. You are also free to delete the source/build directory altogether. (Note that `make install` installs the examples under `PREFIX/share/CitcomS/examples`.)

2.6   Configuration

The `configure` script checks for various system features. As it runs, it prints messages informing you of which features it is checking for. Upon successful completion, it generates a `Makefile` in each source directory of the package. It also generates a `config.h` header file, which contains system-dependent definitions.

The `configure` script will attempt to guess the correct values of various installation parameters. In the event that the default values used by `configure` are incorrect for your system, or `configure` is unable to guess the value of a certain parameter, you may have to specify the correct value by hand.

> **Important:** If the `configure` script fails, and you don't know what went wrong, examine the log file `config.log`. This file contains a detailed transcript of all the checks `configure` performed. More importantly, it includes the error output (if any) from your compiler. When seeking help for `configure` failures on the CIG Mantle Convection Mailing List (`cig-mc@geodynamics.org`), please send `config.log` as an attachment.

Upon successful completion, `configure` will print a brief configuration summary.

If Pyre is enabled, the `configure` script will automatically check for needed Python dependencies, including the Pythia package (which includes the Pyre framework). If necessary, `configure` will download missing Python packages from the Internet and store them under `deps/`. These are Python packages which are required (either directly or indirectly) by CitcomS.

2.6.1 Configure Usage

For a detailed list of `configure` variables and options, give `configure` the `--help` option:

```
$ ./configure --help
```

The following is a summary of the variables and options that are important when installing CitcomS.

2.6.2 Environment Variables

Environment variables may be specified as arguments to `configure`, e.g.,

```
$ ./configure CC=icc # use the Intel compiler
```

Variable	Description

PYTHON	Python interpreter. This is useful if you have Python installed in a non-standard location, e.g.,
	 `./configure \`
	 `     PYTHON=/opt/python2.5/bin/python`
	 By default, `configure` will search for a suitable Python interpreter using your `PATH` environment variable.

CC	C compiler command. This is usually set to the name of an MPI wrapper command, e.g.,
	 `./configure \`
	 `     CC=/opt/mpich-1.2.6/bin/mpicc`
	 See Section 2.6.3 for details and examples.

CFLAGS	C compiler flags. This can be set for optimization flags.
CPPFLAGS	C preprocessor flags; e.g., `-I<dir>` if you have headers in a nonstandard directory.
LDFLAGS	Linker flags; e.g., `-L<dir>` if you have libraries in a nonstandard directory.
LIBS	Library flags; e.g., -l<lib> if additional library is needed

2.6.3 MPI Configuration

By default, `configure` will search for a C compiler using your `PATH` environment variable. It prefers MPI wrapper commands (such as `mpicc`) to ordinary compiler commands (such as `cc` or `gcc`). You may specify the compiler command name manually using the `CC` variable:

```
$ ./configure CC=/opt/mpich-1.2.6/bin/mpicc
```

The `configure` script will test for the presence of the MPI header (`mpi.h`) and an MPI library using the C compiler command. If CC is set to an MPI wrapper command such as `mpicc`, and/or the MPI header and library files are installed in a standard location (i.e., `/usr/include` and `/usr/lib`), these `configure` tests should succeed without difficulty.

But if CC is set to an ordinary compiler command name (e.g., `cc` or `gcc`) and MPI is installed in a non-standard location, you must manually specify `CPPFLAGS` and `LDFLAGS`, so that the compiler can find the MPI header files and libraries.

2.6.3.1 Manually Specifying MPI `include` and `lib` Directories

```
$ ./configure \
CPPFLAGS="-I/opt/mpich-1.2.6/include" \
LDFLAGS="-L/opt/mpich-1.2.6/lib -lmpich"
```

2.6.3.2   Manually Specifying MPI `include` and `lib` Directories and an Alternative Compiler

```
$ ./configure \
CC=icc \
CPPFLAGS="-I/opt/mpich-1.2.6/include" \
LDFLAGS="-L/opt/mpich-1.2.6/lib -lmpich"
```

Note that it may be necessary to specify the name of the MPI library itself in LDFLAGS using the -l compiler option. If a library name is not given – or if the given option doesn't work – configure will automatically try linking using -lmpi and, if that fails, -lmpich.

2.7   Exchanger Configuration (Optional)

This version of CitcomS is capable of solver coupling. Two or more instances of CitcomS solvers can be coupled together to solve a problem with different length and time scales [15]. An external Exchanger package is needed for solver coupling. You can download Exchanger at CIG's Exchanger web page (geodynamics.org/cig/software/packages/cs/exchanger). After you download and untar the package, you can configure and install Exchanger using these commands:

```
$ cd Exchanger-1.0.1/
$ ./configure --prefix=$HOME/cig
$ make
$ make install
```

By default, CitcomS will attempt to auto-detect your Exchanger installation and will disable Exchanger support if it is not found. You may specify the location of your Exchanger installation by setting the PYTHONPATH environment variable to the appropriate installation prefix.

```
$ cd CitcomS-3.2.0/
$ export PYTHONPATH=$HOME/cig/lib/python2.5/site-packages:$PYTHONPATH
$ ./configure --with-exchanger
```

2.8   HDF5 Configuration (Optional)

For writing its output in binary format, CitcomS requires parallel HDF5 (PHDF5). In turn, PHDF5 requires an MPI library with MPI-IO support and a parallel file system. If an existing installation of the PHDF5 library is not available on your cluster, you can compile it from source by following the instructions in the file release_docs/INSTALL_parallel under the HDF5 source tree. Under Debian Linux, you may simply install the libhdf5-mpich, libhdf5-mpich-dev and hdf5-tools packages.

> **NOTE:** Most post-processing and visualization scripts discussed in Chapter 5 only understand ASCII output. An additional step to convert the HDF5 output files to ASCII files in necessary before using those scripts.

By default, CitcomS will attempt to auto-detect your PHDF5 installation, and will disable HDF5 support if it is not found. You may specify the location of your PHDF5 installation by setting the PHDF5_HOME environment variable to the appropriate installation prefix.

```
$ export PHDF5_HOME=/opt/phdf5/1.6.5
$ ./configure --with-hdf5
```

2.8.1   Additional Tools

While the following software is not necessary for the normal operation of CitcomS, you may find it useful for accessing CitcomS data in HDF5 files.

2.8.1.1 NumPy

NumPy is an extension to Python which adds support for multi-dimensional arrays for use in scientific computing. You may download NumPy from the NumPy home page (`numpy.scipy.org`). To compile and install this extension, download it and issue the following commands after extracting it:

```
$ cd numpy-1.0
$ python setup.py install --prefix=$HOME/cig
```

Alternatively, under Debian Linux you can install the `python-numpy` package. On Gentoo Linux, NumPy is available in the `dev-python/numpy` ebuild.

2.8.1.2 PyTables

PyTables is an extension to Python and can expose HDF5 array datasets as Python NumPy arrays. It is available at PyTables (`www.pytables.org`).

To compile and install this extension, download the latest stable version and issue the following commands:

```
$ cd pytables-1.3.3
$ python setup.py install --prefix=$HOME/cig
```

To install on Debian Linux, you may use the `python-tables` package instead. On Gentoo Linux, it is available in the `dev-python/pytables` ebuild.

2.8.1.3 HDFView

HDFView is a visual tool written in Java for browsing and editing HDF5 files. You may download it from the HDFView home page (`hdf.ncsa.uiuc.edu/hdf-java-html/hdfview`).

2.8.1.4 OpenDXutils

In order to import HDF5 files into OpenDX, you need the OpenDXutils package from the Cactus project. Go to the OpenDXutils package website (`www.cactuscode.org/Visualization/openDX`) and follow the instructions to download and install the package. Note that you will need to set both `DXMODULES` and `DXMDF` environment variables before running OpenDX to load the package.

2.9 GGRD Configuration (Optional)

CitcomS can read data from files for initial temperature, boundary conditions, material control and others. By default, these files are in ASCII format, and the data in the files must be ordered in the same way of the node ordering. As a result, whenever the mesh is changed, these data files need to be regenerated to satisfy the ordering requirement. This restriction can be lifted if using GRD data files. GRD files are binary files in NetCDF format (Network Common Data Form). GRD files are widely used in GMT (Generic Mapping Tools) as well.

The GRD file support can be enabled at configuration time. It requires the installation of HC package (`geodynamics.org/cig/software/packages/mc/hc`), a 1D global mantle circulation solver which can compute velocities, tractions, and geoid for simple density distributions and plate velocities. To install HC, you will also need the GMT and NetCDF packages (library and header files). See the `README.TXT` file in HC for instructions on installation. After HC is installed, note the directory (for example: `$HOME/cig/HC-1_0`) of HC installation, and execute these commands:

```
$ export HC_HOME=$HOME/cig/HC-1_0
$ ./configure --with-ggrd
```

You may need to set `GMTHOME` and `NETCDFHOME` environment variables if these packages is not installed in the system directory.

2.10   PETSc Configuration (Optional)

To use the PETSc functionality in CitcomS, CitcomS first needs to be built with the PETSc library. This is done by passing `-with-petsc=yes` option to the `configure` script. If this option is passed to `configure`, `configure` expects PETSc to be installed correctly on the system, with the environment variables `PETSC_DIR` and `PETSC_ARCH` being set appropriately. `configure` will check for the `PETSC_DIR` and `PETSC_ARCH` only if the `-with-petsc=yes` option has been passed to the script.

The PETSc homepage is (`http://www.mcs.anl.gov/petsc/`) and information about installing PETSc can be found at (`http://www.mcs.anl.gov/petsc/documentation/installation.html`)

2.11   Batch System Configuration

If you are installing CitcomS on a cluster with a batch system, you can configure Pyre such that the `citcoms` command automatically submits jobs to the batch queue. Pyre contains support for the LSF, PBS, and Globus batch systems.

The command to submit a batch job depends upon the particular batch system used. Further, the command used in a batch script to launch an MPI program varies from one cluster to the next. This command can vary between two clusters, even if the clusters use the same batch system! On some systems, `mpirun` is invoked directly from the batch script. On others, a special wrapper is used instead. If you need help to configure Pyre for your cluster, you can contact CIG Mantle Convection Mailing List (`cig-mc@geodynamics.org`) for assistance.

Properly configured, Pyre can handle job submissions automatically, insulating users from the details of the batch system and the site configuration. This feature has the most value when the system administrator installs a global Pyre configuration file on the cluster (under `/etc/pythia-0.8`), for the benefit of all users and all Pyre-based applications.

For more information on configuring Pyre for your batch system, see CIG's Pythia page (`geodynamics.org/cig/software/packages/cs/pythia/docs/batch`). For more information on batch system configuration as it pertains to running CitcomS, see Section 3.5.2 on page 42.

2.12   Installing with Pyre

By default, CitcomS 3.2.0 does not install using Pyre. To build CitcomS binaries with the Pyre wrappers (necessary for the example Cookbooks), call `configure` using the `--with-pyre` option:

```
$ ./configure --with-pyre=yes
```

The only system requirements for this configuration are an MPI library and a C compiler. With Pyre the make command will build `pycitcoms` and `mpipycitcoms` as well as the script `citcoms` used for running CitcomS. Without Pyre the `make` command will build two command-line tools, `CitcomSFull` and `CitcomSRegional`, for running the full solver and the regional solver, respectively.

2.13   Installing from the Software Repository

The CitcomS source code is available via a Subversion server at the Geodynamics website (`geodynamics.org`). This allows users to view the revision history of the code and check out the most recent development version of the software.

NOTE: If you are content with the prepared source package, you may skip this section.

2.13.1   Tools You Will Need

In addition to the usual system requirements, you will need a handful of additional development tools installed in order to work with the source from the CIG software repository.

First, you must have a Subversion client installed. To check, type `svn`; it should return a usage message.

```
$ svn
Type 'svn help' for usage.
```

For more information on Subversion, visit the Subversion website (`subversion.tigris.org`).

Second, you must have the GNU tools Autoconf, Automake, and Libtool installed. To check, enter the following commands:

```
$ autoconf --version
$ automake --version
$ libtoolize --version
```

For more information about these GNU tools, see the GNU website (`www.gnu.org/software`). The CitcomS v3.2.0 source package was created with Autoconf 2.68, Automake 1.11.2, and Libtool 2.4.2.

2.13.2 Download Source from Subversion

To check out the latest version of the software, use the `svn checkout` command:

```
$ svn checkout http://geodynamics.org/svn/cig/mc/3D/CitcomS/trunk CitcomS
```

This will create the local directory `CitcomS` (if it doesn't already exist) and fill it with the latest CitcomS source from the CIG software repository.

The `CitcomS` directory thus created is called a *working copy*. To merge the latest changes into an existing working copy, use the `svn update` command:

```
$ cd CitcomS
$ svn update
```

This will preserve any local changes you have made to your working copy.

2.13.3 Generating the GNU Build System

Your working directory should now contain a fresh checkout of CitcomS:

```
$ ls
CitcomS
$
```

Before you can run `configure` or `make`, you must generate the necessary files using the GNU tools. The easiest way to do this is to run `autoreconf -i`:

```
$ cd CitcomS
$ autoreconf -i
$ ./configure
$ make
```

The `autoreconf` tool runs Autoconf to generate the `configure` script from `configure.ac`. It also runs Automake to generate `Makefile.in` from `Makefile.am` in each source directory.

The configure script stores dependency information for source files in hidden subdirectories called `.deps`. If source files are added, deleted, moved, or renamed – which may happen if you run `svn update` to merge the latest changes – the `make` command may report errors for source files which no longer exist. If this happens, clean your existing configuration using the `make distclean` command, and then re-run `configure` and `make`:

```
$ make distclean
$ ./configure
$ make
```

The `make distclean` command deletes all files generated by `configure`, including the Makefiles themselves! Therefore, after running `make distclean`, you will not be able to run `make` again until you re-run `configure`.

Chapter 3

Running CitcomS

3.1 Using CitcomS without Pyre

Regardless of whether you build CitcomS with or without Pyre, two binary executables, `CitcomSRegional` and `CitcomSFull`, are always placed under the `bin` directory. These programs are compiled from pure C code and do not use Python or the Pyre framework. Each program has the same usage:

```
$ mpirun [mpi_options] CitcomSRegional inputfile
$ mpirun [mpi_options] CitcomSFull inputfile
```

Two input file examples, one for a regional spherical model and one for a full spherical model, are provided in the `examples/Regional` and `examples/Full` directories, respectively. The meaning of the input parameters is described in Appendix A on page 101.

The pure C version, compared to the Pyre version, shares the same input parameters and functionality, but is less flexible in changing parameters and in launching parallel jobs. Users are encouraged to use the Pyre version if possible. In the following sections and Chapter 6, we will concentrate on the Pyre version only.

3.2 Using CitcomS with Pyre

If you build CitcomS with the Pyre framework, an additional executable, `citcoms`, is placed under the `bin` directory. The `citcoms` executable is a Python script used for running both the regional and full spherical models using Pyre. Executed without any command line options, `citcoms` will run a regional model with default parameters. It can also run a full spherical model if the correct parameters are set (see Section 6.2 on page 60 for an example).

On input, CitcomS needs numerous parameters to be specified (see Appendix A for a full list). All parameters have sensible default values. Since you will likely want to specify the parameters of your CitcomS runs, you will need to alter both computational details (such as the number of time steps) and controlling parameters specific to your problem (such as the Rayleigh number). These input parameters, or properties in the Pyre terminology, are grouped under several Pyre components.

Most of the properties you will set using CitcomS have names which are identical to the parameters for CitcomS in pure C version, which are described in Appendix A.

3.3 Changing Parameters

There are several methods to set the input parameters for CitcomS: via the command line, or by using a configuration file in `.cfg` format.

3.3.1 Using the Command Line

Pyre uses the following syntax to change properties from the command line. To change the value of a property of a component, use:

```
--[component].[property]=[value]
```

Each component is attached to a facility, so the option above can also be written as:

```
--[facility].[property]=[value]
```

Each facility has a default component attached to it. A different component can be attached to a facility by:

```
--[facility]=[new_component]
```

3.3.2   Using a `.cfg` File

Entering all those parameters via the command line involves the risk of typographical errors, which can lead to undesired results. You may find it easier to write a brief `.cfg` input file that contains the parameters. This file has a format similar to a Windows INI file. The file is composed of one or more sections which are formatted as follows:

```
[CitcomS.component1.component2]
# this is a comment
property1 = value1
property2 = value2  ; this is another comment
```

We strongly recommend that you use `.cfg` files for your work. The files are syntax-colored by the `vim` editor. (Upon termination of each run, all of the parameters are logged in a `.cfg` file.)

3.3.3   Using a `.pml` File

A `.pml` file is an XML file that specifies parameter values in a highly structured format. XML files are intended to be read and written by machines, not edited manually by humans. The `.pml` file format is intended for applications in which CitcomS input files are generated by another program, e.g., a GUI, web application, or a high-level structured editor. This file fomat will not be discussed or used further in the manual. It is composed of nested sections which are formatted as follows:

```
<component name='component1'>
    <component name='component2'>
        <property name='property1'>value1</property>
        <property name='property2'>value2</property>
    </component>
</component>
```

3.3.4   Specification and Placement of Configuration Files

One or more configuration files and command line options may be specified on the command line:

```
$ citcoms a.cfg b.cfg --foo.bar=baz
```

In addition, the Pyre framework searches for configuration files named `CitcomS.cfg` in several predefined locations. You may put settings in any or all of these locations, depending on the scope you want the settings to have:

1. `PREFIX/etc/CitcomS.cfg`, for system-wide settings;

2. `$HOME/.pyre/CitcomS/CitcomS.cfg`, for user settings and preferences;

3. the current directory (`./CitcomS.cfg`), for local overrides.

Parameters given directly on the command line will override any input contained in a configuration file. If more than one configuration files are given on the command line, the later one overrides the former ones. Configuration files given on the command line override all other `CitcomS.cfg` files. The `CitcomS.cfg` files placed in (3) will override those in (2), (2) overrides (1), and (1) overrides only the built-in defaults.

3.4 Uniprocessor Example

CitcomS runs similarly in full spherical or regional modes. For the purpose of this example, you will perform a test run of the regional version on a workstation. Execute the following on the command line:

```
$ citcoms --steps=10 --controller.monitoringFrequency=5 \
--solver.datafile=example0 --solver.mesher.nodex=17 --solver.mesher.nodey=17
```

This runs a default convection problem in a regional domain for 10 time steps and with a mesh of $17 \times 17 \times 9$ nodal points. Since we did not provide the parameter `solver.mesher.nodez`, the default value 9 is used. The model results are written to files `example0.*` with an interval of 5 time steps.

Instead of writing the input parameters on the command line, you can put them in a `.cfg` file. The CitcomS source package contains an `examples` directory (the `make install` command installs the examples under `PREFIX/share/CitcomS/e` where `PREFIX` is the `CitcomS` installation directory). In this directory, you will find a configuration file equivalent to the previous example: `example0.cfg`. You can run the model using:

```
$ citcoms example0.cfg
```

3.4.0.1 Example: Uniprocessor, **example0.cfg**

```
[CitcomS]
steps = 5

[CitcomS.controller]
monitoringFrequency = 1

[CitcomS.solver]
datafile = example0

[CitcomS.solver.mesher]
nodex =  17
nodey =  17
```

3.5 Multiprocessor Example

In order to run this example, you should be on a Beowulf cluster with four or more processors, or on a supercomputer; and you should be in the directory in which the input file is located, in this case, the `examples` directory. CitcomS has been extensively used on both environments, using up to several hundred processors. How to run a multiprocessor CitcomS model depends on your hardware and software settings, e.g., whether a batch system is used, what the names of the computers in a cluster are, and how the file system is organized. This section will lead you through the different settings of a parallel environment.

3.5.0.2 Example: Multiprocessor, **example1.cfg**

```
[CitcomS]
steps = 70

[CitcomS.controller]
monitoringFrequency = 10

[CitcomS.solver]
datafile = example1

[CitcomS.solver.mesher]
nprocx =  2
```

```
nprocy =   2
nodex  = 17
nodey  = 17
nodez  =   9
```

This example uses 2 processors in colatitude (x-coordinate), 2 in longitude (y-direction), and 1 in the radial (z-direction), i.e., it uses 4 processors in total. In addition, there will be 17 nodes in x (theta), 17 nodes in y (fi), and 9 nodes in z (radius_inner). The model will run for 70 time steps and the code will output the results every 10 time steps.

It is important to realize that within the example script (and in finite element method, FEM) the term "node" refers to the mesh points defining the corners of the elements. In example1.cfg, this is indicated with:

```
nodex  = 17
nodey  = 17
nodez  =   9
```

These quantities refer to the total number of FEM nodes in a given direction for the complete problem, and for the example it works out that within a given processor there will be $9 \times 9 \times 9$ nodes. Note that in the x-direction (or y) that for the entire problem there are 17 nodes and there is one node shared between two processors. This shared node is duplicated in two adjacent processors. Unfortunately, "nodes" sometimes also refer to the individual computers which make up a Beowulf cluster or supercomputer. In the example scripts, this is indicated with:

```
nprocx =   2
nprocy =   2
```
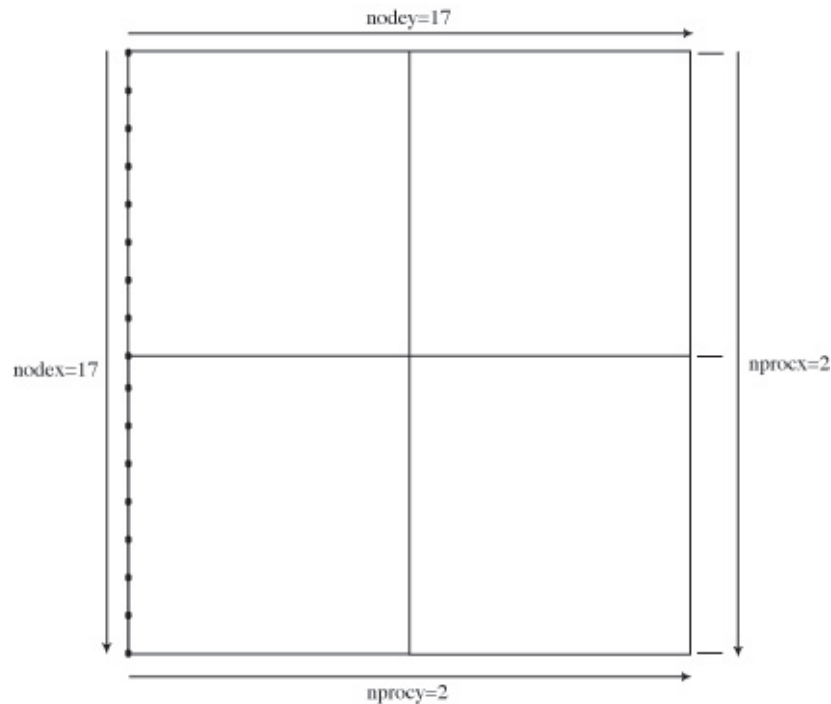

Figure 3.1: Computational Domain. Map view on the configuration of the top layer of the computational nodes and the processors.

3.5.1   Output Directories and Output Formats

CitcomS potentially generates a large number of ASCII files. This means that you will have to organize your directories carefully when running CitcomS so that you can manage these files as well as use a post-processing program contained in this distribution.

How to best manage this large output depends on whether you will use a local file system or a parallel file system. For example, if you have a local hard disk on every machine (node) on a Beowulf cluster, with each hard disk mounted locally to the machine, this scenario is referred to as a local file system in this section. Or you might use some kind of parallel file system on your computer (e.g., NFS, GPFS, PVFS, to name a few), which is mounted on all of the nodes. Usually your home directory is mounted on the parallel file system. The local file system is usually more cost- and time-efficient than the parallel file system.

If you want CitcomS to write its output to the local hard disks, you need to have a common directory structure on all of the local hard disks. For example, if the directory /scratch exists on all local hard disks, you can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=/scratch
```

The additional command line option will override the `datadir` property, which specifies the output directory. The output files are then placed in /scratch on each individual machine with a filename prefix `example1`.

However, if the output directory name on each local hard disk depends on the machine hostname, you can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=/scratch_%HOSTNAME
```

The special string `%HOSTNAME` will be substituted by the hostname of each machine.

As the final example for a local file system, you can specify an arbitrary output directory for each machine. To do so, you must write a program to be executed on each machine which will print the output directory. The program must be named `citcoms_datadir` and must reside on your path. An example of `citcoms_datadir` can be found in the `visual/` directory. Then you can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=%DATADIR
```

The special string `%DATADIR` will be substituted by the output of `citcoms_datadir` for each machine.

If you want CitcomS to write its output to a parallel file system, you have several choices. You can run the example script as follows (substitute *username* with your own username):

```
$ citcoms example1.cfg --solver.datadir=/home/username
```

The output files are then placed in your home directory with a filename prefix `example1`. A potential problem with this approach is that the directory /home/*username* will be flooded with hundreds of files, perhaps even tens of thousands of files if you are running a model using several tens of processors for thousands of time steps. Alternatively you can have each machine write its output to its own directory, according to its MPI rank. You can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=/home/username/%RANK
```

The special string `%RANK` will be substituted by the MPI rank of each processor. You will see four new directories /home/*username*/0, /home/*username*/1, /home/*username*/2, and /home/*username*/3. The processor of MPI rank 0 will write its output in /home/*username*/0 with a filename prefix `example1` (defined by the property `datafile` inside `example1.cfg`) and so on.

The ASCII output can potentially take a lot of disk space. CitcomS can write `gzip` compressed output directly. You can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=/home/username \
--solver.output.output_format=ascii-gz
```

Be warned that the post-process scripts do not understand this output format yet.

The last choice is the most powerful one. Instead of writing many ASCII files, CitcomS can write its results into a single HDF5 (Hierarchical Data Format) file per time step. These HDF5 files take less disk space than all the ASCII files combined and don't require additional post-processing to be visualized in OpenDX. In order to use this feature, you must compile CitcomS with the parallel HDF5 library if you haven't done so already (see Section 2.8 on page 32). You can run the example script with:

```
$ citcoms example1.cfg --solver.datadir=/home/username \
--solver.output.output_format=hdf5
```

The output files will be stored in /home/*username*/ with a filename prefix example1 and a filename suffix h5. See Chapter 4 on page 45 for more information on how to work with the HDF5 output.

3.5.2 Launchers and Schedulers

If you have used MPI before, you know that mpirun requires several command-line options to launch a parallel job. Or if you have used one of the batch systems, you will know that the batch system requires you to write a script to launch a job. Fortunately, launching a parallel CitcomS job is simplified by Pyre's launcher and scheduler facilities. Many properties associated with launcher and scheduler are pertinent to the cluster you are on, and are best customized in a configuration file. Your personal CitcomS configuration file (~/.pyre/CitcomS/CitcomS.cfg) is suitable for this purpose. On a cluster, the ideal setup is to install a system-wide configuration file under /etc/pythia-0.8, for the benefit of all users.

Pyre's scheduler facility is used to specify the type of batch system you are using (if any):

```
[CitcomS]
scheduler = lsf
```

The valid values for scheduler are lsf, pbs, globus, and none.

Pyre's launcher facility is used to specify which MPI implementation you are using:

```
[CitcomS]
launcher = mpich
```

The valid values for launcher include mpich and lam-mpi.

You may find the dry option useful while debugging the launcher and scheduler configuration. To debug the scheduler configuration, use the --scheduler.dry option:

```
citcoms --scheduler.dry
```

This option will cause CitcomS to perform a "dry run," dumping the batch script to the console, instead of actually submitting it for execution (the output is only meaningful if you're using a batch system). Likewise, to debug the launcher configuration, use the --launcher.dry option:

```
citcoms --launcher.dry
```

This option will cause CitcomS to print the mpirun command, instead of actually executing it. (If you're using a batch system, a job will be submitted for execution; when it runs, CitcomS will simply print the mpirun command, and the job will immediately terminate.)

3.5.2.1 Running without a Batch System

On a cluster without a batch system, you need to specify on which machines the job will run. Supposing the machines on your cluster are named n001, n002, ..., etc., but you want to run the job on machines n001, n003, n004, and n005 (maybe n002 is down for the moment). To run the example, create a file named mymachines.cfg which specifies the machines to use:

```
[CitcomS.launcher]
nodegen = n%03d
nodelist = [1,3-5]
```

The nodegen property is a printf-style format string, used in conjunction with nodelist to generate the list of machine names. The nodelist property is a comma-separated list of machine names in square brackets.

Now, invoke the following:

```
$ citcoms example1.cfg mymachines.cfg
```

This strategy gives you the flexibility to create an assortment of `.cfg` files (with one `.cfg` file for each machine list) which can be easily paired with different parameter files.

If your machine list does not change often, you may find it more convenient to specify default values for `nodegen` and `nodelist` in `~/.pyre/CitcomS/CitcomS.cfg` (which is read automatically). Then, you can run any simulation with no additional arguments:

```
$ citcoms example1.cfg
```

Warning: This assumes your machine list has enough nodes for the simulation in question.

You will notice that a machine file `mpirun.nodes` is generated. It will contain a list of the nodes where CitcomS has run. Save the machine file as it will be useful in the postprocessing step.

3.5.2.2 Using a Batch System

The settings which are important when using a batch system are summarized in the sample configuration file which follows.

```
[CitcomS]
scheduler = lsf    ; the type of the installed batch system

[CitcomS.lsf]
bsub-options = [-a mpich_gm]    ; special options for 'bsub'

[CitcomS.launcher]
command = mpirun.lsf    ; 'mpirun' command to use on our cluster

[CitcomS.job]
queue = normal         ; default queue for jobs
walltime = 5*minute    ; run time limit of the job
```

These settings are usually placed in `~/.pyre/CitcomS/CitcomS.cfg` or in a system-wide configuration file. They can be overridden on the command line, where one typically specifies the job name and the allotted time for the job:

```
$ citcoms example1.cfg --job.queue=debug \
    --job.name=example1 --job.walltime=5*minute
```

The number of nodes to allocate for the job is determined automatically, based upon the simulation parameters.

3.5.3 Monitoring Your Jobs

Once launched, CitcomS will print the progress of the model to the standard error stream (stderr). Usually, the stderr is directed to your terminal so that you can monitor the progress. On some system, the stderr is redirected to a file. In any case, the progress is always saved in a log file (e.g., `example1.log`). The log file contains the convergence progress of the computation and, if an error occurs, debugging output. The time file (e.g., `example1.time`) contains the elapsed model time (in non-dimensional units) and CPU time (in seconds) of every time step. The format of the time file can be found in Appendix C on page 121. The log and time files are output by the rank-0 processor only.

Following your successful run, you will want to retrieve the output files from all the nodes and process them so they can be visualized with the visualization program OpenDX (see Chapter 5 on page 51).

3.6   Using CitcomS on the TeraGrid

The TeraGrid is a set of parallel supercomputer facilities at eight partner sites in the U.S. which creates an integrated, persistent computational resource. Since TeraGrid software is based on commodity clusters, Linux/Unix, and Globus, it should be easier to scale from a laboratory development environment to a high-end environment in a straightforward manner which promotes application performance. Although the TeraGrid is a high-end resource, it was developed to be accessible to the general community of scientists and engineers as a production facility. TeraGrid accounts for small allocations are available directly from CIG for investigators in the U.S.

CitcomS has already been installed and tested on several NSF TeraGrid platforms, including NCSA, SDSC, and TACC. To use CitcomS on these machines, please log in to your TeraGrid account and read the instructions at `$TG_COMMUNITY/CIG/CitcomS/TG_README`. See CIG Community Area Software on the TeraGrid (`geodynamics.org/cig/software/csa/`) for additional information on access and to apply for allocation time.

Chapter 4

Working with CitcomS HDF5 Files

4.1   Introduction

A typical run of CitcomS can create thousands if not millions of ASCII output files. This situation is inefficient since it requires an extra post-processing step for assembling the results from each processor (see Chapter 5 on page 51). Since the v2.1 release, CitcomS solves this problem when running the software on computers that have parallel file systems by assembling a binary HDF5 file in parallel I/O mode. You can skip this chapter if you are not using the HDF5 output format.

4.2   About HDF5

The Hierarchical Data Format (HDF) is a portable file format developed at the National Center for Supercomputing Applications (NCSA) (`hdf.ncsa.uiuc.edu/HDF5`). It is designed for storing, retrieving, analyzing, visualizing, and converting scientific data. The current and most popular version is HDF5, which stores multi-dimensional arrays together with ancillary data in a portable self-describing format. It uses a hierarchical structure that provides application programmers with a host of options for organizing how data is stored in HDF5 files.

HDF5 files are organized in a hierarchical structure, similar to a Unix file system. Two types of primary objects, *groups* and *datasets*, are stored in this structure. A group contains instances of zero or more groups or datasets, while a dataset stores a multi-dimensional array of data elements. Both kinds of objects are accompanied by supporting metadata.

A dataset is physically stored in two parts: a header and a data array. The header contains miscellaneous metadata describing the dataset as well as information that is needed to interpret the array portion of the dataset. Essentially, it includes the name, datatype, dataspace, and storage layout of the dataset. The name is a text string identifying the dataset. The datatype describes the type of the data array elements. The dataspace defines the dimensionality of the dataset, i.e., the size and shape of the multi-dimensional array. The dimensions of a dataset can be either fixed or unlimited (extensible). The storage layout specifies how the data arrays are arranged in the file.

The data array contains the values of the array elements and can be either stored together in a contiguous file space or split into smaller *chunks* stored at any allocated location. Chunks are defined as equally-sized multi-dimensional subarrays (blocks) of the whole data array and each chunk is stored in a separate contiguous file space. Extensible datasets whose dimensions can grow are required to be stored in chunks. One dimension is increased by allocating new chunks at the end of the file to cover the extension.

HDF5 also supports access to portions (or selections) of a dataset by *hyperslabs*, which consist of a subarray or strided subarray of the multi-dimensional dataset. The selection is performed in the file dataspace for the dataset. HDF5 also supports parallel I/O. Parallel access is supported through MPI-IO. The file and datasets are collectively created/opened by all participating processes. Each process accesses part of a dataset by defining its own file dataspace for that dataset. When accessing data, the data transfer property specifies whether each process will perform independent I/O or all processes will perform collective I/O.

4.3   Input Parameters

To enable HDF5 output in CitcomS, all you need to do is include the following section in your `.cfg` input file.

```
[CitcomS.solver.output]
output_format = hdf5
```

Alternatively, you can specify the option `--solver.output.output_format=hdf5` on the command line. The resulting filenames will start with the value of your specified `datafile` input parameter and end with `.h5`.

4.3.1   Optimizing Parallel I/O

There are several platform-dependent parameters used by the HDF5 library and the underlying MPI-IO routines to optimize the performance of parallel I/O. The optimal values for these parameters may vary from file system to file system. Ideally, before compiling CitcomS, the build procedure would configure these parameters based on your platform, but this is not implemented currently.

   In order to facilitate the process of gathering I/O performance data from a variety of parallel file systems such as GPFS, PVFS, IBRIX FusionFS, etc., you can specify the following parameters in the CitcomS input file. You may use these parameters to tune the performance of the parallel I/O on your system.

   All values are assumed to be specified in bytes, unless otherwise indicated.

1. MPI file hints for collective buffering file access.

   (a) `cb_block_size`: Target nodes will access data in chunks of this size.

   (b) `cb_buffer_size`: Specifies the total buffer space on each target node. Set this parameter to a multiple of `cb_block_size`.

2. HDF5 file access properties.

   (a) `sieve_buf_size`: Maximum size of data sieve buffer.

   (b) `output_alignment`: Alignment interval size in bytes.

   (c) `output_alignment_threshold`: Allocation requests above this size will be aligned on a memory address that is a multiple of `output_alignment`.

   (d) `cache_rdcc_nelmts`: Maximum number of chunks that can be stored in the raw data chunk cache.

   (e) `cache_rdcc_nbytes`: Size of raw data chunk cache in bytes.

For more details, you can refer to the following references:

- **MPI-2: Extensions to the Message-Passing Interface, section 9.2.8 (`www-unix.mcs.anl.gov/mpi/ mpi-standard/mpi-report-2.0/node182.htm`)** provides a list of MPI-IO reserved file hints, also available in Section 7.2.8 of the MPI-2 reference book.

- **HDF5 documentation (`hdf.ncsa.uiuc.edu/HDF5/doc/UG/08_TheFile.html`)**, Chapter 2, Section 7.3, contains a list of HDF5 file access properties.

- **HDF5 User's Guide: Data Caching (`hdf.ncsa.uiuc.edu/HDF5/doc/Caching.html`)** offers a short explanation of raw data chunk caching.

You should also refer to the documentation for your particular parallel file system and check if there are any other MPI or HDF5 hints that could improve your parallel I/O performance.

   Finally, here is an example section that would appear in a typical CitcomS input file:

```
[CitcomS.solver.output]
cb_block_size = 1048576               # 1 MiB
cb_buffer_size = 4194304              # 4 MiB
sieve_buf_size = 1048576              # 1 MiB
output_alignment = 262144             # 256 KiB
output_alignment_threshold = 524288   # 512 KiB
cache_rdcc_nelmts = 521
cache_rdcc_nbytes = 1048576
```

4.4   Data Layout

Time independent data (e.g., node coordinates, grid connectivity) are saved in a file (for example, `test-case.h5`) at the first output stage. Subsequently, each output stage will save time dependent data (e.g., velocity, and temperature) in a separate file (for example, `test-case.100.h5` contains data of time step 100). Most of the output data from CitcomS is specified at the nodes of a logically Cartesian grid and is therefore well represented by multi-dimensional arrays. A cap dimension is defined for addressing each of the CitcomS caps, followed by three spatial indices (i, j, k) in the case of 3D data, two spatial indices (i, j) in the case of 2D surface data, or one spatial index (k) in the case of 1D radial data. An additional dimension is provided for storing the components of vector and tensor data. These data arrays are stored in different groups. Each group has a descriptive name. In addition, there is an `/input` group archiving the input parameters of the model. Two sample `.h5` files are provided in `visual/samples/` directory.

Dataset	Shape
`/input`	`N/A`
`/coord`	`(caps, nodex, nodey, nodez, 3)`
`/connectivity`	`(cap_elements, 8)`

Table 4.1: Layout of the time-independent data file

Dataset	Shape
`/velocity`	`(caps, nodex, nodey, nodez, 3)`
`/temperature`	`(caps, nodex, nodey, nodez)`
`/viscosity`	`(caps, nodex, nodey, nodez)`
`/pressure`	`(caps, nodex, nodey, nodez)`
`/stress`	`(caps, nodex, nodey, nodez, 6)`
`/geoid`	`(8)` See Section C.6.9 on page 123 for details
`/surf/velocity`	`(caps, nodex, nodey, 2)`
`/surf/heatflux`	`(caps, nodex, nodey)`
`/surf/topography`	`(caps, nodex, nodey)`
`/botm/velocity`	`(caps, nodex, nodey, 2)`
`/botm/heatflux`	`(caps, nodex, nodey)`
`/botm/topography`	`(caps, nodex, nodey)`
`/horiz_avg/temperature`	`(caps, nodez)`
`/horiz_avg/velocity_xy`	`(caps, nodez)`
`/horiz_avg/velocity_z`	`(caps, nodez)`

Table 4.2: Layout of the time-dependent data file

4.5   Accessing Data

As previously indicated, HDF5 is a self-describing binary file format. As such we can use a variety of tools to inspect the structure of an HDF5 file, as well as for retrieving data in any order.

4.5.1   Inspecting Structures

To quickly inspect the structure of an HDF5 file, you can use the command `h5ls` which is included with the HDF5 software:

```
$ h5ls -r file.h5
```

4.5.2   Converting to ASCII Files

You can convert the HDF5 files to the ASCII combined capfiles described in Appendix C.6 for specific time steps by using the command included in CitcomS:

```
$ h5tocap modelname step1 [step2 [...] ]
```

You can also convert the HDF5 files to the velo files described in Appendix C.6.2 on page 122 for restart purposes by using the command included in CitcomS:

```
$ h5tovelo modelname step
```

4.5.3   Accessing Data in Python

The small Python script `h5tocap.py` provides a good example of using the PyTables extension module to access the data contained in the CitcomS HDF5 files. Using PyTables, datasets can be retrieved from disk as NumPy arrays. The retrieval avoids unnecessary copying of data by using hyperslabs, which take advantage of Python's powerful array slice-indexing.

For example, obtaining the node coordinates, temperature, and topography values over the entire surface of the sphere for time step 100 can be done easily with the following code snippet:

```
import tables

h5file = tables.openFile('samples/cookbook1.h5', 'r')
surface_coords = h5file.root.coord[0:12,:,:,-1,:]

data100 = tables.openFile('samples/cookbook1.100.h5', 'r')
surface_temperature = data100.root.temperature[0:12,:,:,-1]
surface_topography = data100.root.surf.topography[0:12,:,:]
```

In this case, the slice `0:12` refers to all caps explicitly, while the empty slice "`:`" refers to the entire extent of the corresponding dimension. The values of -1 above refer to the last z-index, which corresponds to the location of the surface nodes on each of the caps. Finally, note how both HDF5 datasets and groups are conveniently accessible as Python attributes on the PyTables file object.

For more details, refer to the documentation for PyTables (`www.pytables.org`) and NumPy (`numpy.scipy.org`).

4.5.4   Accessing Data Using HDFView

NCSA HDFView is a visual tool for accessing HDF files. You can use it for viewing the internal file hierarchy in a tree structure, creating new files, adding or deleting groups and datasets, and modifying existing datasets. HDFView is capable of displaying 2D slices of multi-dimensional datasets, with navigation arrow buttons that enable you to range over the entire extent of a third dimension. An example of using HDFView is found in Figure 4.1 which uses data from Cookbook 1 in Section 6.2 on page 60.

Figure 4.1: A screenshot of HDFView. The left panel shows the hierarchy of the groups and datasets. The right panel shows a 2D slice of a dataset. The bottom panel shows the metadata associated with the selected group or dataset.

Chapter 5

Postprocessing and Graphics

5.1 Introduction

Once you have run CitcomS, you would have a series of output files (potentially spread throughout the file systems of your Beowulf cluster or in a set of directories on your parallel file system). You now have to retrieve and combine the data for the time step (or age) of interest. To visualize your results, it is recommended that you use the open-source Open Visualization Data Explorer, better known as OpenDX. The software is available from the OpenDX website (`www.opendx.org`). If you are using Linux, OpenDX is usually available as package `dx` or `opendx` in your distribution. If you are using Mac OS X, OpenDX is available via Fink (`fink.sourceforge.net`). We provide experimental scripts for a 3D visualization program called MayaVi2; see Section 5.7 on page 55. Scripts using GMT commands to plot 2D cross sections of temperature field are also provided; see Section 5.8 on page 57.

5.2 Postprocessing on a Beowulf Cluster

Generally, the results from your CitcomS run will be distributed on disks attached to individual nodes of your Beowulf cluster. The output files are written in each node under the directory that you specified as the `datadir` property in the input file. To examine those files, log in to a node and change directories to the one you specified with a prefix. For example, if you set `datadir=/scratch/`*username* and `datafile=test-case` in your input file, then your output files will be written to `/scratch/`*username* and will have the prefix `test-case`.

   If you select HDF5 for the output format, the output files will have a `.h5` suffix. You won't need to postprocess the `.h5` files; you can visualize the results using OpenDX. See Section 5.6 on page 54 for more details.

   If you select compressed ASCII (`ascii-gz`) for the output format, there is no post-processing script for it. You need to decompress and rename the output files before you can use the post-processing script described below.

   If you select ASCII for the output format, you will have many output files. An example of a filename for the velocity output is `test-case.velo.2.10` where `test-case` is the model prefix, `velo` means that this is a velocity data file, `2` corresponds to the processor number (i.e., it is output by the 2nd processor), and `10` corresponds to the time step.

   If your run used the time-dependent velocity boundary conditions (`solver.param.file_vbcs=on`), the log file will also have a `current age` line that lists the time-step numbers and their corresponding times. To choose an age to export for postprocessing, you have to determine which time step corresponds to the age that interests you by looking at the log file.

   When you execute a CitcomS run, your input parameters will be saved in a file `pidxxxxx.cfg` where `xxxxx` is usually a five-digit number for the process ID. This pidfile contains most of the input parameters, which can be useful for archiving and postprocessing.

   The ASCII output files of CitcomS need to be postprocessed before you can perform the visualization. The script `autocombine.py` can postprocess (retrieve and combine) CitcomS output; it will retrieve CitcomS data to the current directory and combine the output into a few files.

   Using `autocombine.py`, retrieve and combine data of time-step 10:

```
$ autocombine.py mpirun.nodes pid12345.cfg 10
```

This reads the MPI machinefile (`mpirun.nodes`) and the CitcomS pidfile (`pid12345.cfg`), then calls other scripts to do the actual job. The general usage for `autocombine.py` is:

```
$ autocombine.py [machinefile] [pidfile] \
[step1] [step2 or more ...]
```

If your Beowulf cluster uses `ssh` (rather than `rsh`) to access the computation nodes, you must manually edit `visual/batchpaste.s` and replace 'rsh' with 'ssh' in the script.

   Once `autocombine.py` has run, you will have 2 files (or 24 files for the full spherical version of CitcomS) formatted as follows:

```
test-case.cap00.10
test-case.cap00.10.general
```

The former file is the data file containing simulation results and is referred to as the "capfile"; its format can be found in Appendix C. The latter file is the OpenDX header for the data.

   If you have enabled some `optional_output`, and the optional fields are node-based (e.g, `comp_nd`, `stress`, or `pressure`), these fields will be combined in separated files, with filenames:

```
test-case.opt00.10
test-case.opt00.10.general
```

The former file is the data file containing optional fields and is referred to as the "optfile." Its format is column-based ASCII data. The latter file is the OpenDX header for the data. The header file contains information on the ordering of the optional fields.

5.3   Postprocessing in a Non-Cluster Environment

If you run CitcomS in a non-cluster environment or all of your data can be accessed from the local machine, you can still use `autocombine.py` to combine the data. In this case, the `machinefile` is not needed and can be replaced by `localhost`, such as:

```
$ autocombine.py localhost [pidfile] \
[step1] [step2 or more ...]
```

5.4   Using OpenDX for Regional Sphere Visualization

OpenDX modules designed for CitcomS can be found in the source directory called `visual`. The optional `make install` command installs the OpenDX modules under `PREFIX/share/CitcomS/visual` (where `PREFIX` defaults to `/usr/local`).

   In this example, you will use `visRegional.net` to visualize the results of regional CitcomS.

   1. Launch OpenDX by typing:

      ```
      $ dx
      ```

      You will see an OpenDX Data Explorer window.

   2. Click Edit Visual Programs and select `visRegional.net` from the file selector.

   3. You will see a Visual Program Editor window.

   4. Select the import tab in the Visual Program Editor's main window and double-click on the FileSelector block, which will open a Control Panel window.

   5. In the CitcomSImport filename input box, select the header file of your postprocessed data, e.g.,

```
samples/regtest.cap00.100.general
```

6. In the pull-down menu, select Execute ▷ Execute on Change.

7. A new window will appear with the image of the model.

8. If you want to zoom, rotate, change projection, and otherwise manipulate the view of the model, experiment with the menu Options ▷ View Control.
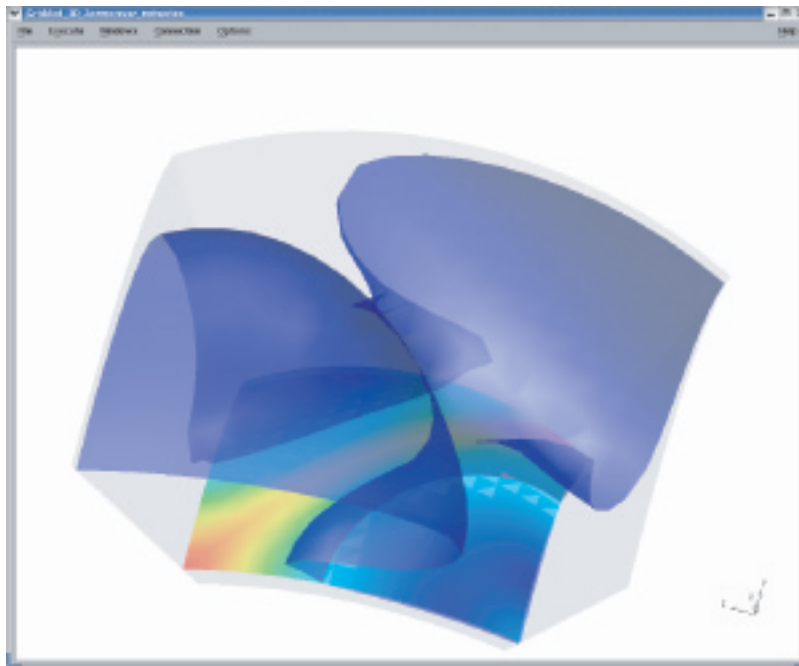
Figure 5.1: Regional Model Visualized with OpenDX. A snapshot of an upwelling (blue isosurface) with a slice of the temperature field (bisecting plane).

Additional options in the control panel window for the regional model include:

- **CitcomSImport reduced** can increase or reduce the resolution of the velocity vectors and grids. Reducing resolution is often necessary for visualizing large dataset interactively. Note that the resolution of other fields (e.g., temperature and viscosity) is not reduced.

- **Core radius** is the size of the orange sphere which represents the core-mantle boundary.

- **Isosurface value** is the temperature isosurfaces. You can change the values of the isosurfaces, including adding additional isosurfaces or deleting existing ones.

- **Slab cut dimension** is the direction of the slab (an OpenDX term for cross-section).

- **Slab cut position** is the position of the slab.

You can change any of the parameters, visualization, or set-up by going back to the main window and clicking on each tab. If you click on each block, you will be able to change the settings for that function.

5.5   Using OpenDX for Full Sphere Visualization

1. After launching OpenDX, you will see an OpenDX Data Explorer window.

2. Click Edit Visual Programs and select `visFull.net` from the file selector.

3. You will see a Visual Program Editor window.

4. Select the import tab in the Visual Program Editor's main window and double-click on the FileSelector block, which will open a Control Panel window.

5. In the Format String of CitcomSFullImport input box, select one of the 12 header files of your postprocessed data, e.g.,

        samples/fulltest.cap00.100.general

6. The results of a full spherical CitcomS consist of 12 cap files. In order to import the 12 cap files at the same time, edit the filename with the cap number replaced by printf-styled format string `%02d`, e.g.,

        samples/fulltest.cap%02d.100.general

7. In the pull-down menu, select Execute ▷ Execute on Change.

8. A new window will appear with the image of the model.

9. If you want to zoom, rotate, change projection, and otherwise manipulate the view of the model, experiment with the menu Options ▷ View Control.

Additional options in the control panel window for the spherical model include:

- **CitcomSFullImport reduced** can increase or reduce the resolution of the velocity vectors and grids. Reducing resolution is often necessary for visualizing large dataset interactively. Note that the resolution of other fields (e.g., temperature and viscosity) is not reduced.

- **Core radius** is the size of the orange sphere which represents the core-mantle boundary.

- **Isosurface value** is the temperature isosurfaces. You can change the values of the isosurfaces, including adding additional isosurfaces or deleting existing ones.

- **Latitude of normal axis** and **Longitude of normal axis** are the directions of the normal axis to the cross-section plane.

5.6   Using OpenDX for HDF5 Visualization

If you use the HDF5 output format (`solver.output.output_format=hdf5`), you can directly visualize the data without postprocessing. First, you need to install and set up the OpenDXutils package (see Section 2.8.1.4 on page 33). Then, open either `visRegional.net` or `visFull.net` in OpenDX.

1. In the pull-down menu, select File ▷ Load Macro, and select the file CitcomSImportHDF5.net to load it.

2. In the Tools panel of the main window, select the CitcomSImportHDF5 module in the Macros category (highlighted in Figure 5.2).

3. Place the module in the work space and rewire the network as shown in Figure 5.2.

4. There are four input tabs in the CitcomSImportHDF5 module.

    (a) The first tab (connected to the left FileSelector module) specifies the HDF5 file containing time-independent information (e.g., `samples/cookbook1.h5`).
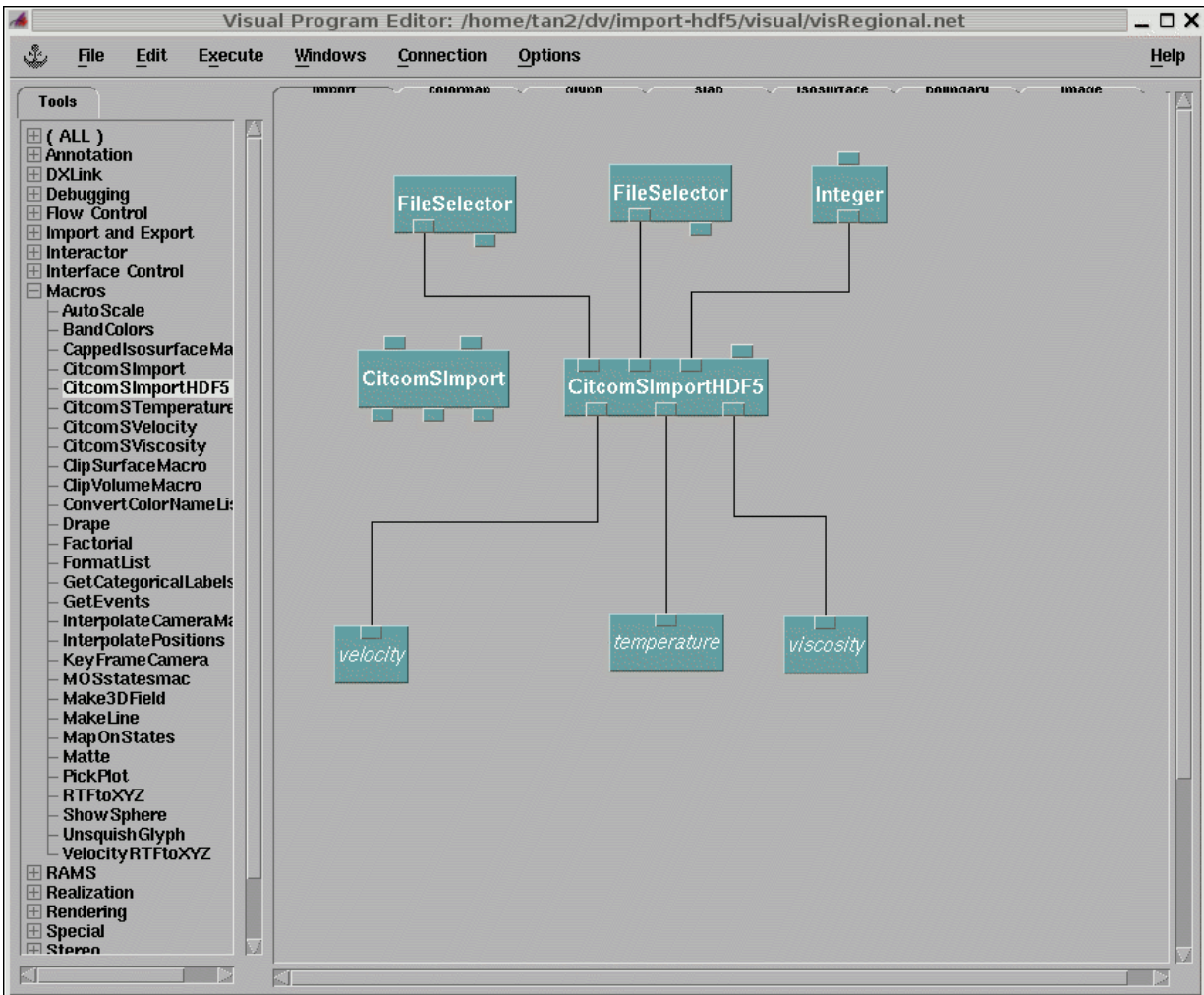
Figure 5.2: How to import CitcomS HDF5 data. The CitcomSImportHDF5 module is highlighted in the Tools panel.

      (b) The second tab (connected to the right FileSelector module) specifies the HDF5 file containing time-dependent information (e.g., samples/`cookbook1.100.h5`).

      (c) The third tab (connected to the Integer module) specifies the resolution reduction factor.

      (d) The fourth tab (unconnected, default to 0) specifies which cap(s) to import.

          i. To visualize a regional model, leave this tab unchanged.

         ii. To visualize a full spherical model, double-click this module and change the value of this tab to `{0,1,2,3,4,5,6,7,8,9,10,11}`.

        iii. You can also specify a subset of caps to visualize.

5. After the data are imported, the visualization can be manipulated as described in previous sections.

5.7 Using MayaVi for Visualization

This distribution also comes with scripts for visualizing CitcomS using MayaVi2. MayaVi2 is the successor of MayaVi for 2D/3D scientific data visualization. It is an interactive program allowing elaborate plots of scientific data. MayaVi2 relies on the Visualization Toolkit (VTK) and allows easy scripting in Python. To install MayaVi2, you should follow the instructions on the MayaVi2 website (`https://svn.enthought.com/enthought/wiki/`

GrabbingAndBuilding) and on the SciPy website (`www.scipy.org/Cookbook/MayaVi/Installation`).
Besides MayaVi2, before using the script you will need to install PyTables (see Section 2.8.1.2 on page 33) and
PyVTK; see PyVTK website (`cens.ioc.ee/projects/pyvtk`) for instructions.

The script acts as an extension module of MayaVi2. The installation of the script is still preliminary. You will
need to include `PREFIX/share/CitcomS/visual/Mayavi2/citcoms_plugins/` in your `PYTHONPATH`
environment variable. You also need to create a directory called `~/.mayavi2` and copy into it the following:

```
PREFIX/share/CitcomS/visual/Mayavi2/mayavi_custom_ui.py
```

To run the script, type this command:

```
$ mayavi2_citcoms_display.py file.step.h5
```

This will launch MayaVi2 and load the data from `file.step.h5`. An example of using this script is found in Figure
5.3. You may adjust your visualization pipeline by adding any appropriate VTK filters and modules. For more details
about this process, refer to *The Visualization Toolkit User's Guide* (ISBN 1-930934-13-0) or see the VTK website
(`www.vtk.org`).
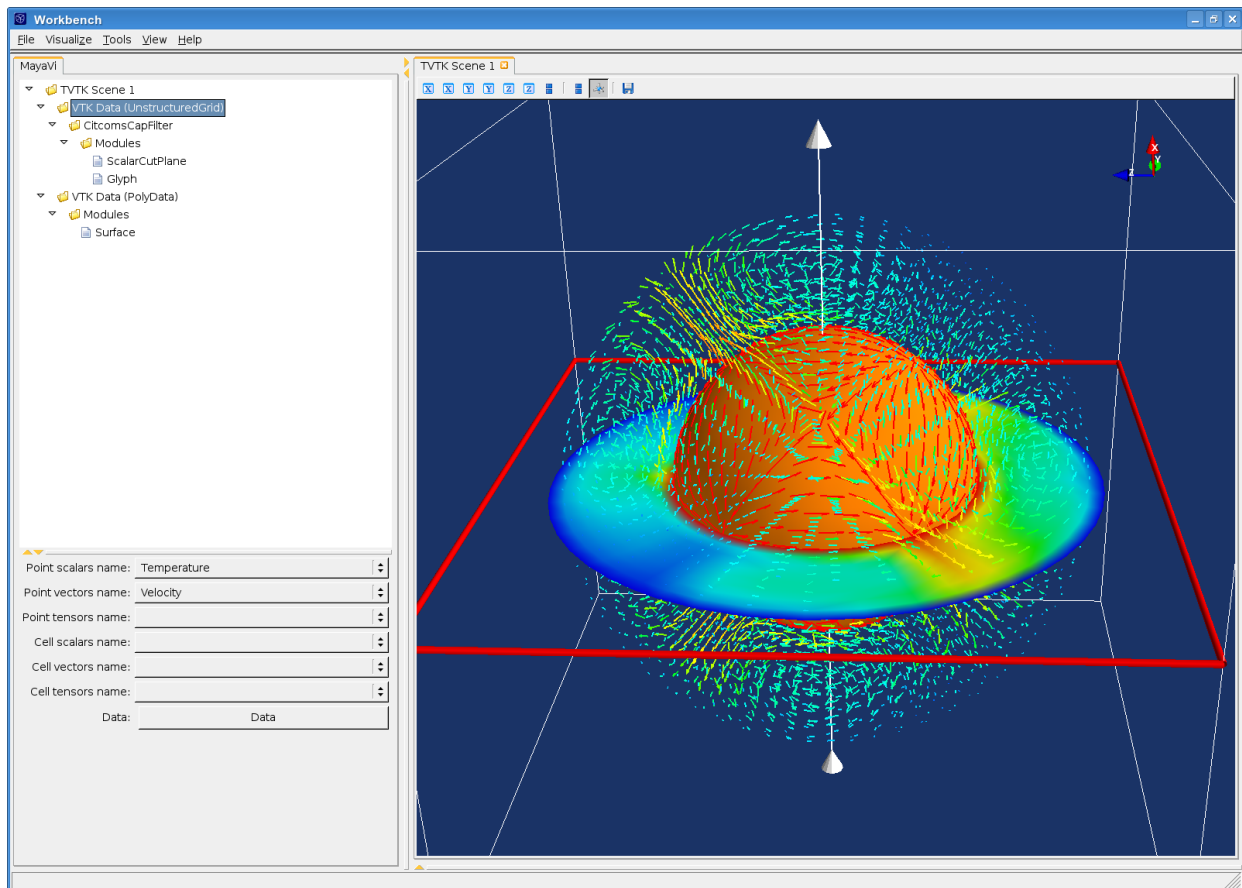
Figure 5.3: Example MayaVi2 visualization of `cookbook1.100.h5`. Here we display the velocity field as vectors, as
well a slice of the temperature field. Note the visualization pipeline in the tree view on the left panel.

5.8 Using GMT Commands for Visualization

The Generic Mapping Tools (GMT) is a collection of command-line tools for manipulating geographic and Cartesian data that produces PostScript (PS) or Encapsulated PostScript File (EPS) illustrations. GMT is widely used in the geophysics community. Two scripts `plot_layer.py` and `plot_annulus.py`, which can plot the temperature field in horizontal and radial cross sections, respectively, are provided. These scripts use GMT commands to generate EPS images. GMT is very customizable. Users might wish to customize the scripts for their need.

The usage of `plot_layer.py` is:

```
$ plot_layer.py modelname caps step layer
```

The script will look for the capfile(s) `modelname.cap00.step`, if `caps` is 1, or `modelname.cap00.step`, `modelname.cap01.step`, ... through `modelname.cap11.step`, if `caps` is 12. A slice of the capfile at the specified radial layer is then plotted in Mercator projection, if `caps` is 1, or in Hammer-Aitoff projection, if `caps` is 12.
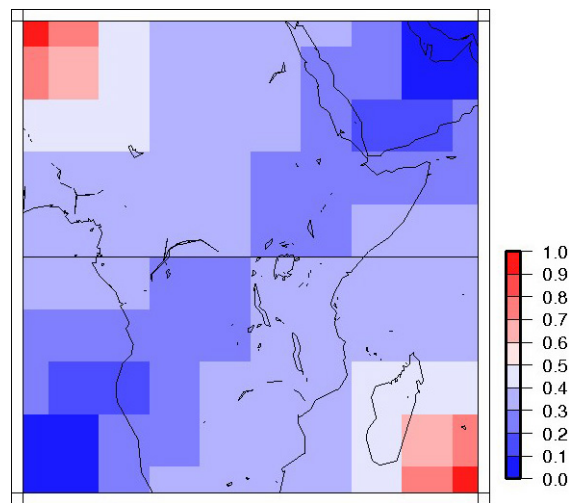
Figure 5.4: Temperature field generated by `plot_layer.py`. This image is the mid-layer (layer 5) of the sample data `visual/samples/regtest.cap00.100`. The resolution of the image is poor because the data has only 9×9×9 nodes.

The usage of `plot_annulus.py` is:

```
$ plot_annulus.py modelname step
```

The script will ask you a few questions on how to specify the great circle path. There are three options: (1) a starting point and an azimuth, (2) a starting point and another point on the great circle, and (3) a starting point and a rotation pole. The great circle path is used to construct the radial cross section.
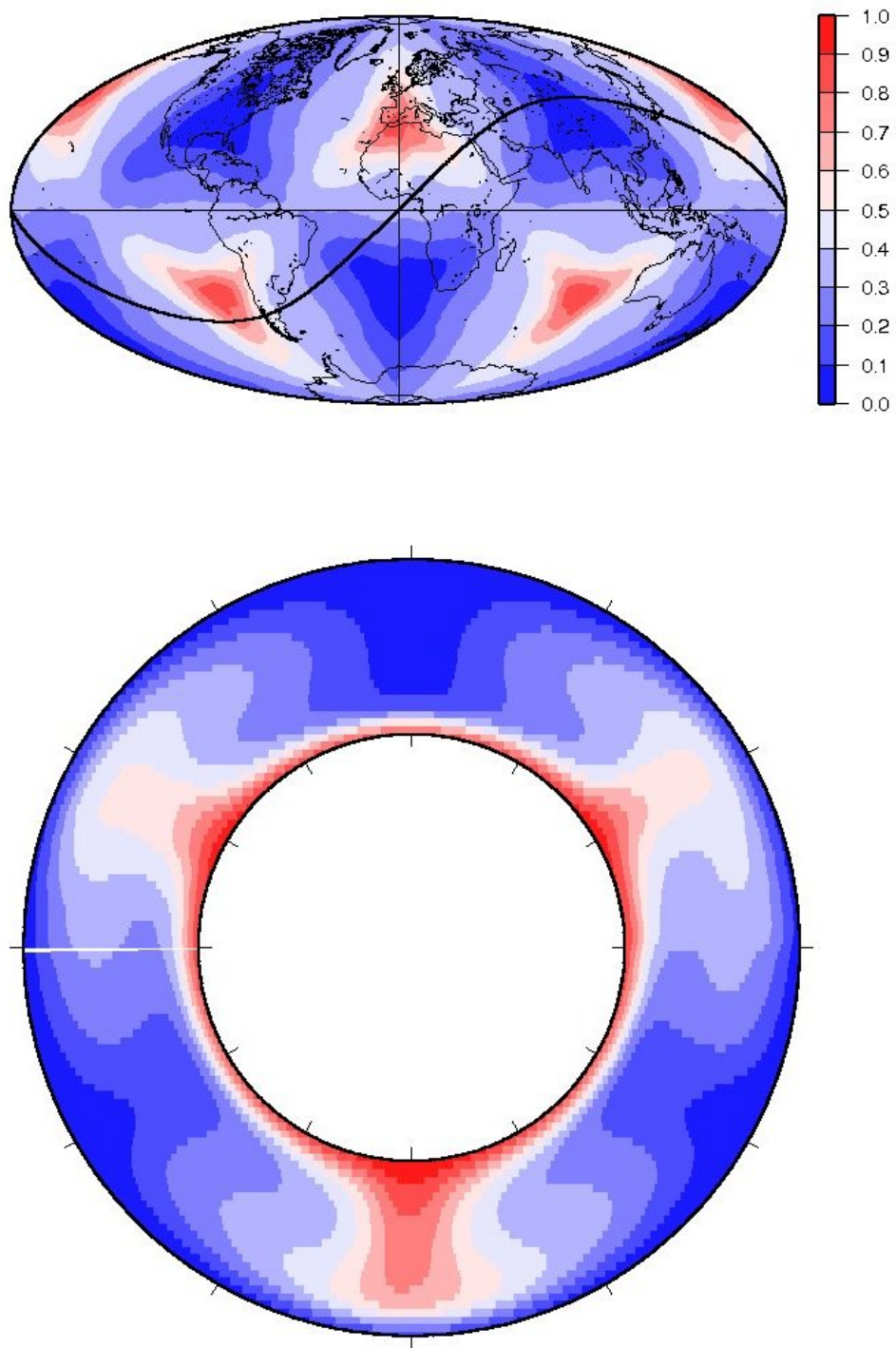
Figure 5.5: Temperature fields generated by `plot_annulus.py`. The top panel is the horizontal cross section at the mid layer in Hammer-Aitoff projection. The thick line marks the surface track of the radial cross section. The bottom panel is the radial cross section. The cross section starts at $0°$ latitude and $0°$ longitude and has an azimuth of $45°$. The image is from the sample data `visual/samples/fulltest.cap*.100`. There is always a gap on the left (starting point) of the cross section. Users familiar with GMT are welcome to contribute a fix to the script.

Chapter 6

Cookbooks

6.1 Introduction

These cookbook examples are meant to serve as a guide to some of the types of problems CitcomS can solve. Each of these cookbook problems will only run with CitcomS if Pyre is enabled. Cookbook examples range from regional to full spherical shell problems that address traditional mantle convection problems. These cookbook examples are distributed with the package under the `examples` directory. However, you might need to edit these example scripts slightly to launch the job on your cluster (see Section 3.5 on page 39 for more information).

Cookbooks 1 to 4 introduce the basic parameters and are suitable for all users. Cookbook 5 introduces time-dependent velocity boundary conditions, reading in initial temperature field from files and tuning of the advection solver. Cookbook 6 introduces the pseudo-free-surface formulation for studying short wavelength dynamics topography. Cookbook 7 introduces thermo-chemical convection problem and tuning of the Conjugate Gradient velocity solver. Cookbook 8 introduces compressible convection problem, checkpointing/restarting, geoid and tuning of the Multigrid and Uzawa velocity solver. Cookbook 9 introduces embedding one CitcomS domain within another CitcomS domain, and further tuning of the advection solver. Cookbook 10 introduces how to convert the convection field to seismic velocities and how to generate synthetic seismograms using SPECFEM3D_GLOBE at the CIG Seismology Web Portal.

6.2   Cookbook 1: Global Model

6.2.1   Problem

This example solves for thermal convection within a full spherical shell domain. The full spherical version of CitcomS is designed to run on a cluster that decomposes the spherical shell into 12 equal "caps" and then distributes the calculation for caps onto separate processors. To run CitcomS with the full solver parameter set, it is recommended that you have a minimum of 12 processors available on your cluster.
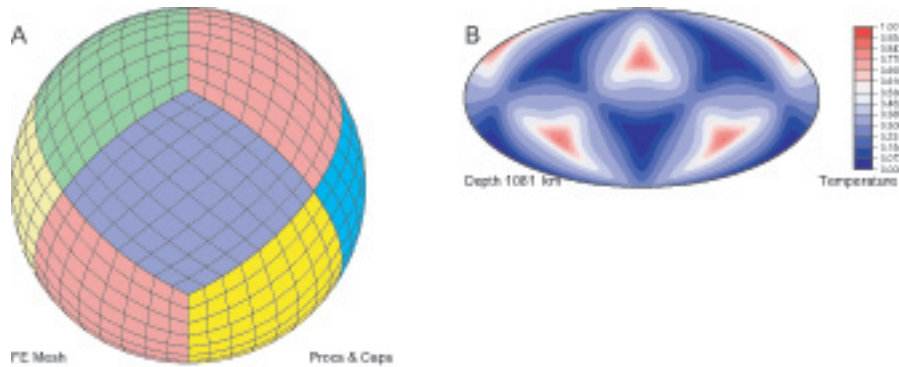
Figure 6.1: Global Model "Caps." Left (A): Three-dimensional perspective image showing seven of the 12 spherical caps used in a full CitcomS run. Right (B): The temperature field at 1081 km depth from a Cookbook 1 run.

6.2.2   Solution

You will use `cookbook1.cfg`. The first set of parameters specifies that you are going to use the full spherical version of the solver. The default is to use the regional spherical version, so this must be set.

```
solver = full
```

The second set of parameters specifies the number of time steps (100), how often full outputs of the computation are created (25), and the prefix of output filenames (cookbook1).

```
steps = 100
monitoringFrequency = 25
datafile = cookbook1
```

The `solver.ic` facility controls the temperature field for the initial conditions. The last set of parameters includes the number of perturbations to the initial temperature (1), the number of nodal lines of the perturbation in the longitudinal direction, e.g., the spherical harmonic order (3), the number of nodal lines in the latitudinal direction, e.g., the spherical harmonic degree (2), which layer the perturbation is on (5), and the amplitude of the perturbation (0.05). Note that although the number of perturbations is assigned here as `num_perturbations=1`, that is actually the default value.

```
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 5
perturbmag = 0.05
```

This example is executed by typing

```
$ citcoms cookbook1.cfg
```

6.2.2.1   Example: Global Model, `cookbook1.cfg`

```
[CitcomS]
solver = full
steps = 100                 ; number of time steps

[CitcomS.controller]
monitoringFrequency = 25    ; how often outputs are created

[CitcomS.solver]
datafile = cookbook1        ; prefix of output filenames

[CitcomS.solver.ic]
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 5
perturbmag = 0.05
```

Once you have run the model, you can visualize the results using OpenDX, described in the previous chapter. When you invoke "Edit Visual Program," select `visFull.net`.
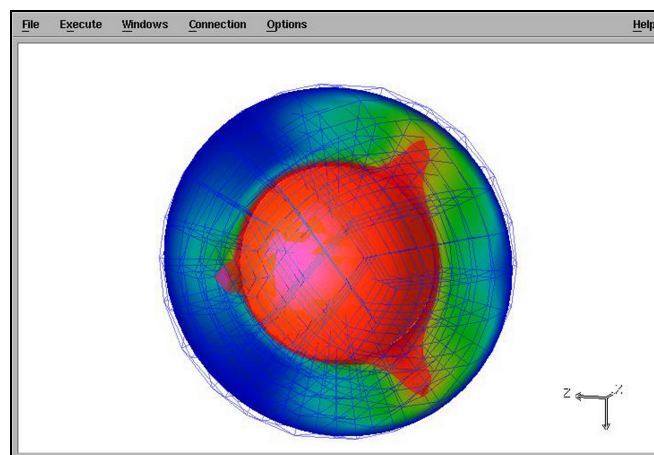
Figure 6.2: Cookbook 1: Global Model. This image, created by OpenDX, depicts a slice through a spherical model of convection, with warmer colors indicating upwelling and the cooler colors showing downwelling.

6.2.3   Discussion

You have generated a simple example of the full CitcomS model, with minimal parameter alterations. With a default Rayleigh number of 10^5 and perturbation on the initial temperature field which has a degree-3 and an order-2 pattern, after 100 time steps, the convection pattern remains relatively steady.

   As a side note, it is not required that 12 processors, with one spherical cap per processor, be used. As an end-member possibility, for example, 12 different jobs could be run on a single computer (`n001` in this example) by invoking:

```
$ citcoms cookbook1.cfg --launcher.nodegen="n%03d" \
--launcher.nodelist=[1,1,1,1,1,1,1,1,1,1,1,1]
```

This is not particularly efficient, but it does illustrate the flexibility of both MPI and Pyre.

6.3   Cookbook 2: Domain Size and Velocity Boundary Conditions

6.3.1   Problem

This example solves for thermal convection with velocity boundary conditions imposed on the top surface within a given region of a sphere. This requires using the regional version of CitcomS.

6.3.2   Solution

You will use `cookbook2.cfg`. The parameters specify the number of time steps (60), the prefix of the output filenames (`cookbook2`), and how often outputs will be created (30).

```
steps = 60
monitoringFrequency = 30
datafile = cookbook2
```

The `solver.mesher` facility has several properties involved in the generation of the computational mesh. Continue to use the default values for the physical portion of the domain in which you are interested. However, try modifying the layout of the mesh as shown. The parameters specify two processors per cap in the x- and y-direction, one processor per cap in the z-direction (by default), 17 nodes per cap in the x- and y-direction, 9 nodes in the z-direction, and the minimum/maximum extents in the colatitudal, longitudal, and radial (`theta`, `fi`, `radius`) directions. The unit for `theta` and `fi` is radian.

```
nprocx =   2
nprocy =   2
nodex   = 17
nodey   = 17
nodez   =  9

theta_min = 0.7854
theta_max = 1.5708
fi_min = 0.0
fi_max = 0.7854
radius_inner = 0.55
radius_outer = 1.0
```

The `solver.bc` facility allows you to impose a uniform velocity across the top surface. You have a velocity which is purely in the colatitude direction with a non-dimensional velocity of 100 (see Equation 1.14 on page 21 for how to dimensionalize it).

```
topvbc     =    1
topvbxval = 100
topvbyval =    0
```

In addition, the initial temperature field has a linear conductive profile. The amplitude of initial temperature perturbation is set to zero using the `solver.ic` facility.

```
num_perturbations = 1
perturbmag        = 0.0
```

6.3.2.1   Example: Velocity Boundary Conditions, `cookbook2.cfg`

```
[CitcomS]
steps = 60                       ; number of time steps

[CitcomS.controller]
```

```
monitoringFrequency = 30     ; how often outputs are created

[CitcomS.solver]
datafile = cookbook2        ; prefix of output filenames

# Modify the layout of the mesh.
[CitcomS.solver.mesher]
nprocx =  2
nprocy =  2
nodex  = 17
nodey  = 17
nodez  =  9

theta_min = 0.7854
theta_max = 1.5708
fi_min = 0.0
fi_max = 0.7854
radius_inner = 0.55
radius_outer = 1.0

# Impose a uniform velocity across the top surface.
[CitcomS.solver.bc]
topvbc    =    1
topvbxval = 100
topvbyval =    0

# In addition, set the initial temperature perturbation to zero.
[CitcomS.solver.ic]
num_perturbations = 1
perturbmag        = 0.0
```

6.3.3 Discussion

Using OpenDX to visualize the results (Figure 6.3), this model allows you to create a plate-driven convection in which there is a thermal upwelling on one wall, a thermal downwelling on another, and uniform horizontal velocity across the top. The downwelling is not exactly subduction because the sidewalls have reflecting boundary conditions. This means that there is a symmetrical downwelling in a vertical domain on the other side.
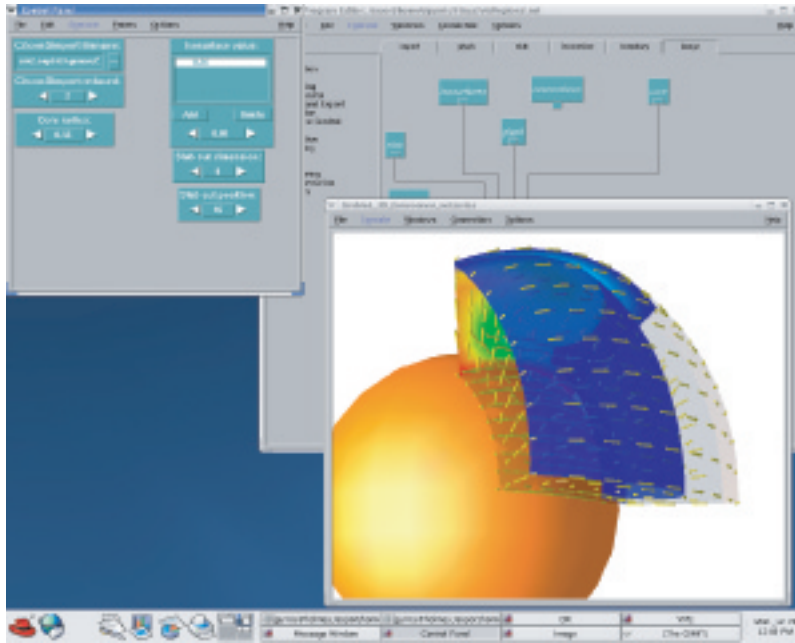
Figure 6.3: Cookbook 2: Velocity Boundary Conditions. This model, visualized with OpenDX, highlights a region of the sphere and the heated upwellings (warm colors), downwellings (cool colors), and the velocities (yellow arrows).

6.4 Cookbook 3: Temperature-Dependent Viscosity

6.4.1 Problem

A common problem in geophysics is the exploration of natural convection in the presence of variable viscosity, including temperature-dependent or stress-dependent viscosity.

6.4.2 Solution

You will use `cookbook3.cfg`. The parameters specify the number of time steps (200), how often outputs will be created (25), the prefix of the output filenames (`cookbook3`), and the Rayleigh number (10^6).

```
steps = 200
monitoringFrequency = 25
datafile = cookbook3
rayleigh = 1e6
```

The `solver.visc` facility assigns the viscosities. The parameters specify whether the viscosity should be updated at every time step (`on`), the number of viscous layers (4), the viscosity of each layer (1,1,1,1), whether the viscosity is temperature dependent (`on`), the type of viscosity law to use (4), the activation energy of each layer (0.2,0.2,0.2,0.2), the temperature offset of each layer (0,0,0,0), the activation volume of each layer (0,0,0,0), whether to apply the minimum cutoff (`on`), the value of the minimum cutoff (1.0), whether to apply the maximum cutoff (`on`), and the value of the maximum cutoff (100.0).

```
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
rheol = 4
viscE = 0.2,0.2,0.2,0.2
viscT = 0,0,0,0
```

```
viscZ = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0
```

The range of the layers are determined by the following parameters: layer 1 extends from the top surface to a depth of `solver.const.z_lith` (default to 0.014, or 90 km dimensionally); layer 2 is below layer 1 and extends to a depth of `solver.const.z_410` (default to 0.06435, or 410 km dimensionally); layer 3 is below layer 2 and extends to a depth of `solver.const.z_lmantle` (default to 0.105, or 670 km dimensionally); layer 4 is below layer 3 and extends to the bottom. These depth parameters also control the depth of various phase transitions.

There are several viscosity laws coded in the program, which can be selected by the `rheol` parameter. All available viscosity laws can be found in Appendix A.1.11. For `rheol=4`, the temperature dependence of the viscosity of each layer is determined by:

$$visc = visc0 \times exp\left(\frac{viscE + viscZ \times (1-r)}{T^* + viscT} - \frac{viscE + viscZ \times (1 - r_{inner})}{1 + viscT}\right) \qquad (6.1)$$

where $T^* = \min(\max(T, 0), 1)$. This equation is non-dimensionalized. The last term on the right-hand side normalizes the viscosity such that $visc = visc0$ when $T = 1$ and $r = r_{inner}$. Comparing Equation 6.1 with the dimensional Arrhenius activation equation:

$$
\begin{aligned}
\eta &= \eta_0 exp\left(\frac{E_a + PV_a}{RT}\right) = \eta_0 exp\left(\frac{E_a + PV_a}{R\Delta T\left(T' + T'_0\right)}\right) \\
&= \eta_0 exp\left(\frac{E_a + \rho g\left(1 - r\right)V_a}{R\Delta T\left(T' + T'_0\right)}\right) = \eta_0 exp\left(\frac{E_a/R\Delta T + \left(1 - r\right)\rho g V_a/R\Delta T}{T' + T'_0}\right)
\end{aligned} \qquad (6.2)
$$

where E_a and V_a are the activation energy and activation volume, P is the hydrostatic pressure, R is the universal gas constant, and other symbols are as defined in Section 1.5, it is clear that

$$viscE = \frac{E_a}{R\Delta T} \qquad (6.3)$$

$$viscZ = \frac{\rho g V_a}{R\Delta T} \qquad (6.4)$$

$$viscT = T_0 \qquad (6.5)$$

6.4.2.1 Example: Temperature-Dependent Viscosity, `cookbook3.cfg`

```
[CitcomS]
steps = 200                     ; number of time steps

[CitcomS.controller]
monitoringFrequency = 25    ; how often outputs are created

[CitcomS.solver]
datafile = cookbook3        ; prefix of output filenames
rayleigh = 1e6              ; Rayleigh number

# Modify the layout of the mesh.
[CitcomS.solver.mesher]
nprocx =   2
nprocy =   2
nodex  = 17
nodey  = 17
nodez  =  9
```

```
# Assign the viscosities.
[CitcomS.solver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
rheol = 4
viscE = 0.2,0.2,0.2,0.2
viscT = 0,0,0,0
viscZ = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0
```
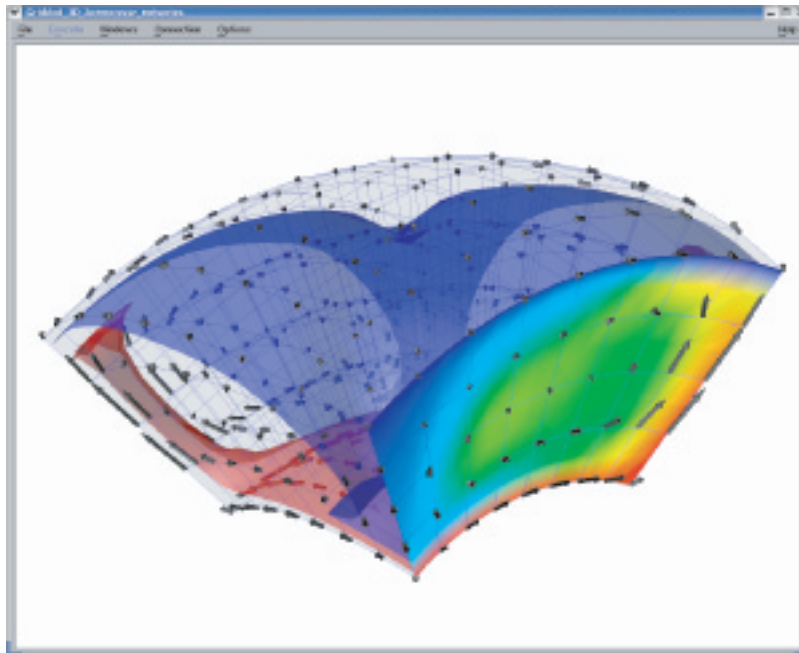

Figure 6.4: Cookbook 3: Temperature-Dependent Viscosity. This model, visualized with OpenDX, highlights a region that features both the heated upwelling (warm colors) and the even distribution of the velocities (arrows).

6.5 Cookbook 4: Regionally Refined Meshes

6.5.1 Problem

Frequently for convection problems, particularly those with variable viscosity, there are features with strong gradients in temperature or viscosity that can be better resolved with refined meshes. For example, for the problem just studied in Cookbook 3, temperature-dependent viscosity, a higher resolution is required for a narrow hot upwelling while a lower resolution is sufficient for the wider cold downwelling.

6.5.2 Solution

The parameter that controls whether a mesh is to be uniform or refined is `solver.mesher.coor`. Set it to 1 (`solver.mesher.coor=1`) in order to read the uneven mesh point coordinates from an input file (specified by `coor_file`). The format of the coordinate input file is described in Appendix B.2 on page 117.

```
coor = 1
coor_file = coor.dat
```

The computational domain is bounded in colatitude between radian 1 and 2, in latitude between radian 0 and 1, and in radius between 0.55 and 1, as determined by the content of `coor_file`.

6.5.2.1 Example: Regionally Refined Meshes, `cookbook4.cfg`

```
[CitcomS]
steps = 250                 ; number of time steps

[CitcomS.controller]
monitoringFrequency = 10    ; how often outputs are created

[CitcomS.solver]
rayleigh = 1e6              ; Rayleigh number
datafile = cookbook4        ; prefix of output filenames

[CitcomS.solver.ic]
num_perturbations = 1
perturbmag = 0.05
perturblayer = 10

# Perturb the initial temperature gradient in the longitudinal
# direction.
perturbl = 1
perturbm = 0

[CitcomS.solver.mesher]
# Read uneven mesh point coordinates from 'coor.dat'.
coor = 1
coor_file = coor.dat

nprocx = 2
nprocy = 1
nprocz = 1
nodex = 33
nodey = 17
nodez = 17
```

```
[CitcomS.solver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
rheol = 4
viscE = 0.2,0.2,0.2,0.2
viscT = 0,0,0,0
viscZ = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0
```
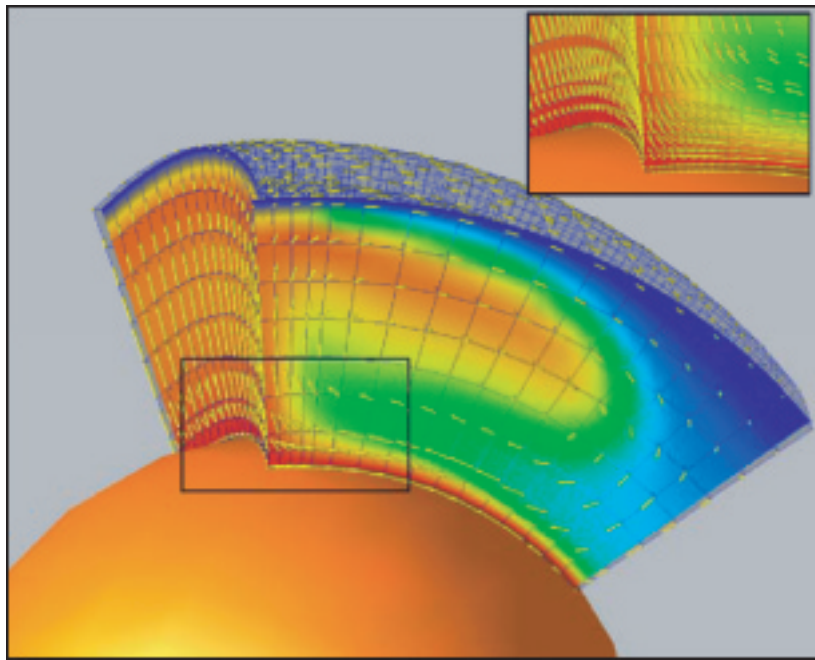

Figure 6.5: Cookbook 4: Regionally Refined Mesher. This model shows the temperature (upwelling – warm colors, downwelling – cool colors) and the uneven distribution of the velocities (yellow arrows). Note the refined mesh for the left and bottom regions of the model (inset).

6.5.3   Discussion

The resulting model is like a 2D model, but extends in the longitudinal direction. To set up this type of model, the initial temperature gradient was perturbed only in the longitudinal direction, by setting the parameters `perturbl=1` and `perturbm=0`. The model results show a thin thermal upwelling on one wall and a wide thermal downwelling on the opposite wall. Also, at the bottom of the model a thin layer of hot material can be shown. Note the higher resolution in the narrow regions with hot material and the lower resolution for the wide thermal downwelling region.

6.6 Cookbook 5: Subduction Models with Trench Rollback

6.6.1 Problem

A common issue to address is the problem arising when the position of the oceanic trench is not constant in time (trench rollback) for a subduction zone. In addition, the trench rollback speed may vary in time, which can be caused, for example, by a rotation pole jump.

6.6.2 Solution

In order to introduce in a convection model a trench rollback you have to prepare the velocity files. The following scenario is proposed for this cookbook: there are two plates centered along the equator, with two different Euler poles (see Figure 6.6). Initially, both plates have Euler poles situated far apart, so the velocities are approximately constant (about 5 cm/yr for the left plate and about 2 cm/yr for the right plate). After 30 Ma, a pole jump occurred for the right slab only, so the Euler pole moved closer.

Since we impose a top velocity boundary in our model, the following parameters should be turned on:

```
[CitcomS.solver.bc]
topvbc = 1

[CitcomS.solver.param]
file_vbcs = on
```

The following two lines specify the location of the velocity files and the starting age for the model:

```
start_age = 55
vel_bound_file = ./velocity/bvel.dat
```

Since the starting age is set to 55 Ma, there will be 57 velocity files, one for each Ma (`vel.dat0`, `vel.dat1`, `...vel.dat55`, `vel.dat56`). The format of the velocity file is described in Appendix B.3 on page 118. Note that the velocity file uses a unit of cm/yr.

When `tic_method=-1` is set, the initial temperature field is read from setup files. The files have the same naming scheme and format as the CitcomS velo output, as described in Appendix C.6.2 on page 122. The location and prefix of the file is specified in `datadir_old` and `datafile_old`, and the time step of the velo file in `solution_cycles_init`. In this example, a processor of MPI rank n will read file `./ic/cookbook5.velo.n.0`

```
[CitcomS.solver]
datadir_old = ./ic
datafile_old = cookbook5

[CitcomS.solver.ic]
tic_method = -1
solution_cycles_init = 0
```

The descending slab will cause some numerical instability in the temperature solver. To reduce the numerical instability, you will use a smaller time-step size (0.75 of the maximum time-step size for a stable solution). The change in maximum temperature will also be monitored. If the maximum temperature increases too much (> 5%) between time steps, the temperature solver will rerun with half time-step size.

```
[CitcomS.solver.tsolver]
finetunedt = 0.75
monitor_max_T = on
```
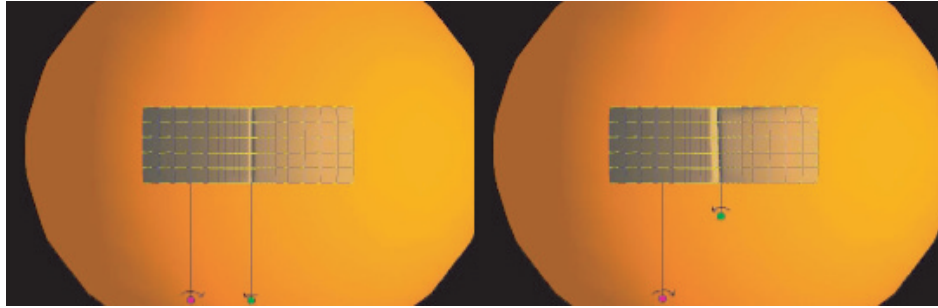
Figure 6.6: Cookbook 5: Left (A): Initially, both plates have Euler poles (magenta and green dots) situated far apart from the plate, so the velocities are approximately constant (about 5 cm/yr for the left plate and about 2 cm/yr for the right plate). Right (B): After 30 Ma a pole jump occurred for the right slab only, so the Euler pole moved closer.

6.6.2.1   Example: Subduction Models with Trench Rollback, `cookbook5.cfg`

```
[CitcomS]
steps = 1100                    ; number of time steps

[CitcomS.controller]
monitoringFrequency = 100   ; how often outputs are created

[CitcomS.solver]
datafile = cookbook5
datadir_old = ./ic
datafile_old = cookbook5
rayleigh = 4.07e+08

[CitcomS.solver.bc]
topvbc = 1

[CitcomS.solver.param]
file_vbcs = on
start_age = 55

# Since the starting age is set to 55 Ma, there will be 57 velocity
# files, one for each Ma (bvel.dat0, bvel.dat1, ... bvel.dat56).
vel_bound_file = ./velocity/bvel.dat

[CitcomS.solver.ic]
tic_method = -1
solution_cycles_init = 0

[CitcomS.solver.mesher]
coor = 1
coor_file = ./coor.dat
nprocx = 1
nprocy = 2
nprocz = 1
nodex = 17
nodey = 65
nodez = 33
```

```
[CitcomS.solver.tsolver]
finetunedt = 0.75
monitor_max_T = on

[CitcomS.solver.visc]
num_mat = 4
visc0 = 100,0.003,1,2
TDEPV = on
viscE = 24,24,24,24
viscT = 0.182,0.182,0.182,0.182
VMIN = on
visc_min = 0.01
VMAX = on
visc_max = 100.0
```
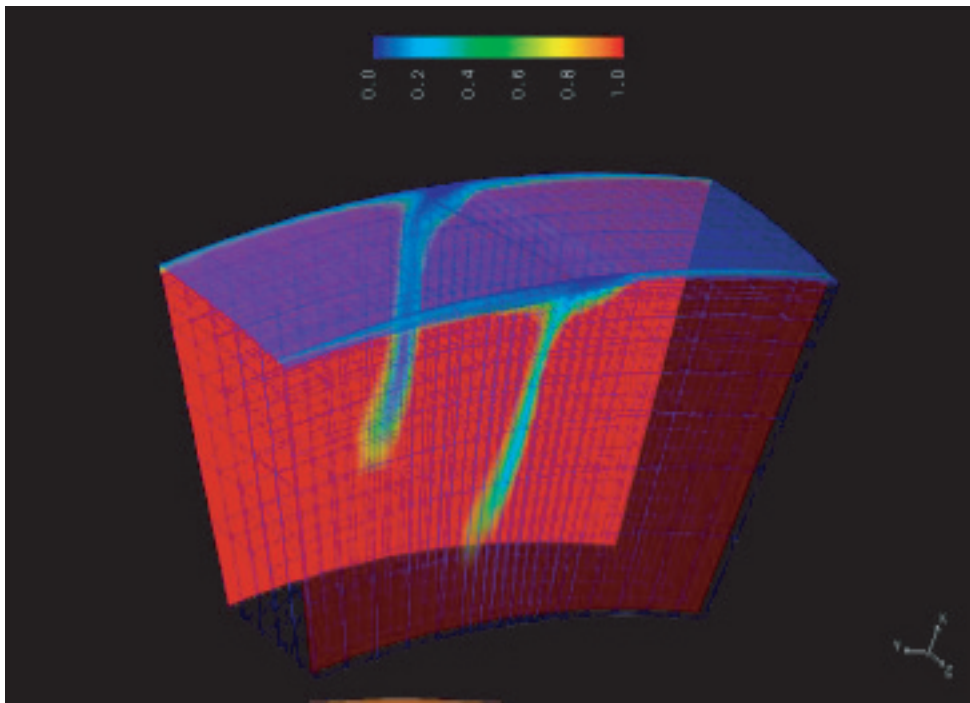

Figure 6.7: Cookbook 5: The pole jump after 30 Ma produced a flat slab on one side (fore side) and a steep slab on the other side (back side).

6.6.3 Discussion

The results for this problem are presented in Figure 6.7. Since the two Euler poles are kept fixed for the first 30 Ma, the shape of the subducting slab will be the same along the trench. At 25 Ma, the Euler pole for the right plate jumps toward the plate. Therefore, the velocity along the trench varies from about 1 cm/yr to about 2.5 cm/yr. This will produce in time a flat slab at one side of the model, and a steep slab at the other side.

6.7   Cookbook 6: Pseudo-Free-Surface Formulation

6.7.1   Problem

Free-slip boundary conditions are typically applied on the top surface of mantle convection models, and the dynamic topography is obtained by assuming that the normal stress on the top surface is instantaneously compensated by the deformed surface. This type of boundary condition works well for long-wavelength topography, but a free-surface formulation becomes necessary in cases where intermediate to short wavelength topography is of interest or the lithosphere has a very high effective viscosity. Another situation where free-surface formulation is desired is when two Pyre solvers, Snac and Citcom, are coupled.

The basic algorithm [16, 17] consists of four steps.

1. On the nodes of the top surface, compute the topography increment by integrating normal velocity over time.

2. Calculate the normal traction on the top surface based on the accumulated topography up to the current time step, and add it to the forcing term in Equation 1.31.

3. Update the velocity field with the changed forcing term.

4. If the velocity field has not converged yet, repeat steps 1 to 3.

6.7.2   Solution

To verify that the above algorithm works, you will run two different CitcomS models with each boundary condition (BC) (free-slip and pseudo-free-surface) and compare the topography computed accordingly. The scripts in `cookbook6.cfg` include the following parameters.

- Domain size: $45° \times 45° \times 1200\,\mathrm{km}$

- Mesh size: $61 \times 61 \times 25$ nodes with mesh refinement (`coor=1`)

- Boundary Conditions (BC): free-slip/free-surface for top; free-slip for all the other surfaces

- Initial Conditions (IC): spherical hot blob with diameter of $\frac{1}{4}$ of the radial dimension placed at the center of the domain

The pseudo-free-surface boundary condition is enabled by:

```
[CitcomS.solver.bc]
topvbc = 2
pseudo_free_surf = on
```

The time step size is fixed to 7.77×10^{-10} (about 1000 yrs), instead of determined dynamically by the velocity solution.

```
[CitcomS.solver.tsolver]
fixed_timestep = 7.77e-10
```

6.7.3   Discussion

The plots of the topography profile are consistent with results described in [16]. In the graphs in Figure 6.8, the solid lines indicate free-slip and the dashed lines indicate free-surface.
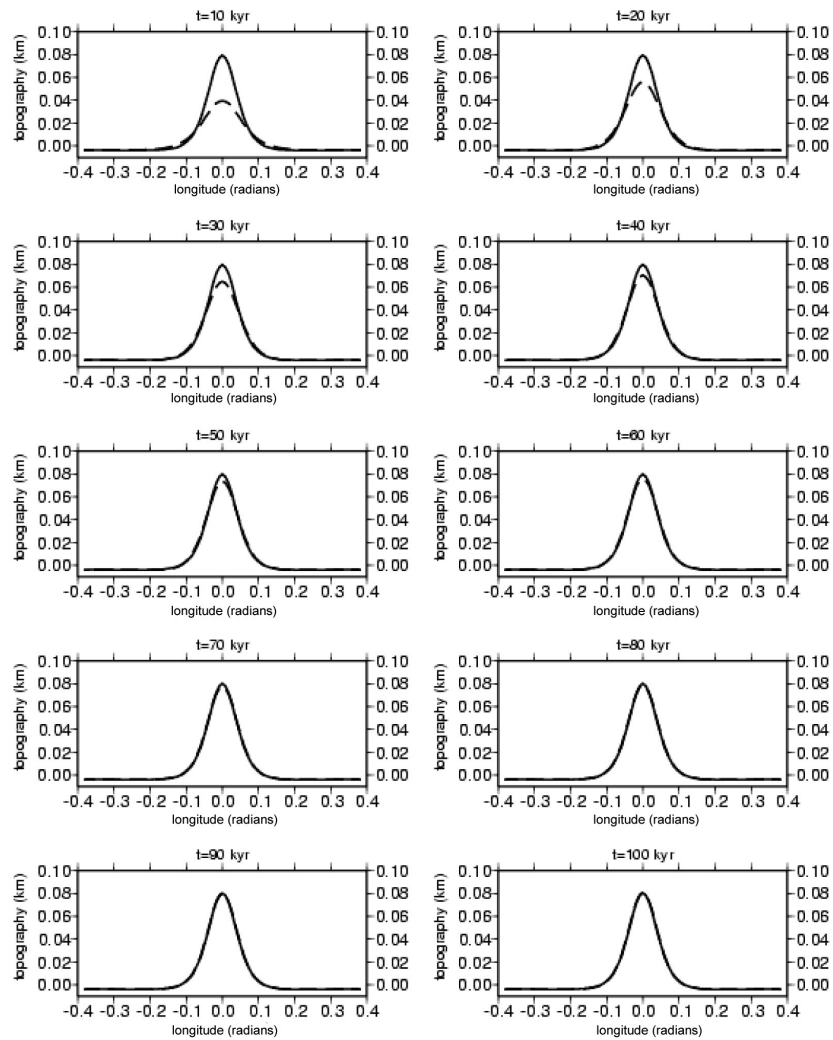
Figure 6.8: Cookbook 6: Graphs of topography profiles.

6.8   Cookbook 7: Thermo-Chemical Convection

6.8.1   Problem

This example solves for thermo-chemical convection within a full spherical shell domain. Composition heterogeneity exists in the Earth mantle. The density anomalies due to the composition heterogeneity, as well as due to the thermal heterogeneity, drive the convection flow.

6.8.2   Solution

You will use `cookbook7.cfg`. Most of the parameters you have encountered in previous cookbooks. The initial condition is the same as in Cookbook 1, and the viscosity law is the same as in Cookbook 3.

A large number of ASCII files will be output. In order to keep the current directory tidy, the output files can be put in a subdirectory `output/` by specifying

```
datadir = output
```

Since you are interested in the composition field, the compostion output should be enabled and some output files disabled:

```
output_optional = tracer,comp_nd
```

The most important parameters are in the `CitcomS.solver.tracer` section. Turn on the tracer module:

```
tracer = 1
```

The number of tracers and their initial location must be set. Here, you specify `tracer_ic_method=0`. The tracers will be generated pseudo-randomly, with a total number equal to

```
tracers_per_element×(total number of finite elements).
```

If `tracer_ic_method=1`, all processors will read the location (and flavors; see next paragraph) of the tracers from the same file specified by `tracer_file`. If `tracer_ic_method=2`, each processor will read the location (and flavors; see next paragraph) of the tracers from the file specified by `datafile_old` (in the `CitcomS.solver` section) and `solution_cycles_init` (in the `CitcomS.solver.ic` section).

```
tracer_ic_method = 0
tracers_per_element = 20
tracer_file = tracer.dat
```

Each tracer can have a "flavor" attached to it. The meaning of the flavor depends on the application. Here, the flavor indicates the chemical species of the tracer. There are two flavors of tracers (`tracer_flavors=2`). A tracer of flavor 0 is of the "normal," or ambient, chemical composition, while a tracer of flavor 1 is of the "anomalous" chemical composition. Because the tracers are automatically generated, you need to specify how to assign the flavor to each tracer. If `ic_method_for_flavors=0`, tracers above `z_interface` are assigned to flavor 0, and tracers below `z_interface` to flavor 1.

```
tracer_flavors = 2
ic_method_for_flavors = 0
z_interface = 0.7
```

The thermo-chemical convection module is turned on by

```
chemical_buoyancy = 1
```

The composition field is determined by the ratio method (`buoy_type=1`) [19]. The density anomaly of the anomalous chemical composition is defined by $B = \Delta\rho_{ch}/(\rho_0\alpha_0\Delta T)$, the buoyancy ratio.

```
buoy_type = 1
buoyancy_ratio = 0.5
```

The code keeps track of the sum of the bulk composition. In a perfect world, the sum of the bulk composition would not change with time. But due to numerical issues, the sum of the bulk composition tends to decrease with time. If `tracer_ic_method=2`, the code will read in the location of the tracers, as well as the initial sum of the bulk composition, from the previous run.

The regular grid is an auxiliary grid that helps locate the tracers [18]. The optimal grid spacing of the regular grid depends on the size of the CitcomS mesh. A general rule of thumb is that the grid spacing of the regular grid should be less than $18/(nodex \times nprocx)$. These parameters are used only in the full spherical version.

```
regular_grid_deltheta = 1.0
regular_grid_delphi = 1.0
```

If you encounter any error, look at the end of the tracer log files (`cookbook7.tracer_log.*`) for error messages.

You will use the conjugate gradient solver to solve the matrix equation $\mathbf{A}x = b$ for x. The conjugate gradient solver is more efficient than the multigrid solver (`Solver=multigrid`) for small problems (e.g., less than $17 \times 17 \times 17$ nodes per processor). The desired accuracy and maximum iterations are set by `accuracy` and `vlowstep`. For the Uzawa algorithm, the maximum iterations are set by `piterations`. Both `vlowstep` and `piterations` should be large integers, but you can experiment with a larger value for `accuracy` to speed up the computation.

```
Solver = cgrad
accuracy = 1e-03
vlowstep = 1000
piterations = 1000
```

6.8.2.1 Example: Thermo-Chemical Convection, `cookbook7.cfg`

```
[CitcomS]
solver = full
steps = 15                   ; number of time steps

[CitcomS.controller]
monitoringFrequency = 5      ; how often outputs are created

[CitcomS.solver]
datadir = output             ; path to output directory
datafile = cookbook7         ; prefix of output filenames
rayleigh = 1e7

[CitcomS.solver.ic]
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 5
perturbmag = 0.05

[CitcomS.solver.output]
output_optional = tracer,comp_nd

[CitcomS.solver.tracer]
tracer = on
tracer_ic_method = 0
tracers_per_element = 20
tracer_file = tracer.dat
```

```
tracer_flavors = 2
ic_method_for_flavors = 0
z_interface = 0.7

chemical_buoyancy = 1
buoy_type = 1
buoyancy_ratio = 0.5

regular_grid_deltheta = 1.0
regular_grid_delphi = 1.0

[CitcomS.solver.vsolver]
Solver = cgrad
accuracy = 1e-04
vlowstep = 1000
piterations = 1000

# Assign the viscosities.
[CitcomS.solver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
rheol = 4
viscE = 0.2,0.2,0.2,0.2
viscT = 0,0,0,0
viscZ = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0
```
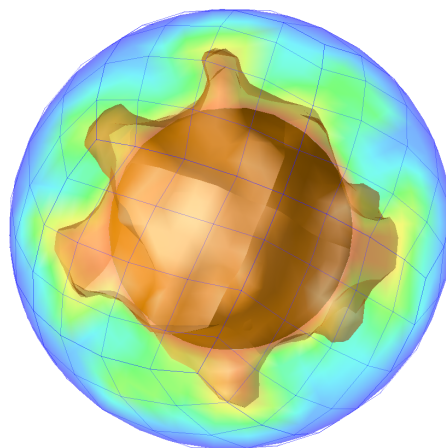

Figure 6.9: Cookbook 7: The composition and velocity field at the 15th step. The arrows are the velocity vectors. The composition field is shown in an isosurface of 0.7 and in a cross section.

6.8.3 Discussion

When the model is running, it will output the progress of the run to the screen. This line has information about the grid:

```
    Problem has 9 x 9 x 9 nodes per cap, 6930 nodes and 6144 elements in total
```

The following lines give the radial coordinate and reference density of each nodes and their viscosity layer:

```
        nz      radius      depth    rho              layer
         1    0.550000   0.450000 1.000000e+00        4
         2    0.606250   0.393750 1.000000e+00        4
         3    0.662500   0.337500 1.000000e+00        4
         4    0.718750   0.281250 1.000000e+00        4
         5    0.775000   0.225000 1.000000e+00        4
         6    0.831250   0.168750 1.000000e+00        4
         7    0.887500   0.112500 1.000000e+00        4
         8    0.943750   0.056250 1.000000e+00        2
         9    1.000000   0.000000 1.000000e+00        1
```

This line gives the perturbation parameters used to construct the initial temperature:

```
    Initial temperature perturbation:  layer=5  mag=0.05  l=3  m=2
```

This line gives the magnitude the right-hand side vector in Equation 1.31:

```
    Momentum equation force 2.207120371e+03
```

The following lines give the convergence progress of the Stokes solver, where `v` is the volume averaged norm of velocity, `p` is the volume averaged norm of pressure, `div/v` is the volume averaged norm of $\nabla \cdot (\bar{\rho}v)$ divided by `v`, `dv/v` is the volume averaged norm of velocity change divided by `v`, and `dp/p` is the volume averaged norm of pressure change divided by `p`. The convergence of the Stokes solver is achieved if either (1) `div/v` is less than `accuracy` or (2) both `dv/v` and `dp/p` are less than `accuracy` for two consecutive iterations. In this example, the second condition is met.

```
    (000)    7.0 s v=1.470010e+02 p=0.000000e+00 div/v=5.37e+00 dv/v=1.00e+00 dp/p=1.00e+00
    ⋮
    (090) 151.3 s v=1.012752e+02 p=1.304499e+04 div/v=5.54e-04 dv/v=1.84e-05 dp/p=9.20e-05
    (091) 151.8 s v=1.012752e+02 p=1.304512e+04 div/v=5.66e-04 dv/v=2.07e-05 dp/p=7.45e-05
```

This line gives the rotation angle and the angular coordinates of rotation pole of the removed net angular momentum:

```
    Angular momentum: rot=9.917258e-02 tr=8.924735e+01 fr=1.083630e+02
```

These lines give the heat flux across the top and bottom surfaces:

```
    surface heat flux= 2.227892
    bottom heat flux= 2.216542
```

The surface heat flux H_{surf} can be converted to the Nusselt number Nu_{surf} by:

$$Nu_{surf} = H_{surf} \times (r_{outer} - r_{inner}) \frac{r_{outer}}{r_{inner}} \tag{6.6}$$

The results for this problem are presented in Figure 6.9. The buoyancy ratio in this model is too low to stabilize the chemical layer. A few thermo-chemical plumes are rising from the lower mantle, especially the ones at the 4, 6, 9, 10, and 12 o'clock directions. The resolution of this model is fairly low. The composition isosurface is slightly discontinuous across the cap boundary. A model of higher resolution will not have this kind of artifact.

6.9   Cookbook 8: Compressible Steady-State Convection

6.9.1   Problem

This example is a benchmark problem for compressible thermal convection. The Stokes solver in CitcomS has been benchmarked and validated against a semi-analytical solution. However, no analytical solution exists for the benchmark on the energy equation solver, which is nonlinear. The steady-state solution is usually used for the comparison with other numerical solutions.

6.9.2   Solution

This cookbook example will run for 10,000 time steps to reach steady state. It will use 12 processors and take 1 to 2 days to finish on a modern computer. At every 1,000th time-step interval, a checkpoint for the internal state of the solver is saved.

```
checkpointFrequency = 1000
```

If the solver is interrupted before finishing the computation, one can resume the computation from the checkpointed state. To shorten the computation time, a checkpoint at the 9,000th time step (`CitcomS-cookbook8- restart.tar.gz`) is provided at CIG's CitcomS web page (`geodynamics.org/cig/software/packages/mc/citcoms`). (Note that the checkpoint files are produced by an x86 machine and may not be usable by other types of machines, e.g., PowerPC.) To resume the computation from the 9,000th time-step checkpoint, untar the package in the `examples/Cookbook8/` directory and set these parameters:

```
[CitcomS.solver.ic]
restart = on
solution_cycles_init = 9000
```

If you restart from the checkpoint, the computation will resume from the 9,000th time-step. Note that the `coord` files are only output at the 0th time-step, so you will need to run the model without restarting for one time-step to get the `coord` files.

A compressible convection model has four dimensionless numbers: the Rayleigh number, the dissipation number, the Gruneisen parameter $\gamma = \alpha_0 K_{S0}/\rho_0 c_{P0}$, and the non-dimensionalized absolute surface temperature, which are defined in Section 1.5. The Rayleigh number of CitcomS is scaled by the radius of the Earth. If scaled to the thickness of the mantle, the effective Rayleigh number is 7×10^3 ($= 7.68175583 \times 10^4 \times (r_{outer} - r_{inner})^3$). Similarily, the effective dissipation number is 0.275 ($= 0.5 \times (r_{outer} - r_{inner})$). Under these non-dimensional numbers, the convection is of low vigor and low compressibility.

```
rayleigh = 7.68175583e4
dissipation_number = 0.5
gruneisen = 1.25
surfaceT = 0.1
```

Since we are going to use the multigrid solver, the grid size is specified by:

```
nodex = 33
nodey = 33
nodez = 33
levels = 5
```

The additional parameter `levels` specifies the nested levels of multigrid units and is subjected to the following constraint:

$$\text{nodex} = 1 + \text{nprocx} \times \text{mgunitx} \times 2^{levels-1} \tag{6.7}$$

where `mgunitx` must be an integer. In the pure C version, `mgunitx` is an input parameter.

If `reference_state=1`, then constant gravity, heat capacity, thermal expansivity, and $\rho_r = exp\left(\frac{D_i}{\gamma}(1-r)\right)$ are used as the reference state. If `reference_state=0`, the reference state is read from a file `refstate_file`. See Appendix A for the file format.

```
reference_state = 1
refstate_file = ref.dat
```

We are interested in the geoid, dynamic topography, and heat flux. The dynamic topography and heat flux are computed on the surface grids. The geoid is computed in the spherical harmonics, with a maximal degree of 20.

```
output_optional = geoid,surf,botm
output_ll_max = 20
```

The initial temperature is a conductive profile with a single spherical harmonic perturbation. The perturbation is located at mid-depth and is defined as:

$$mag \times \sin\left(\frac{(r - r_{in})\pi}{r_{out} - r_{in}}\right) (\sin(m\phi) + \cos(m\phi)) P_{lm}(\cos\theta)$$

```
tic_method = 3
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 17
perturbmag = 0.01
```

You will need the output of dynamic topography and the geoid. The dynamics topography will be computed by the Consistent Boundary Flux (CBF) method, and the effect of self-gravitation is included in the geoid. The maximum spherical harmonics degree for the geoid is 20.

```
output_optional = geoid,surf,botm
use_cbf_topo = on
self_gravitation = on
output_ll_max = 20
```

Various parameters tune the performance of the solver. The maximum size of each time step is determined dynamically by the Courant criterion. To enhance the stability of the energy equation solver, you will only use three quarters of the maximum Courant time-step size.

```
finetunedt = 0.75
```

You will use the multigrid solver to solve the matrix equation $\mathbf{A}x = b$ for x. The multigrid solver is more efficient than the conjugate gradient solver (`Solver=cgrad`) for larger problems (e.g., more than $17 \times 17 \times 17$ nodes per processor). Several parameters control the behavior of the multigrid solver: `mg_cycle=1` for the V cycle and 2 for the W cycle; `down_heavy` and `up_heavy` are the number of smoothing cycles for downward/upward smoothing; `vlowstep` and `vhighstep` are the number of smoothing passes at lowest/highest levels; and `max_mg_cycles` is the maximum number of multigrid cycles per solve. All these parameters should be small integers.

```
Solver = multigrid
mg_cycle = 1
down_heavy = 2
up_heavy = 2
vlowstep = 20
vhighstep = 2
max_mg_cycles = 50
```

The following parameter turn on the pre-conditioner for the matrix equation solver (either multigrid or conjugate gradient).

```
precond = on
```

The stiffness matrix uses augmented Lagrangian formulation to improve the convergence for large viscosity variations [3]. These parameters specify whether to enable the formulation and how much weight to use for the formulation.

```
aug_lagr = on
aug_number = 2.0e3
```

The discrete Stokes equations 1.30 and 1.31 are solved using the Uzawa algorithm, which iteratively updates the pressure and velocity solutions. Three variations of the Uzawa algorithm are used in CitcomS, one for the incompressible case, and the other two for the compressible case. One parameter, `piterations,` common to the three variations, specifies the maximum number of iterations and the desired residual level for the continuity equation 1.30. Sometimes, larger value of `piterations` is required for convergence if complicated velocity boundary conditions are used.

```
piterations = 375
```

For the compressible case, two choices of the Uzawa algorithm are available. If `uzawa=cg`, the algorithm described in Equation 1.33 is used. In this case, an additional parameter controls the maximum number of outer iterations.

```
uzawa = cg
compress_iter_maxstep = 100
```

If `uzawa=bicg`, the algorithm described in Equation 1.34 is used, and no additional parameter is needed.

The overall accuracy of the velocity solver is controlled by a single parameter. The solver is converged if the residuals of Equation 1.30 and 1.31 both are smaller than `accuracy`, or if the changes in the velocity and pressure both are smaller than `accuracy` for the last two iterations.

```
accuracy = 0.001
```

Finally, the net angular momentum of the velocity solution is removed. The net angular momentum and rigid body rotation are unconstrained by the Stokes equations, if free-slip boundary conditions are used for the top and bottom boundaries in a full spherical model. That is, you can add an arbitrary amount of rotation to the velocity solution, and the resultant velocity is still a valid solution of the Stokes equations. Since no external torque is applied to the mantle in free-slip boundary conditions, the angular momentum must be constant in time. Enforcing the angular momentum to be zero by removing it from the velocity solution is often desirable.

```
remove_rigid_rotation = off
remove_angular_momentum = on
```

However, for models with imposed plate velocity, it is advisable to turn off both `remove_rigid_rotation` and `remove_angular_momentum`.

6.9.2.1   Example: Compressible Steady-State Convection, cookbook8.cfg

```
# Cookbook 8: Compressible Model and Checkpointing

[CitcomS]
solver = full
steps = 10000

[CitcomS.controller]
monitoringFrequency = 1000
checkpointFrequency = 1000

[CitcomS.solver]
datadir = output
datafile = cookbook8
datadir_old = restart
```

```
datafile_old = cookbook8

rayleigh = 7.68175583e4
dissipation_number = 0.5
gruneisen = 1.25
surfaceT = 0.1

[CitcomS.solver.mesher]
nodex = 33
nodey = 33
nodez = 33
levels = 5

coor = 1
coor_file = coord.dat

[CitcomS.solver.param]
reference_state = 1
refstate_file = ref.dat

[CitcomS.solver.output]
output_optional = geoid,surf,botm
use_cbf_topo = on
self_gravitation = on
output_ll_max = 20

[CitcomS.solver.ic]
tic_method = 3
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 17
perturbmag = 0.01

restart = off
solution_cycles_init = 9000

[CitcomS.solver.visc]
VISC_UPDATE = on
visc_smooth_method = 1

TDEPV = on
rheol = 1
num_mat = 4
viscE = 2.99573,2.99573,2.99573,2.99573
viscT = 0.5,0.5,0.5,0.5
visc0 = 1,1,1,1

VMIN = on
visc_min = 0.001
VMAX = on
visc_max = 1e+06

[CitcomS.solver.tsolver]
```

```
finetunedt = 0.75

[CitcomS.solver.vsolver]
uzawa = cg
Solver = multigrid
mg_cycle = 1
down_heavy = 2
up_heavy = 2
vlowstep = 20
vhighstep = 2
max_mg_cycles = 50

aug_lagr = on
aug_number = 2.0e3
precond = on

piterations = 375
accuracy = 0.001
compress_iter_maxstep = 100

remove_rigid_rotation = off
remove_angular_momentum = on
```

6.9.3   Discussion

The results for this problem are presented in Figure 6.10. A tetrahedral symmetric pattern is developed for the convection. The surface heat flux H_{surf} at the steady state is 3.892, and the bottom heat flux H_{botm} is 12.817. The heat flux imbalance ($H_{botm}r_{inner}^2/H_{surf}r_{outer}^2 - 1$) is -0.38%. The Nussult number, converted from the surface heat flux by Equation 6.6, is 3.182. The total viscous heating is 7.68991, and the total adiabatic cooling is 7.71719. Under a steady state, these two terms should be exactly balanced.

   The geoid is output as spherical harmonic coefficients. A post-processing program is provided to project the geoid coefficients to a regular (longitude, latitude) grid. To use a regular grid of 1° spacing, run this command:

```
$ visual/project_geoid cookbook8.geoid.0.10000 geoid.xyz 361 181
```

It will generate a file geoid.xyz. There are 3 columns in the file, which are (longitude, latitude, geoid). The geoid is in a unit of meters. Several dimensional constants are required for the geoid computation. These constants have sensible default values (in SI units) for the Earth. Note that the temperature drop from the core-mantle boundary to the surface (ΔT in Equation 1.16) is derived from these constants and the Rayleigh number.

```
[CitcomS.solver.const]
radius=6.371e+06
density=3340
thermdiff=1e-06
gravacc=9.81
thermexp=3e-05
refvisc=1e+21
cp=1200
density_above=1030
density_below=6600
```
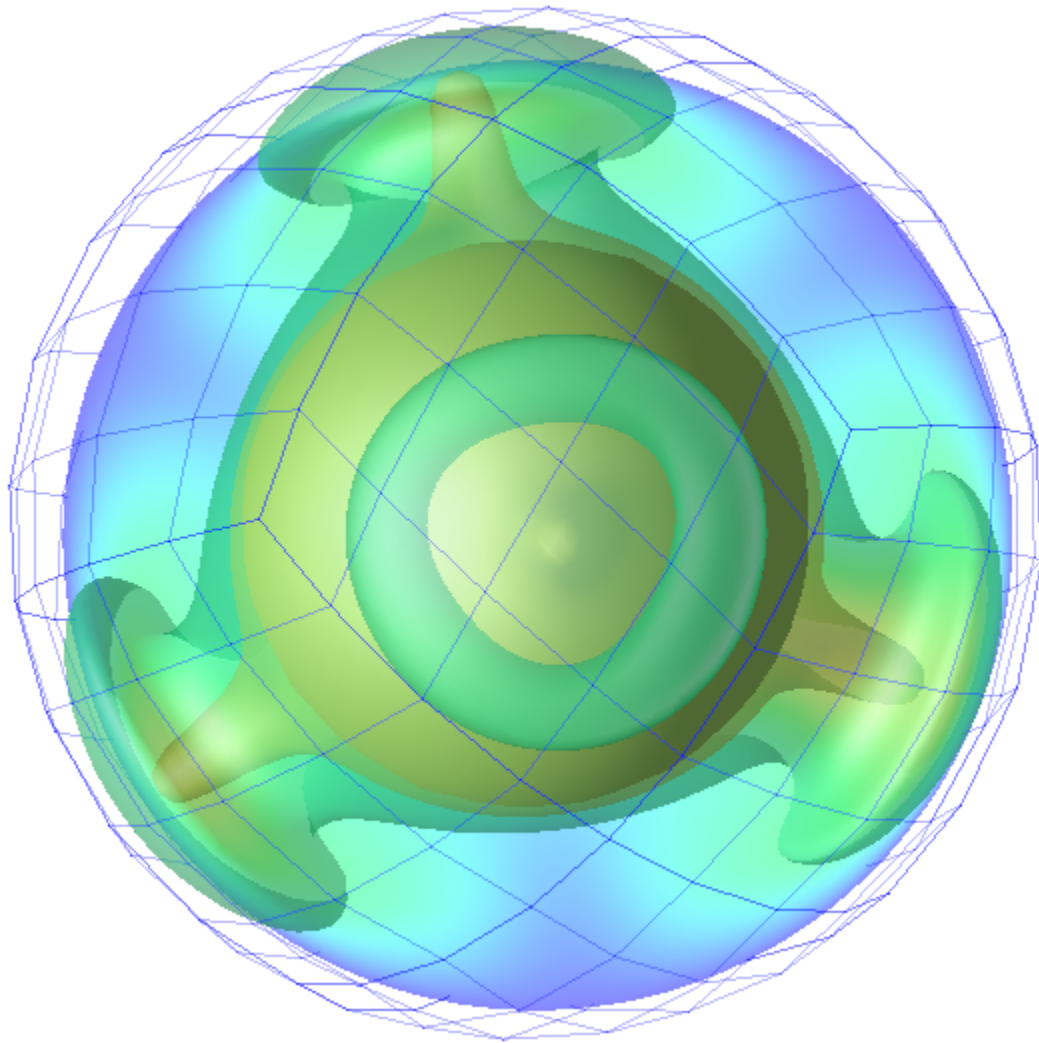
Figure 6.10: Cookbook 8: The steady state temperature field at the 10,000th time step. A tetrahedral symmetric convection pattern is developed. Two temperature isosurfaces of 0.4 and 0.8 are shown.

6.10   Cookbook 9: Nested Solver Coupling for Ridge-Plume Interaction

To run this cookbook, you need to install the Exchanger package. See Section 2.7 on page 32 for installation instructions.

6.10.1   Problem

In order to model the interaction between a segment of a mid-ocean ridge and a plume, a small grid spacing is required to resolve the thin plume conduit and the flow near the ridge. In addition, the plume must be placed sufficiently away from the sidewalls to avoid possible boundary effects. Satisfying both of these requirements in a model entails a long computation time. Using solver coupling, a high-resolution model with a smaller domain can be nested within a low-resolution model, and the computation time significantly reduced.

6.10.2   Solution

You will use two solvers in the model. A special command-line option is required for a coupled model. Type the following command to run this cookbook example:

```
$ citcoms --coupled cookbook9.cfg
```

The embedded solver (esolver) is nested within the domain of the containing solver (csolver). The velocity boundary conditions of the esolver are fixed normal velocity and shear stress, whose values are received from the esolver. The containing solver can be either a full CitcomS solver or a regional one. The embedded solver can only be a regional one. Both solvers are instances of a regional CitcomS solver in the cookbook example.

```
csolver = regional      ; containing solver
esolver = regional      ; embedded solver
```

You will use four processors for this model. Each solver will use two processors. The rank-0 and rank-1 processors will be assigned to the csolver, and the rank-2 and rank-3 processors will be assigned to the esolver.

```
[CitcomS.layout]
containing_group = [0-1]
embedded_group = [2-3]
```

The procedure for the nested solver coupling is described elsewhere [15] and only briefly described below:

1. The containing solver solves the velocity and computes its time-step size dt_c.

2. The containing solver interpolates the velocity, stress and temperature onto the boundary of the embedded model.

3. The embedded model solves the velocity and temperature, using the boundary conditions from step 2, with a time-step size dt_e; dt_e is always smaller than dt_c.

4. Step 3 is repeated until the sum of dt_e is equal to dt_c.

5. Optionally (if `two_way_communication` is on), the containing solver updates its temperature according to the embedded solver's temperature.

6. The containing solver solves the temperature with a time-step size dt_c.

7. The entire process repeats beginning at step 1.

The two solver processes are separated and only communicate through the couplers, which in turn use the exchanger package to pass messages. The containing coupler and controller (ccoupler and ccontroller) are associated with the csolver, and the embedded coupler and controller (ecoupler and econtroller) with the esolver. Each solver will track its own number of time steps. The esolver has a smaller time-step size and, hence, a larger number of time steps. The model will finish when either of the solvers reaches the 200th time step. The csolver will output for every 2 steps and the esolver for every 10 steps. Additional output will occur when the embedded solver is at procedure 4 above.

```
[CitcomS]
steps = 200

[CitcomS.ccontroller]
monitoringFrequency = 2

[CitcomS.econtroller]
monitoringFrequency = 10
```

A few parameters must be identical for the ccoupler and ecoupler. You will use two-way communication, which enables the ecoupler to send temperature information to the ccoupler. Otherwise the communication is one way, ccoupler to ecoupler only, and the csolver is not affected by the esolver.

```
two_way_communication = on
```

There is an option to exchange initial temperature, which could ensure that the initial temperature field of both solvers is consistent. The initial temperature field is read from velo files, which already contain consistent temperature fields and don't need to exchange that information again.

```
exchange_initial_temperature = off
```

A good initial guess of pressure field can speed up the convergence of the iterative Stokes solver. We will use the pressure solution of the containing solver as the initial guess of pressure of the embedded solver.

```
exchange_pressure = on
```

Three additional parameters are for the ecoupler only. The following two parameters specify whether the top and bottom boundary of the esolver will be imposed with the velocity and temperature from the csolver. For models with prescribed top or bottom boundary conditions, you can turn on these two parameters:

```
exclude_top = off
exclude_bottom = off
```

The next parameter deserves a little more explanation. The continuity equation 1.1 can be rearranged according to Gauss's divergence theorem to become:

$$\oint_{surface\ area} \rho_0 \vec{u} \cdot \vec{n} dA = 0 \tag{6.8}$$

This equation requires that the normal velocity $\vec{u}$ imposed on the embedded solver must have zero outflow. Due to finite accuracy of the containing solver and the interpolation process, the normal velocity received by the embedded solver might not have zero outflow, which could cause a convergence problem in the embedded solver. One can amend the received normal velocity slightly to satisfy Equation 6.8 by setting:

```
amending_outflow = on
```

Without turning on side_sbcs, the model will fail to run.

```
[CitcomS.esolver.bc]
side_sbcs = on
```

Plate motion is imposed on top of the esolver, which has a mid-ocean ridge with a 5 cm/yr half-spreading rate. A transform fault cuts through the ridge. Setting start_age to 0, the plate motion is read from the file velocity/bvel.dat0 and will be constant in time.

```
[CitcomS.csolver.bc]
topvbc = 1

[CitcomS.csolver.param]
file_vbcs = on
vel_bound_file = velocity/bvel.dat
start_age = 0
```

The domain of the csolver is bigger than that of the esolver. The radial dimension of the esolver will shrink slightly
with respect to the csolver so that the domain of the esolver is completely inside the domain of the csolver. The radial
coordinates of the csolver is refined near the top and bottom boundaries (coor=2), with the lower 10% of the mesh
divided by 15% of the nodes, the upper 10% of the mesh divided by 20% of the nodes, and the remaining 80% of the
mesh divided by 75% of the nodes.

   Therefore, when setting the values of coor_refine (see below), be careful not to set the first or third value (in
example below, 0.1) too low, or the second or fourth value (in example below, 0.15 and 0.2) too high. This can
cause the mesh size to change too rapidly across an element, which will generate pronounced numerical artifacts in
the temperature solver.

```
[CitcomS.csolver.mesher]
nprocz = 2
nodex = 17
nodey = 17
nodez = 25
radius_outer = 1.0
radius_inner = 0.55
theta_min = 1.171
theta_max = 1.971
fi_min = 0
fi_max = 0.8
coor = 2
coor_refine = 0.1,0.15,0.1,0.2

[CitcomS.esolver.mesher]
nprocz = 2
nodex = 21
nodey = 21
nodez = 49
radius_outer = 0.999
radius_inner = 0.551
theta_min = 1.421
theta_max = 1.721
fi_min = 0.25
fi_max = 0.55
```

The temperature solver has several parameters to tune its behavior. The temperature solver is turned on (ADV). A
Lenardic-type filter, which removes numerical artifacts while keeping total energy conserved, is disabled (filter_temp).
The maximum temperature can be monitored between time steps (monitor_max_T). If the maximum temperature
increases too much (> 5%) between time steps, the temperature solver will rerun with half time-step size. The time-step
size is usually determined dynamically according to Courant criterion and is reduced by a fraction (finetunedt) to
improve accuracy. The time-step size can also be specified statically in fixed_timestep, if fixed_timestep
is non-zero. The temperature solver uses an explicit predictor-corrector algorithm. Using 0.5 for the predictor
(adv_gamma) and 2 iterations for the corrector (adv_sub_iterations), this algorithm is second-order accu-
rate.

```
ADV = on
```

```
filter_temp = off
monitor_max_T = off
finetunedt = 0.9
fixed_timestep = 0
adv_gamma = 0.5
adv_sub_iterations = 2
```

The purpose of the csolver is to provide the proper boundary condition for the esolver, and we don't need high accuracy for that. So we will use low accuracy for the csolver and moderate accuracy for the esolver.

```
[CitcomS.csolver.vsolver]
accuracy = 2e-2

[CitcomS.esolver.vsolver]
accuracy = 1e-3
```

6.10.2.1 Example: Nested Solver Coupling for Ridge-Plume Interaction, cookbook9.cfg

```
# Cookbook 9: Nested Solver Coupling for Ridge-Plume Interaction

[CitcomS]
steps = 200
csolver = regional       ; containing solver
esolver = regional       ; embedded solver

[CitcomS.ccoupler]
two_way_communication = on
exchange_initial_temperature = off
exchange_pressure = on

[CitcomS.ecoupler]
two_way_communication = on
exchange_initial_temperature = off
exchange_pressure = on
amending_outflow = on
exclude_top = off
exclude_bottom = off

# assigning processors to csolver and esolver
[CitcomS.layout]
containing_group = [0-1]
embedded_group = [2-3]

[CitcomS.ccontroller]
monitoringFrequency = 2

[CitcomS.econtroller]
monitoringFrequency = 10

[CitcomS.csolver]
datadir_old = ic
datafile_old = cntn
datadir = output
datafile = cntn
rayleigh = 1e8
```

```
[CitcomS.csolver.mesher]
nprocz = 2
nodex = 17
nodey = 17
nodez = 25
radius_outer = 1.0
radius_inner = 0.55
theta_min = 1.171
theta_max = 1.971
fi_min = 0
fi_max = 0.8
coor = 2
coor_refine = 0.1,0.15,0.1,0.2

[CitcomS.csolver.bc]
topvbc = 1

[CitcomS.csolver.param]
file_vbcs = on
vel_bound_file = velocity/bvel.dat
start_age = 0

[CitcomS.csolver.ic]
tic_method = -1
solution_cycles_init = 0

[CitcomS.csolver.tsolver]
ADV = on
filter_temp = off
monitor_max_T = off
finetunedt = 0.9
fixed_timestep = 0
adv_gamma = 0.5
adv_sub_iterations = 2

[CitcomS.csolver.vsolver]
accuracy = 2e-2

[CitcomS.csolver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
viscE = 1.6,1.6,1.6,1.6
viscT = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0

##############################################

[CitcomS.esolver]
```

```
datadir_old = ic
datafile_old = embd
datadir = output
datafile = embd
rayleigh = 1e8

[CitcomS.esolver.mesher]
nprocz = 2
nodex = 21
nodey = 21
nodez = 49
radius_outer = 0.999
radius_inner = 0.551
theta_min = 1.421
theta_max = 1.721
fi_min = 0.25
fi_max = 0.55

[CitcomS.esolver.ic]
tic_method = -1
solution_cycles_init = 0

[CitcomS.esolver.vsolver]
accuracy = 1e-3

[CitcomS.esolver.tsolver]
ADV = on
filter_temp = off
monitor_max_T = off
finetunedt = 0.9
fixed_timestep = 0
adv_gamma = 0.5
adv_sub_iterations = 2

[CitcomS.esolver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
viscE = 1.6,1.6,1.6,1.6
viscT = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0

[CitcomS.esolver.bc]
side_sbcs = on
```

6.10.3 Discussion

The solution of this problem is presented in Figure 6.11. The plume head spreads below the lithosphere, and the plume conduit is elongated in the ridge-parallel direction. The lithosphere subducts at the left and right edges of the csolver. If the domain of the csolver were bigger, the plume would be further away from the subducted slabs.
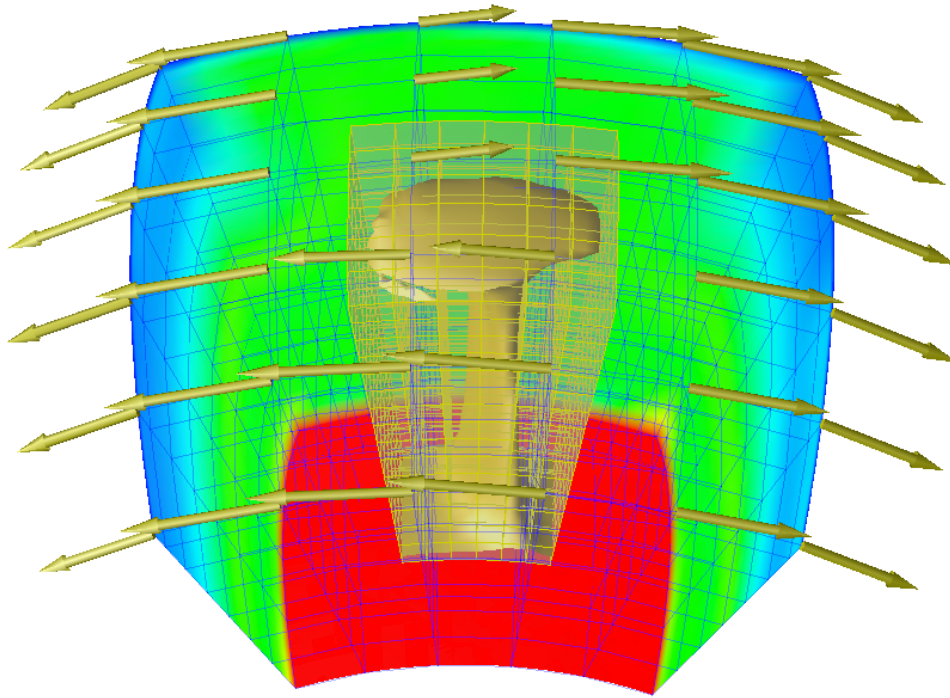
Figure 6.11: Cookbook 9: The plume head spreads below the lithosphere, and the plume conduit is elongated in the ridge-parallel direction. The temperature isosurface is at 0.8. The grid spacings of both meshes are reduced approximately threefold for better visualization.

6.11 Cookbook 10: Synthetic Seismograms from Mantle Convection Models

6.11.1 Problem

This example is a step-up of Cookbook 6.9, thermo-chemical convection within a full spherical shell domain. Composition heterogeneity exists in the Earth mantle. The density anomalies due to the composition heterogeneity, as well as due to the thermal heterogeneity, drive the convection flow. The same composition heterogeneity causes seismic velocity anomalies. The goal is to convert the mantle convection models, with the aid of a mineral physics model, to seismic anomalies, and then generate synthetic seismograms using SPECFEM3D_GLOBE.

6.11.2 Solution

This cookbook uses CitcomS and SPECFEM3D_GLOBE. SPECFEM3D_GLOBE is a spectral element code to simulate seismic wave propagation in the global scale. To use SPECFEM3D_GLOBE, you can either download the code from this link (`geodynamics.org/cig/software/packages/seismo/specfem3d-globe/`) and install it on your machine, which requires a Fortran 90 compiler and a cluster, or you can go to CIG Seismology Web Portal (`https://crust.geodynamics.org/portals/seismo/`) to launch a job, which only requires a browser. We will use the later approach in the cookbook.

6.11.2.1 Running CitcomS

Most of the parameters are copied from Cookbook 6.9. We will highlight a few differences. We use a higher Rayleigh number.

```
rayleigh = 1e9
```

The radius of the bottom surface is set to 0.546 in the cookbook, which must be smaller than the CMB radius in SPECFEM3D_GLOBE. (If PREM is used as the 1D reference model in SPECFEM3D_GLOBE, the CMB radius is 0.5462.)

```
radius_inner = 0.546
```

We convert the temperature and composition fields to seismic velocities using a mineral phyiscs model. Currently, there is only one model implemented, based on the model of *Trampert, Vacher, and Vlaar*[20]. In their paper, the (depth dependent) temperature and composition derivatives of seismic velocities are given as polynomial coefficients. Note that the paper has its own reference profile, and is only valid between 1000 km < depth < 2600 km. We will extend the model to whole mantle and use PREM as the reference profile. This clearly is over-stretching the model, but we are using it for demonstration purposes.

```
mineral_physics_model = 3
```

We will output the converted density and seismic velocities for SPECFEM3D_GLOBE consumption. This option enables the binary seismic output (`*.seismic.*` files), as well as other binary output (`*.domain` and `*.coord_bin.*` files) that SPECFEM3D_GLOBE will read. The formats of these binary files are provided in Appendix C.8.

```
output_optional = tracer, comp_nd, seismic
```

6.11.2.2 Example: Synthetic Seismograms from Mantle Convection Model, cookbook10.cfg

```
# Cookbook 10: Synthetic Seismograms from Mantle Convection Models
[CitcomS]
solver = full
steps = 15

[CitcomS.controller]
monitoringFrequency = 5
```

```
[CitcomS.solver]
datadir = output
datafile = cookbook10
rayleigh = 1e9

[CitcomS.solver.mesher]
radius_inner = 0.546

[CitcomS.solver.ic]
num_perturbations = 1
perturbl = 3
perturbm = 2
perturblayer = 5
perturbmag = 0.05

[CitcomS.solver.output]
output_optional = tracer,comp_nd,seismic

[CitcomS.solver.param]
mineral_physics_model = 3

[CitcomS.solver.tracer]
tracer = on
tracer_ic_method = 0
tracers_per_element = 20
tracer_file = tracer.dat

tracer_flavors = 2
ic_method_for_flavors = 0
z_interface = 0.7

chemical_buoyancy = 1
buoy_type = 1
buoyancy_ratio = 0.5

regular_grid_deltheta = 1.0
regular_grid_delphi = 1.0

[CitcomS.solver.vsolver]
Solver = cgrad
accuracy = 1e-04
vlowstep = 1000
piterations = 1000

# Assign the viscosities.
[CitcomS.solver.visc]
VISC_UPDATE = on
num_mat = 4
visc0 = 1,1,1,1
TDEPV = on
rheol = 4
viscE = 0.2,0.2,0.2,0.2
viscT = 0,0,0,0
```

```
viscZ = 0,0,0,0
VMIN = on
visc_min = 1.0
VMAX = on
visc_max = 100.0
```

6.11.2.3   Running SPECFEM3D_GLOBE from CIG Seismology Web Portal

Using your favorite browser, go to the CIG Seismology Web Portal (`https://crust.geodynamics.org/portals/seismo/`). Free registration is required to use the portal. Your initial account has 10,000 SUs (CPU-hours) allocated. A short (20 minutes of seismograms), low-resolution SPECFEM3D_GLOBE run consumes about 450 SUs. A short, high-resolution SPECFEM3D_GLOBE run consumes about 1,000 SUs. Further SUs can be allocated upon request.

After you login to the portal, take a few minutes to read the instructions and familiarize yourself with the interface. You will see a toolbar with big icons on the top and several grayed-out tabs below the toolbar. The toolbar allows you to specify the earthquake source (`Events`), the receivers (`Stations`), and simulation parameters (`3D Parameters`), including the resolution (`Mesh`) and the seismic velocity model for the crust and mantle (`3D Models`). In the cookbook, we will upload the result of CitcomS as a 3D Model and upload our own fictitious stations and event.
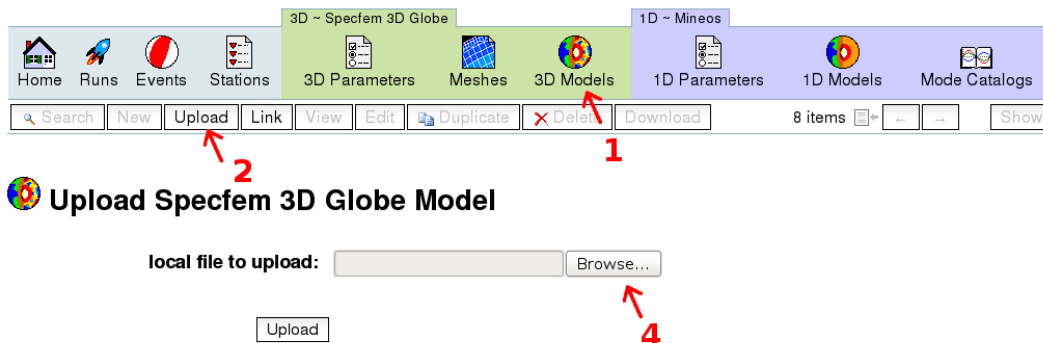
Click on the `3D Models` icon (1), and the `Upload` tab (2), then click on the link `citcoms_isotropic_no_crust.tgz` (3) to download the tar file to your machine. The tar file you just downloaded contains the code that reads CitcomS output and feeds the seismic velocities to SPECFEM3D_GLOBE. However, the tarball does not contains the actual CitcomS output, which will be provided by you later. As you might have guessed from the filename, the code will generate an isotropic mantle without an overlay of a 3D crust, such as the CRUST2.0 model. The 3D crust model obeys the continent-ocean distribution of current Earth. Since our CitcomS model has no notation on where is the Pacific and where is Asia, we do not want to impose a 3D crust model. You can untar the file by running:

```
$ gunzip -c citcoms_isotropic_no_crust.tgz | tar xf -
```

You will supply the CitcomS output to the code. Copy these CitcomS output files `cookbook.domain`, `cookbook.coord_bin.*`, and `cookbook.seismic.*.15` to the directory `citcoms_isotropic_no_crust/shared/`, so that the content of the directory looks like:

```
$ ls citcoms_isotropic_no_crust/shared/
cookbook10.coord_bin.0    cookbook10.seismic.0.15
cookbook10.coord_bin.1    cookbook10.seismic.10.15
cookbook10.coord_bin.10   cookbook10.seismic.11.15
cookbook10.coord_bin.11   cookbook10.seismic.1.15
cookbook10.coord_bin.2    cookbook10.seismic.2.15
cookbook10.coord_bin.3    cookbook10.seismic.3.15
cookbook10.coord_bin.4    cookbook10.seismic.4.15
cookbook10.coord_bin.5    cookbook10.seismic.5.15
cookbook10.coord_bin.6    cookbook10.seismic.6.15
cookbook10.coord_bin.7    cookbook10.seismic.7.15
cookbook10.coord_bin.8    cookbook10.seismic.8.15
cookbook10.coord_bin.9    cookbook10.seismic.9.15
cookbook10.domain
```

These files contain the coordinate, density, and seismic velocities data. We will need to tell SPECFEM3D_GLOBE where to find the CitcomS output. Edit the header file `citcoms_isotropic_no_crust/citcoms_parm.h` to become:

```
/* filename prefix of citcoms output */
const char citcoms_model_filename_base[] = "@THIS_DIR@/shared/cookbook10";
/* time step of citcoms output */
const int citcoms_step = 15;
```

The portal has a few conventions on where to put the data. First, the magic string `@THIS_DIR@` will be replaced by the absolute path when the tar file is expanded by the portal. Second, the tar file will be distributed to all computer nodes when portal launches the job. Third, the subdirectory `shared/` is special such that files in this directory will not be distributed to all computer nodes. Data files of huge size should be put in this directory. You might want to edit `citcoms_isotropic_no_crust/description.txt` to provide a description of your model. The text in this file will be displayed on the portal. The final step before uploading is to create a new tar file containing the code and data.

```
$ tar cf cookbook10.tar citcoms_isotropic_no_crust/
$ gzip cookbook10.tar
```

Now, you can upload the data by clicking on the `Browse` button (4), choosing `cookbook10.tar.gz` from the resulting dialog box, then clicking on the `Upload` button. After the portal confirms that the upload is successful, click on the `3D Models` icon again; you will see `cookbook10` is among the available 3D models.
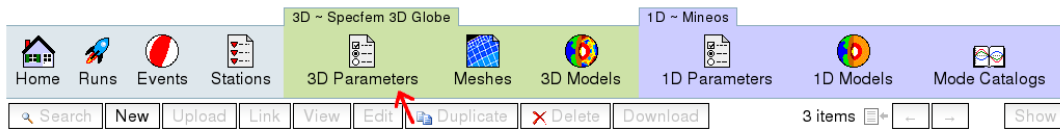
New Specfem 3D Globe Parameters

name: cookbook10

mesh: Global 27s Nex=160

model: cookbook10

☐ oceans
☑ gravity
☑ attenuation
☐ topography
☑ rotation
☐ ellipticity

Save

You have to select a few parameters for a SPECFEM3D_GLOBE run. Click on the `3D Parameters` icon (5), the `New` tab (6), select the parameters as shown in the figure above, and save the parameters for later use. We will use a global mesh that is capable of resolving seismic waves of 27 second period. Since CitcomS mesh is a perfect sphere, you need to disable `topography` and `ellipticity` to have a matching mesh in SPECFEM3D_GLOBE. The `oceans` is disabled because we don't have a 3D crust.

We will provide our own fictitious earthquake source and seismic stations. The earthquake source is defined in `cmt-solution.cookbook10` in the cookbook directory. The source is located at 15 km depth of 0°N, 0°E. The half duration of the source is 0 second, which means a step function is used. Click on the `Events` icon and the `upload` tab to upload the file `cmt-solution.cookbook10`. The stations are defined in `stations.cookbook10` in the cookbook directory. The stations are on the Equator and are 70 to 100 degrees away from the source. Click on the `Stations` icon and the `upload` tab to upload the file `stations.cookbook10`.

New Run

event: my-cmt-solution

station list: my-stations

parameters: cookbook10

record length: 30.0 minutes

Save

Finally, we are ready to launch a SPECFEM3D_GLOBE simulation. Click on the `Runs` icon (7), then the `New` tab (8), and select our recently uploaded event, stations and parameters. Set the record length to 30 minutes, which will give us synthetic seismograms of 30 minutes. Click the `Save` button to save the settings.

You will be presented with a summary of the simulation settings, including a map showing the location of the events and stations. After you have reviewed all settings, scroll to the bottom of the page. Click on the `Start` button. The request for the simulation is sent to the TeraGrid supercomputing center. Your simulation will be waiting in the queue and will be launched within several hours. You can log off the portal for now.

When your simulation is finished, the portal will send you an e-mail notification. Log in to the portal, click on the `Runs` icon, where there is a list of finished and unfinished runs. Click on the finished run, and you will see a list of output. Click on the `specfem3dglobe.tar.gz` link to download the tar file. Expand the file:

```
$ gunzip -c specfem3dglobe.tar.gz | tar xf -
```

You will find the synthetic seismograms `*.sem.sac` in the directory `OUTPUT_FILES/`.

6.11.3   Discussion

The dimensional value of total temperature contrast across the mantle is derived from the Rayleigh number in Equation 1.25 and the dimensional parameters in the `[CitcomS.solver.const]` section. In the very beginning of the simulation, the total temperature contrast across the mantle is displayed on the screen. This value will be used to scale the non-dimensional temperature when converting the temperature anomaly to seismic velocities.

```
Total temperature contrast = 3934.055176 K
```

The event and stations are all on the equatorial plane. Figure 6.12 shows the temperature field of the equatorial slice. A large warm upwelling is beneath 60°E. We should be able to observe its effect on delaying teleseismic waves in the 70° to 90° range.
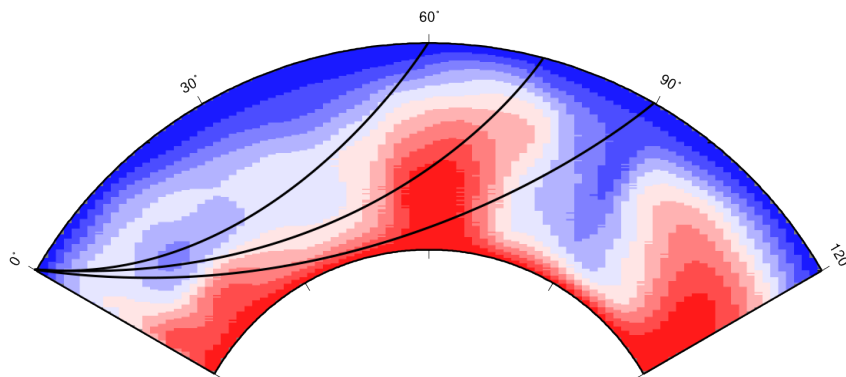
Figure 6.12: The equatorial slice of temperature from the CitcomS result. Three S wave paths probing the mantle are shown.

The synthetic seismograms need to be post-processed. The post-processing programs we will use can be downloaded from the portal. Follow the instructions on the portal to build the programs. We will band-pass filter within the period of 30 and 500 seconds, and convolve the synthetics with a gaussian source time function of 50 seconds half duration, and append `conv` to the output filenames.

```
$ process_syn.pl -S -t 30/500 -h 50 -x conv *.sac
```

Optionally, you can rotate the synthetics from East-North components to Transversal-Radial components.

```
$ rotate.pl *LHE*.conv
```

Part III

Appendices

Appendix A

Input Parameters for CitcomS

A.1 Input Parameters Grouped by Functionality

This section explains the meaning of the input parameters for CitcomS. These parameters are grouped by their functionality. Parameters are given with their default values.

A.1.1 Parameters that Control Input Files

`reference_state=1` `refstate_file="refstate.dat"`	If `reference_state` is set to `1`, a simple reference state of $p_r = \exp\left((1-r)D_i/\gamma\right)$ is used, with constant gravity, thermal expansivity, and heat capacity. If `reference_state` is set to `0`, the reference state is read from a file `refstate_file`.
`mineral_physics_model=3`	Using which mineral physics model to convert the seismic velocities.
`file_vbcs=off` `vel_bound_file="bvel.dat"`	If `file_vbcs` is set to `on`, the top surface velocity boundary conditions are read in from files which have location and name specified by `vel_bound_file`. Requires setting `topvbc=1` to take effect. If you wish to have a uniform top surface velocity boundary condition or some simple geometric pattern, then `file_vbcs` should be set to zero.
`mat_control=off` `mat_file="mat.dat"`	If `mat_control` is set to `on`, then the time- and positional-dependent viscosity factor is defined from the files specified by `mat_file`. These parameters allow you to define the material group of each element (such as a moving weak zone). Not working in this version.

`lith_age=off`
`lith_age_file="age.dat"`
`lith_age_time=off`
	If `lith_age` is set to `on`, then the age of each surface nodes is read from the files specified by `lith_age_file`. These parameters control the thermal age of the top thermal boundary condition. If `lith_age_time` is `on`, the files are time-dependent.

A.1.2   Parameters that Control Output Files

`output_format=ascii`	Choose the format and layout of the output files. Can be either `ascii`, `ascii-gz` or `hdf5`. If `ascii-gz` is chosen, the code places gzipped files into `data_dir`, and will put all time-step output into subdirectories of `data_dir`. The same naming logic holds for reading old velo files.
`output_optional="surf, botm,tracer"`	Choose additional output, including `surf`, `botm`, `geoid`, `seismic`, `stress`, `pressure`, `connectivity`, `horiz_avg`, `tracer`, `heating`, `comp_el` and `comp_nd`.
`datadir="."`	Controls the location of output files.
`datafile="regtest"`	Controls the prefix of output file names such as `regtest.xxx`. Cannot contain the "/" character if `output_format=ascii`.
`storage_spacing=10` (in non-Pyre version) or `monitoringFrequency=100` (in Pyre version)	Controls the interval between output files. CitcomS dynamically determines the size of the time step; this means that you might not get an output at the exact time required, but you can always get close depending on how small this number is. Do not make this number too small since outputs slow the code down and you may end up with an unmanageable number of output files.
`checkpointFrequency=100`	The time-step interval between checkpoint output, which can be used later to resume the computation.
`output_ll_max=20`	This parameter controls the maximum degree of spherical harmonics coefficients for geoid output.
`self_gravitation=off`	Considering the effect the self gravitation on the geoid or not.
`use_cbf_topo=off`	Using the Consistent Boundary Flux (CBF) method to compute the dynamic topography or not.

A.1.3   Mesh and Processors Setup

`nproc_surf=1`	This specifies the number of spherical caps of the mesh; must be `1` for regional spherical model and `12` for full spherical model.
`nprocx=1` `nprocy=1` `nprocz=1`	These specify the number of processors in each spherical cap. For a full spherical model, `nprocx` must be equal to `nprocy`
`nodex=9` `nodey=9` `nodez=9`	These specify the number of FEM nodes in each spherical cap. These parameters are not used in the C version if multigrid solver is used. For a full spherical model, `nodex` must be equal to `nodey`
`mgunitx=8` `mgunity=8` `mgunitz=8` `levels=1`	These specify the nested level of multigrid units. Used by multigrid solver only. These parameters are not completely independent to each other. The constraint of Equation 6.7 must be satisfied. These parameters are not used in the C version if conjgrad solver is used. For a full spherical model, `mgunitx` must be equal to `mgunity`

A.1.4 Domain Size

`theta_min=1.0708`
`theta_max=2.0708`
`fi_min=0`
`fi_max=1`
	These parameters specify the horizontal extent of the computational domain. `theta_min` and `theta_max` are the colatitude measured in radians from the north pole. `fi_min` and `fi_max` are the longitudes measured from the prime meridian eastward in radians. Only in regional CitcomS.

`radius_inner=0.55` `radius_outer=1.0`	These parameters specify the radial extent of the computational domain. `radius_inner` and `radius_outer` are the inner and outer radii in non-dimensional units. It is probably more convenient to normalize lengths by the radius of the Earth. If you do this, then the Rayleigh number must be calculated with the radius of the Earth, not the thickness of the mantle. The core mantle boundary is close to having a non-dimensional radius of 0.55.

`coor=0`
 	
`coor_file="coor.dat"`
`coor_refine=0.1,0.15,0.1,0.2`
	If `coor=0`, there will be uniform mesh in the latitudinal, longitudinal, and radial directions.
	If `coor=1`, the coordinate is reading from the file specified by `coor_file`. This is used to have a regular but uneven spacing between elements.
	If `coor=2`, there will be uniform mesh in the latitudinal and longitudinal directions. The mesh in the radial direction is generated according to `coor_refine`, which is a vector of 4 numbers. The 1st value of `coor_refine` specifies the radius fraction of the bottom layer, the 2nd value specifies the fraction of the nodes in the bottom layer, the 3rd value specifies the top layer fraction, and the last value specifies the top layer node fraction.

A.1.5 Restarting the Code

`restart=off`	If `restart` is `on`, each processor will resume the computation from the checkpoint files.
`post_p=off`	Similar to `restart`, except that the model will then only run for 1 time step, which can be useful to regenerate the flow field and calculate the associated observables.

`datadir_old="."`
`datafile_old="regtest"`
`solution_cycles_init=0`
	If `restart` is `on`, for example, processor #5 will read its initial conditions from checkpoint file `regtest.chkpt.5.0` in this case.

A.1.6 Run Length

`minstep=1`
`maxtotstep=1000000`
(only in pure C version)
or
`steps=1`
(only in Pyre version)
	The maximum and minimum number of time steps for the model, including the 0th time step.

`cpu_limits_in_seconds=` `   360000000`	Controls the termination of the code based on total wall clock time used. Available only in pure C version.

A.1.7 Initial Conditions

`tic_method=0`	Which method to use to generate the initial temperature field.

`datadir_old="."`
 `datafile_old="regtest"`
 `solution_cycles_init=0`
 `zero_elapsed_time=on`
	If `tic_method=-1`, the initial temperature is read from files. For example, processor #5 will read its initial temperature from old velo file `regtest.velo.5.0` in this case. If `zero_elapsed_time` is `on`, the initial time is set to zero. If it is `off` and `tic_method=-1`, the initial time is read in from the old velo files. Note that this option has no effect when `restart=on`.

`num_perturbations=1`
 `perturbmag=0.05`
 `perturbl=1`
 `perturbm=1`
 `perturblayer=5`
 	
 `half_space_age=40`
 `mantle_temp=1.0`
 	
 `blob_center=[-999,-999,-999]`
 `blob_radius=0.063`
 `blob_dT=0.18`
	If `tic_method=0`. The initial temperature is a linear temperature gradient with perturbations at specific layers, where `num_perturbations` specifies the number of perturbations, and `perturblayer` specifies the layers to be perturbed, representing the number of the mesh node in radial direction. There must be as many entries as `num_perturbations` in a comma-separated list. The perturbation added to each layer is given by:
	
	 $$mag \times \cos(m\phi) \times P_{lm}(\cos\theta)$$
	 for the full sphere, and by:
	
	 $$mag \times \cos\left(\frac{(\theta - \theta_{min})\, l\pi}{\theta_{max} - \theta_{min}}\right) \times \cos\left(\frac{(\phi - \phi_{min})\, m\pi}{\phi_{max} - \phi_{min}}\right)$$
	
	 for the regional sphere.
	 If `tic_method=1`, T is `1` everywhere, except a cold thermal boundary layer at the top, whose temperature is determined by the half-space cooling model and `half_space_age` (in million of years, Myrs).
	 If `tic_method=2`, T is `mantle_temp` everywhere, except for a warm spherical blob and a cold thermal boundary layer at the top, whose temperature is determined by the half-space cooling model and `half_space_age` (in Myrs). The location of the blob is default to the center of the computational domain.
	 If `tic_method=3`, the initial temperature is a conductive profile with perturbations to all layers. The perturbation is given by:
	
	 $$mag \times \sin\left(\frac{(r - r_{in})\pi}{r_{out} - r_{in}}\right) (\sin(m\phi) + \cos(m\phi))\, P_{lm}(\cos\theta)$$
	
	 for the full sphere, and by:
	
	 $$mag \times \sin\left(\frac{(r - r_{in})\pi}{r_{out} - r_{in}}\right) \times \cos\left(\frac{(\theta - \theta_{min})\, l\pi}{\theta_{max} - \theta_{min}}\right) \times \cos\left(\frac{(\phi - \phi_{min})\, m\pi}{\phi_{max} - \phi_{min}}\right)$$
	
	 for the regional sphere.
	 If `tic_method=4`, the initial temperature is read from grd files.
	 If `tic_method=10`, T is `mantle_temp` everywhere, except for a cold thermal boundary layer at the top and perturbations at all layers, similar to `tic_method=3`.
	 If `tic_method=11`, T is `mantle_temp` everywhere, except for a hot thermal boundary layer at the bottom and perturbations at all layers, similar to `tic_method=3`.
	 If `tic_method=12`, T is `mantle_temp` everywhere, except for a cold thermal boundary layer, a hot thermal boundary layer at the bottom and perturbations at all layers, similar to `tic_method=3`.
	 If `tic_method=90`, T is `0` everywhere, except for a single perturbation at the middle layer. This initial temperature is good for comparison with analytical solutions.

A.1.8 Boundary Conditions

`topvbc=0`
`topvbxval=0.0`
`topvbyval=0.0`
	Surface velocity boundary condition parameters. If `topvbc` is 0, `topvbxval` and `topvbyval` specify the tangential surface stress (stress BC). If `topvbc` is 1, `topvbxval` and `topvbyval` specify the tangential surface velocity (velocity BC). The surface normal velocity is zero in these two cases (impermeable BC).

`botvbc=0`
`botvbxval=0.0`
`botvbyval=0.0`
	As above, but for bottom velocity boundary conditions.

`side_sbcs=off`	Enable traction boundary condition for the sidewalls or not. Must be `on` for coupled model.
`pseudo_free_surf=off`	Enable pseudo free surface or not.
`toptbc=1` `toptbcval=0.0`	Surface temperature boundary conditions. If `toptbc` is 0, `toptbcval` specifies the surface heat flux (not working in this version). If `toptbc` is 1, the `toptbcval` specifies the surface temperature.
`bottbc=1` `bottbcval=1.0`	As above, but for bottom temperature boundary conditions.

`temperature_bound_adj=off`
`depth_bound_adj=0.157`
`width_bound_adj=0.08727`
`lith_age_depth=0.0314`
	Additional parameters for temperature boundary conditions when `lith_age` is on.

A.1.9 Non-Dimensional Numbers

`rayleigh=1.0e+5`	This specifies the Rayleigh number, which is one of the most important parameters you may want to change.
`dissipation_number=0.0`	The dissipation number.
`gruneisen=0.0`	The Gruneisen parameter. When this parameter is 0, the code treats it as infinity (i.e., incompressible case).
`surfaceT=0.1`	The non-dimensional value of surface temperature.
`Q0=0.0`	This specifies the internal heating number.

A.1.10 Depth Information

`z_lith=0.014`
`z_410=0.06435`
`z_lmantle=0.105`
`z_cmb=0.439`
	These specify the non-dimensional depth of the Moho, 410km discontinuity, 660km discontinuity and D". These parameters are used to determine the depth of viscosity layers and phase changes (see next two sections). The names are only suggestive. You are free to refer `z_lith` to an arbitrary depth, for example.

A.1.11 Viscosity

`Viscosity=system`	This parameter must be set as indicated.
`visc_smooth_method=3`	This specifies which method to use to smooth viscosity projection for the multigrid solver.
`VISC_UPDATE=on`	If `VISC_UPDATE` is `on`, viscosity will be updated every time step. Otherwise, viscosity will be time-independent.

`num_mat=4`	This specifies the number of material layers. Material 1 is at depth between 0 and `z_lith`, material 2 between `z_lith` and `z_410`, material 3 between `z_410` and `z_lmantle`, and material 4 between `z_lmantle` and the bottom. If `mat_control` is on, then a multiplicative factor is applied to the viscosity, as defined below.
`visc0=1,1,1,1`	The pre-exponent factor of layered viscosity structure (η_0 in the equations below). There must be as many entries as `num_mat` in a comma-separated list.
`TDEPV=off`	Enable temperature dependence or not.
`rheol=3`	When `rheol=1`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(E_\eta(T_\eta - T))$ When `rheol=2`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(-T/T_\eta)$ When `rheol=3`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(\frac{E_\eta}{T^*+T_\eta} - \frac{E_\eta}{1+T_\eta})$, where $T^* = \min(\max(T,0),1)$. When `rheol=4`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(\frac{E_\eta + Z_\eta(1-r)}{T^*+T_\eta})$ When `rheol=5`, same as `rheol=3`, except the viscosity cut-off is applied before `mat_control`. When `rheol=6`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(E_\eta(T_\eta - T^*) + Z_\eta(1-r))$ When `rheol=7`, temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(\frac{E_\eta + Z_\eta(1-r)}{T+T_\eta} - \frac{E_\eta + Z_\eta(1-r_{inner})}{1+T_\eta})$, where r_{inner} is the inner radius of the mesh. When `rheol=8`, same as `rheol=3`, except viscosity reduction is applied when the temperature exceeds the solidus. When `rheol=9`, same as `rheol=3`, except using T, not T^*. When `rheol=10`, same as `rheol=8`, except using T, not T^*.

`viscE=1,1,1,1`
`viscT=1,1,1,1`
`viscZ=1,1,1,1`
	Parameters defining viscosity law (E_η, T_η, and Z_η in the equations above, respectively). There must be as many entries as `num_mat` in a comma-separated list.

`SDEPV=off`	Enable stress dependence (non-Newtonian) or not.
`sdepv_expt=1,1,1,1` `sdepv_misfit=0.001`	If `SDEPV` is on, these specify the exponent in the viscosity law and the criterion of convergence test. There must be as many entries as `num_mat` in a comma-separated list.
`PDEPV=off`	Pseudo-plastic rheology, implemented by adding a plastic viscosity $\eta_p = \frac{\sigma_y}{(2\epsilon_{II}+10^{-7})+\eta_p^0}$ where the yield stress is defined as $\sigma_y = \min\left(a + b\left(1-z\right), y\right)$ and ϵ_{II} is the second shear strain rate invariant (all non-dimensional). The effective viscosity η' is computed from η and η_p as $\eta' = \frac{\eta_p \eta}{(\eta+\eta_p)}$ (pdevp_eff=on) or $\eta' = \min\left(\eta, \eta_p\right)$ (pdepv_eff=off).

`pdepv_a=1e20,1e20,1e20,1e20`
`pdepv_b=0,0,0,0`
`pdepv_y=1e20,1e20,1e20,1e20`
	Parameters for σ_y.

`pdepv_eff=on`	Effective or minimum viscosity "plasticity" (see above).
`pdepv_offset=0`	Offset for plastic viscosity η_p^0.
`CDEPV=off`	Compositionally dependent viscosity pre-factor (only for `tracer=on`). Will assign two pre-multipliers for $C = 0$ and $C = 1$ and compute a geometric mean for all elements depending on the nodal composition. Only works for two flavors and assuming C varies between $[0;1]$.
`cdepv_ff=1,1`	Flavor-wise viscosity pre-factors for $C = 0$ and $C = 1$, respectively.
`low_visc_channel=off` `low_visc_wedge=off`	Used in conjunction with tracers. The tracers define the upper boundary of the subducted slab.

`lv_min_radius=0.9764`
`lv_max_radius=0.9921`
`lv_channel_thickness=0.0047`
`lv_reduction=0.5`
	If `low_visc_channel` or `low_visc_wedge` is on, this specifies the radial extents of the low viscosity zones and the viscosity reduction factor, respectively.

`VMIN=off` `visc_min=0.001`	If `VMIN` is on, minimum viscosity is cut off at `visc_min`.
`VMAX=off` `visc_max=1000`	If `VMAX` is on, maximum viscosity is cut off at `visc_max`.

A.1.12 Phase Change Information

`Ra_410=0.0`
`clapeyron410=0.0235`
`transT410=0.78`
`width410=0.0058`
	These specify the phase change parameters (phase change Rayleigh number, Clapeyron slope, ambient temperature, and phase change width, respectively). The depth of this phase change is specified by `z_410`.

`Ra_670=0.0`
`clapeyron670=-0.0235`
`transT670=0.875`
`width670=0.0058`
	As above. The depth of this phase change is specified by `z_lmantle`.

`Ra_cmb=0.0`
`clapeyroncmb=-0.0235`
`transTcmb=0.875`
`widthcmb=0.0058`
	As above. The depth of this phase change is specified by `z_cmb`.

A.1.13 Momentum Equation Solver Parameters

`stokes_flow_only=off`	If you wish only to solve for the velocity once (e.g., Stokes flow) then change this parameter to `on`. However, if you want to do a convection problem, this should be `off`.
`remove_rigid_rotation=on` `remove_angular_momentum=on`	Whether to remove rigid body rotation component or net angular momentum from the velocity solution. Only effective for global models.
`Solver=cgrad`	Can be either `cgrad` for conjugate gradient solver or `multigrid` for multigrid solver for the outer loop of the momentum solver.
`node_assemble=on`	Whether to assemble stiffness matrix at the node level or not.

`mg_cycle=1`
`down_heavy=3`
`up_heavy=3`
`vlowstep=1000`
`vhighstep=3`
`max_mg_cycles=50`
	Parameters for `multigrid` and `cgrad` solvers. For `multigrid` solver: `mg_cycle=1` for V cycle and 2 for W cycle; `down_heavy` and `up_heavy` are the number of smoothing passes for downward/upward smoothing; `vlowstep` and `vhighstep` are the number of smoothing passes at lowest/highest levels; `max_mg_cycles` is the maximum number of multigrid cycles used per solve; all these parameters should be small integers.
	For `cgrad` solver, `vlowstep` is the maximum iterations of the conjugate gradient solver and should be a large integer.

`piterations=1000`	Maximum iterations of the outer loop for the momentum solver.
`accuracy=1.0e-4`	Convergence criterion for the momentum solver.
`uzawa=cg` `compress_iter_maxstep=100`	Can be either `cg` or `bicg`. If set to `cg`, additional parameters control the maximum iterations.
`precond=on`	Whether to use the preconditioner.
`aug_lagr=on` `aug_number=2.0e3`	Whether to use augmented stiff matrix and the weight of the augmented stiff matrix.

A.1.14   Energy Equation Solver Parameters

`ADV=on`	If on, solves the energy equation.
`fixed_timestep=0.0`	If it is equal to 0, the size of the time step is variable and is determined dynamically. Otherwise, the size of the time step is fixed at the specified value.
`finetunedt=0.9`	Set the size of the time step to the specified fraction of a maximum stable advection time step. Must be between 0 and 1.
`adv_sub_iterations=2` `adv_gamma=0.5`	The number of iterations and the weight of each iteration for the energy predictor-corrector solver.
`filter_temp=off`	Using a Lenardic filter to remove the overshoots and undershoots of the temperature field or not. The filter conserves the total energy.
`monitor_max_T=on`	If on, the maximum value of the current and previous temperature fields are compared. If the maximum temperature increases more than 5%, the energy equation solver is rerun with a smaller time-step size. Keep this parameter on to prevent numerical instability.
`inputdiffusivity=1`	Currently, don't change this parameter. It is used only in problems which are integrated backward in time.

A.1.15   Age Information

`start_age=40.0`	Set initial age (in Myrs). This age determines which files of various time-dependent input to read in.
`reset_startage=off`	If on, the initial age is set to `start_age`. If it is `off` and `tic_method=-1`, the initial age is read in from previous output.

A.1.16   Debugging Information

`DESCRIBE=off` `BEGINNER=off` `VERBOSE=off`	These parameters affect the echo behavior of the CitcomS parser. Only in non-Pyre version.
`verbose=off`	This is used for debugging. If verbose is `on`, additional information is output to a `.info` file.
`see_convergence=on`	If `on`, the velocity residual will be output on the screen for every iteration of the momentum solver.

A.1.17   HDF5 Output Parameters

`cb_block_size=1048576` `cb_buffer_size=4194304`	Size for collective buffer in MPI-IO.
`sieve_buf_size=1048576`	Size of data sieve buffer.
`output_alignment=262144` `output_alignment_threshold=` `   524288`	Memory alignment.
`cache_mdc_nelmts=10330` `cache_rdcc_nelmts=521` `cache_rdcc_nbytes=1048576`	Cache size for chunked dataset.

A.1.18 Tracer Parameters

`tracer=off`	If on, enables the tracers.

`tracer_ic_method=0`
`tracers_per_element=10`
`tracer_file="tracer.dat"`
	Specify the initial location of the tracers. If `tracer_ic_method=0`, the tracers are generated randomly, with the number of tracers per element specified by `tracers_per_element`. If `tracer_ic_method=1`, the location of the tracers is read from a file specified in `tracer_file`. If `tracer_ic_method=2`, the location of the tracers is read from the old tracer output, similar to `tic_method=-1`.

`tracer_flavors=0`	The number of flavors among the tracers. If set to 0, flavor counting is turned off.
`ic_method_for_flavors=0` `z_interface=0.7`	Specify the initial flavors of the tracers. Used only when `tracer_ic_method=0`. Currently only `ic_method_for_flavors=0` is supported. A layered structure is generated. `z_interface` must be a comma-separated list with (`tracer_flavors-1`) entries. Tracers above the 1st radius in `z_interface` are of flavor 0, between the 1st and 2nd radii are of flavor 1, ... etc.
`regular_grid_deltheta=1.0` `regular_grid_delphi=1.0`	The grid spacing of the regular grid. The regular grid is an auxiliary grid to help locate the tracers.
`chemical_buoyancy=on`	If on, enables thermo-chemical convection.
`buoy_type=1`	If `buoy_type=1`, the composition field is determined by the ratio method [19]. (No other methods are implemented yet.)
`buoyancy_ratio=1.0`	The ratio of chemical density anomaly to the reference density, must be a comma-separated list with (`tracer_flavors-1`) entries.
`itracer_warnings=on`	The warning level of the tracer module.
`tracer_enriched=off` `Q0_enriched=0.0`	Whether the composition anomaly is associated with radioactive heating anomaly. If `on`, specifies the internal heating number inside the composition anomaly.

A.1.19 Dimensional Information

`radius=6371e3`
`density=3340.0`
`thermdiff=1.0e-6`
`gravacc=9.81`
`thermexp=3.0e-5`
`refvisc=1.0e+21`
`cp=1200`
`density_above=1030.0`
`density_below=6600.0`
	Various dimensional information in SI units.

A.1.20 Required Information

`Problem=convection` `Geometry=sphere`	For this version of CitcomS, all of these parameters must be set as indicated.

A.1.21 PETSc Related Flags

`use_petsc=off`	Set to `on` to use PETSc functionality. Turning on this flag only will cause the PETSc version of the Uzawa algorithm to be used in the Stokes solver
`petsc_schur=off`	Set to `on` to use the "Schur complement reduction" approach in the Stokes solver

A.2   CitcomS Facilities and Properties

This section lists the facilities and properties in the Pyre version of CitcomS. Most of the properties have names which are identical to the parameters used in the non-Pyre version of CitcomS and are explained in the section above. This section highlights those which have changed and those which are entirely new. Parameters are given with their default values.

A.2.1   Top-Level Facilities and Properties

`steps=1`	How many time steps to run.
`launcher=mpich`	A facility specifying which launcher to use. Choices include `mpich` and `lam-mpi`.
`scheduler=none`	A facility specifying which scheduler to use. Choices are `lsf`, `pbs`, and `globus`.
`controller`	A facility. User cannot change it.
`solver=regional`	A facility specifying which solver to use. Must be either `regional` or `full`.

A.2.2   `launcher`

The launcher facility controls how CitcomS, an MPI application, is executed on multiple processors. It is the equivalent to `mpirun` in MPI.

`dry=off`	If on, prints the `mpirun` command line and exits without launching the job.
`nodegen`	A printf-styled format string, used in conjunction with `nodelist` to generate a list of machine names. Example: `n%03d`
`nodelist`	A comma-separated list of machine names in square brackets. Example: `[101-103,105,107]`
`command`	`The command used to launch the job.  The default value should be customized if using any job scheduler, otherwise the default value should work well.`

A.2.3   `scheduler`

The scheduler facility controls how CitcomS submits jobs to a batch scheduler. Available schedulers include: `none` (default, not using a batch scheduler), `lsf` (for Load Sharing Facility batch scheduler), `pbs` (for Portable Batch System batch scheduler), `sge` (for Sun Grid Engine batch scheduler), and tacc-ranger (a variant of PBS, customized for the Ranger cluster at Texas Advanced Computing Center). Only the command options for these schedulers are listed below. For more information on configuring Pyre for your batch system, see CIG's Pythia page (`geodynamics. org/cig/software/packages/cs/pythia/docs/batch`).

`dry=off`	If `on`, prints the batch script and exits without scheduling the job.
`wait=off`	If `on`, waits for batch jobs to finish before exiting.

A.2.4   `job`

The `job` facility controls options for individual batch jobs.

`name`	The name of the job.
`queue`	The name of the queue to which the job is scheduled.
`walltime`	Time limit for the job, specified using units, e.g., `5*minute`, `2*hour`.
`stdin=/dev/null`	File to read as the input stream.
`stdout=stdout.txt`	File to write for the output stream.
`stderr=stderr.txt`	File to write for the error stream.

A.2.5 `controller`

`monitoringFrequency=100`	The time-step interval between disk output. It replaces the `storage_spacing` parameter in the (old) CitcomS input file.
`checkpointFrequency=100`	The time-step interval between checkpoint output, which can be used later to resume the computation.

A.2.6 `solver`

`mesher`	A facility. Must be either `full-sphere` or `regional-sphere`. User does not need to specify it. It is set by the `solver` facility automatically.
`tsolver`	A facility for the temperature solver using Petrov-Galerkin time integration.
`vsolver`	A facility for the velocity solver using Boussinesq approximation and the Uzawa algorithm.
`bc`	A facility of boundary conditions.
`const`	A facility for dimensional constants.
`ic`	A facility for initial conditions.
`output`	A facility for output options.
`param`	A facility for some additional input parameter files.
`phase`	A facility for phase change parameters.
`tracer`	A facility for tracer parameters.
`visc`	A facility for viscosity parameters.
`datadir="."`	
`datafile="regtest"`	
`datadir_old="."`	
`datafile_old="regtest"`	
`rayleigh=100000`	
`dissipation_number=0.0`	
`gruneisen=0.0`	
`surfaceT=0.1`	
`Q0=0`	
`stokes_flow_only=off`	
`verbose=off`	
`see_convergence=on`	

A.2.7 `solver.mesher`

`nprocx=1`	
`nprocy=1`	
`nprocz=1`	
`coor=0`	
`coor_file="coor.dat"`	
`coor_refine=0.1,0.15,0.1,0.2`	
`nodex=9`	
`nodey=9`	
`nodez=9`	
`levels=1`	
`radius_outer=1`	
`radius_inner=0.55`	
`theta_min=1.0708`	
`theta_max=2.0708`	
`fi_min=0`	
`fi_max=1`	

A.2.8 `solver.tsolver`

`ADV=on`	
`filter_temp=off`	
`monitor_max_T=on`	
`finetunedt=0.9`	
`fixed_timestep=0.0`	
`inputdiffusivity=1`	
`adv_gamma=0.5`	
`adv_sub_iterations=2`	

A.2.9 `solver.vsolver`

`Solver=cgrad`	
`node_assemble=on`	
`precond=on`	
`accuracy=1.0e-4`	
`uzawa=cg`	
`compress_iter_maxstep=100`	
`mg_cycle=1`	
`down_heavy=3`	
`up_heavy=3`	
`vlowstep=1000`	
`vhighstep=3`	
`max_mg_cycles=50`	
`piterations=1000`	
`aug_lagr=on`	
`aug_number=2000`	
`remove_rigid_rotation=on`	
`remove_angular_momentum=on`	

A.2.10 `solver.bc`

`side_sbcs=off`	
`pseudo_free_surf=off`	
`topvbc=0`	
`topvbxval=0`	
`topvbyval=0`	
`botvbc=0`	
`botvbxval=0`	
`botvbyval=0`	
`toptbc=1`	
`toptbcval=0`	
`bottbc=1`	
`bottbcval=1`	
`temperature_bound_adj=off`	
`depth_bound_adj=0.157`	
`width_bound_adj=0.08727`	

A.2.11 `solver.const`

`radius=6.371e+06`	
`density=3340.0`	
`thermdiff=1e-06`	
`gravacc=9.81`	
`thermexp=3e-05`	
`refvisc=1e+21`	
`cp=1200`	
`density_above=1030.0`	
`density_below=6600.0`	
`z_lith=0.014`	
`z_410=0.06435`	
`z_lmantle=0.105`	
`z_cmb=0.439`	

A.2.12 `solver.ic`

`restart=off`	
`post_p=off`	
`solution_cycles_init=0`	
`zero_elapsed_time=on`	
`tic_method=0`	
`num_perturbations=1`	
`perturbl=1`	
`perturbm=1`	
`perturblayer=5`	
`perturbmag=0.05`	
`half_space_age=40`	
`mantle_temp=1.0`	
`blob_center=[-999,-999,-999]`	
`blob_radius=0.063`	
`blob_dT=0.18`	

A.2.13 `solver.output`

`output_format="ascii"`	
`output_optional="surf,botm,` `tracer"`	
`output_ll_max=20`	
`self_gravitation=off`	
`use_cbf_topo=off`	
`cb_block_size=1048576`	
`cb_buffer_size=4194304`	
`sieve_buf_size=1048576`	
`output_alignment=262144`	
`output_alignment_threshold=` `    524288`	
`cache_mdc_nelmts=10330`	
`cache_rdcc_nelmts=521`	
`cache_rdcc_nbytes=1048576`	

A.2.14 `solver.param`

`reference_state=1`	
`refstate_file="refstate.dat"`	
`mineral_physics_model=3`	
`file_vbcs=off`	
`vel_bound_file="bvel.dat"`	
`mat_control=off`	
`mat_file="mat.dat"`	
`lith_age=off`	
`lith_age_file="age.dat"`	
`lith_age_time=off`	
`lith_age_depth=0.0314`	
`start_age=40`	
`reset_startage=off`	

A.2.15 `solver.phase`

`Ra_410=0`	
`clapeyron410=0.0235`	
`transT410=0.78`	
`width410=0.0058`	
`Ra_670=0`	
`clapeyron670=-0.0235`	
`transT670=0.78`	
`width670=0.0058`	
`Ra_cmb=0`	
`clapeyroncmb=-0.0235`	
`transTcmb=0.875`	
`widthcmb=0.0058`	

A.2.16 `solver.tracer`

`tracer=off`	
`tracer_ic_method=0`	
`tracers_per_element=10`	
`tracer_file="tracer.dat"`	
`tracer_flavors=0`	
`ic_method_for_flavors=0`	
`z_interface=0.7`	
`itracer_warnings=on`	
`regular_grid_deltheta=1.0`	
`regular_grid_delphi=1.0`	
`chemical_buoyancy=on`	
`buoy_type=1`	
`buoyancy_ratio=1.0`	
`tracer_enriched=off`	
`Q0_enriched=0.0`	

A.2.17 `solver.visc`

`Viscosity="system"`	
`visc_smooth_method=3`	
`VISC_UPDATE=on`	
`num_mat=4`	
`visc0=1,1,1,1,`	
`TDEPV=off`	
`rheol=3`	
`viscE=1,1,1,1,`	
`viscT=1,1,1,1,`	
`viscZ=1,1,1,1,`	
`SDEPV=off`	
`sdepv_misfit=0.001`	
`sdepv_expt=1,1,1,1,`	
`PDEPV=off`	
`pdepv_a=1e20,1e20,1e20,1e20`	
`pdepv_b=0,0,0,0`	
`pdepv_y=1e20,1e20,1e20,1e20`	
`pdepv_eff=on`	
`pdepv_offset=0`	
`CDEPV=off`	
`cdepv_ff=1,1`	
`low_visc_channel=0`	
`low_visc_wedge=0`	
`lv_min_radius=0.9764`	
`lv_max_radius=0.9921`	
`lv_channel_thickness=0.0047`	
`lv_reduction=0.5`	
`VMIN=off`	
`visc_min=0.001`	
`VMAX=off`	
`visc_max=1000`	

A.2.18 `layout`

The following facilities are only used in the coupled CitcomS solver.

`containing_group=[0-11]`	The processors to be assigned to the csolver.
`embedded_group=[12]`	The processors to be assigned to the esolver.

A.2.19 `ccoupler`

`si_unit=off`	Whether to exchange information in SI units.
`cartesian=off`	Whether to exchange information in Cartesian coordinate.
`two_way_communication=on`	Whether to transfer information from esolver to csolver.
`exchange_initial_temperature` `=on`	Whether to ensure consistent initial temperature between csolver or esolver.
`exchange_pressure=on`	Whether to send the pressure solution to esolver.

A.2.20 `ecoupler`

`si_unit=off`	Whether to exchange information in SI units.
`cartesian=off`	Whether to exchange information in Cartesian coordinate.
`two_way_communication=on`	Whether to transfer information from esolver to csolver.
`exchange_initial_temperature=on`	Whether to ensure consistent initial temperature between csolver or esolver.
`exchange_pressure=on`	Whether to receive the initial guess of pressure from csolver.
`exclude_top=off`	Whether to exclude the top boundary when receiving boundary conditions from the csolver. If the esolver has imposed plate velocity and constant temperature at the surface, set this to on.
`exclude_bottom=off`	Whether to exclude the bottom boundary when receiving boundary conditions from the csolver.
`amending_outflow=off`	Whether to amend the velocity boundary conditions to satisfy the continuity equation.

A.2.21 `journal`

The Pyre facility `journal` provides five types of debugging output for conceptually different types of information. The journal output stream can be instantiated as separated channels multiple times, and each channel can be individually activated or deactivated, and sent to different locations (the terminal, sockets, files, devices, etc.). The streams and their default states of the journal streams are:

`debug`	Debugging information. Default off.
`error`	Unrecoverable runtime error. Default on.
`firewall`	Fatal programming error. Default on.
`info`	Descriptive information. Default off.
`warning`	Recoverable runtime error. Default off.

For coupled solvers, there is a large amount of debugging information that outputs through the journal facility. That output can be turned on/off with command line options. The most important ones are `journal.debug.Exchanger` and `journal.debug.CitcomS-Exchanger`. Other less important options can be found in `tests/coupled.cfg`. To enable the journal output, try running the scripts with the following options:

```
[CitcomS.journal.debug]
Exchanger = on
CitcomS-Exchanger = on
```

Appendix B

CitcomS Input File Format

B.1 Introduction

CitcomS expects Unix-styled ASCII files (i.e., no carriage character following new line character) for all input files. This can be a nuisance in DOS/Windows systems. You may want to find a text editor that can write Unix-style ASCII files. In the following, words in normal `courier` must be input exactly as shown, while ***italicized*** words should be substituted by your values. All parameters are in non-dimensional units unless specified.

B.2 Coordinate Files

For regional version of CitcomS, the mesh must be regular, but the mesh spacing may be unequal. The `coor_file` has the format:

```
nsd= 1
1       theta1
2       theta2
...     ...
nodex theta_nodex
nsd= 2
1       phi1
2       phi2
...     ...
nodey phi_nodey
nsd= 3
1       r1
2       r2
...     ...
nodez r_nodez
```

For the full spherical version of CitcomS, the mesh of each cap must be regular and equidistant in the horizontal dimension. Only the vertical dimension is specified by `coor_file`. The `coor_file` has the format:

```
nsd= 3
1       r1
2       r2
...     ...
nodez r_nodez
```

B.3   Velocity Boundary Condition Files

If `vel_bound_file` is set to `bvel.dat`, then it is necessary to have one `bvel.dat` file per cap for each million-year interval. For example, if `start_age=83`, then the following files are needed for the regional mesh:

```
bvel.dat84
bvel.dat83
bvel.dat82
...
bvel.dat0
```

> **TIP:** Even though the model starts at 83 million years before the present, by default it will attempt to read in both a file for 84 and a file for 83 million years ago. To deal with this, create a duplicate copy of `bvel.dat83` and call it `bvel.dat84`

In this example, the model age will start at 83 Ma and decrease toward 0 Ma. At any particular age, the velocity boundary conditions are interpolated in time according to the nearest `bvel.dat` files. Once the age becomes negative, the velocity boundary conditions are specified by the content of `bvel.dat0`.

> **TIP:** By setting `start_age=0` and providing identical `bvel.dat0` and `bvel.dat1`, you can effectively get time-invariant velocity boundary conditions.

For the global mesh, each of the 12 caps requires one file for each million-year interval. For example, these files are needed for an 82-million-year age:

```
bvel.dat82.0
bvel.dat82.1
bvel.dat82.2
...
bvel.dat82.11
```

Each velocity boundary condition file has the format:

> ***Vx Vy***

The units of `Vx` and `Vy` are cm/yr.

B.4   Material Files

In this version of CitcomS, the implementation of material support is not working. The material output has been disabled and is documented here for completion. If `mat_file` is set to `mat.dat`, then it is necessary to have one `mat.dat` file for each million-year interval. For example, if `start_age=83`, then the following files are needed:

```
mat.dat84
mat.dat83
mat.dat82
...
mat.dat0
```

The same note about `vel_bound_file` (see Section B.3 above) applies. The format of `mat_file` is:

> ***n viscosity_factor***

B.5 Lithosphere Age Files

If `lith_age_file` is set to `lith.dat`, then it is necessary to have one `bvel.dat` file for each million-year interval. For example, if `start_age=83`, then the following files are needed for the regional mesh:

```
lith.dat84
lith.dat83
lith.dat82
...
lith.dat0
```

The same note about `vel_bound_file` (see Section B.3 above) still applies. The input age is in millions of years. For the global mesh, each of the 12 caps requires one file for each million-year interval. For example, these files are needed for an 82-million-year age:

```
lith.dat82.0
lith.dat82.1
lith.dat82.2
...
lith.dat82.11
```

The format of `lith_age_file` is:

> ***n age***

B.6 Tracer Files

This file contains the initial location of all tracers. The first line is the number of tracers and the number of columns in the file. The first three columns are the coordinates of the tracers. The fourth column, if present, indicates the flavor of the tracers.

> ***num_tracers num_columns***
> ***theta phi radius [flavor]***

B.7 Reference State Files

This file contains the profiles of the reference state. This file must contain at least `nodez` lines, and each line must contain 7 columns, where the meaning of each column is:

> ρ_r g α c_P ***reserved reserved reserved***

Appendix C

CitcomS Output File Format

C.1 Introduction

The format of the output files of CitcomS is described here. In the following sections, the model prefix is assumed as `test-case`, the processor number as 0, and the time step as 10. All outputs are in non-dimensional units unless specified.

C.2 Postprocessed Cap Output (`test-case.cap00.10`)

The command `autocombine.py` produces 1 cap file for regional CitcomS and 12 cap files for the full CitcomS. The first line of the cap file is a comment describing the node geometry (`nodex` × `nodey` × `nodez`). The rest of the file is column-based, where the meaning of each column is:

```
colatitude longitude radius vel_colat vel_lon vel_r temperature viscosity
```

C.3 Postprocessed Opt Output (`test-case.opt00.10`)

If the optional output contains node-based fields (e.g., `comp_nd`, `pressure`, and `stress`), the command `autocombine.py` produces 1 opt file for regional CitcomS and 12 opt files for the full CitcomS. The first line of the opt file is a comment describing the node geometry (`nodex` × `nodey` × `nodez`). The rest of the file is column-based, where the meaning of each column is defined in the corresponding `.general` file. For example, if the `.general` file contains these two lines, then the first column in the opt file is the composition, the 2nd column is the pressure, and the last six columns are the stress.

```
field = composition, pressure, stress
structure = scalar, scalar, 6-vector
```

C.4 Postprocessed Surf Output (`test-case.surf0.10`)

An undocumented (and unmaintained) post-processing script `batchsurf.py` can combine the `coord`, `surf`, and `botm` output. The format of the combined surf file is listed for completion. The first line of the surf file is a comment describing the node geometry (`nodex` × `nodey`). The rest of the file is column-based, where the meaning of each column is:

```
colatitude longitude topography heat_flux vel_colat vel_lon
```

C.5   Time Output (`test-case.time`)

This file reports non-dimensional elapsed model time and spent CPU time (in seconds), and it is only outputted on computer node 0. The meaning of each column is:

```
step total_t delta_t total_cpu_time step_cpu_time
```

C.6   ASCII Output

C.6.1   Coordinate Output (`test-case.coord.0`)

This file is only outputted at the 0th time step. The first line is a header. The rest of the file is column-based, where the meaning of each column is:

```
colatitude longitude radius
```

C.6.2   Velocity and Temperature Output (`test-case.velo.0.10`)

The first two lines of this file are headers. The rest of the file is column-based, where the meaning of each column is:

```
vel_colat vel_lon vel_r temperature
```

C.6.3   Viscosity Output (`test-case.visc.0.10`)

The first line of this file is a header. The rest of the file is column-based, where the meaning of the only column is:

```
viscosity
```

C.6.4   Material Output (`test-case.mat.0`)

In this version of CitcomS, the implementation of material support is not working. The material output has been disabled and is documented here for completion. This file is only outputted at the 0th time step. There is no header. The meaning of each column is:

```
element_number layer material
```

C.6.5   Surface Variables Output (`test-case.surf.0.10` and `test-case.botm.0.10`)

The first line of each file is a header. The rest of each file is column-based, where the meaning of each column is:

```
topography heat_flux vel_colat vel_lon
```

C.6.6   Stress Output (`test-case.stress.0.10`)

The first two lines of the file are headers. The rest of the file is column-based, where the meaning of each column is:

$S_{\theta\theta}$ $S_{\phi\phi}$ S_{rr} $S_{\theta\phi}$ $S_{\theta r}$ $S_{\phi r}$

You can use the above values to form the following symmetric stress tensor:

$$\begin{bmatrix} S_{\theta\theta} & S_{\theta\phi} & S_{\theta r} \\ S_{\phi\theta} & S_{\phi\phi} & S_{\phi r} \\ S_{r\theta} & S_{r\phi} & S_{rr} \end{bmatrix} \tag{C.1}$$

C.6.7 Pressure Output (`test-case.pressure.0.10`)

The first line of the file is a header. The rest of the file is column-based, where the meaning of the only column is:

    pressure

C.6.8 Horizontal Average Output (`test-case.horiz_avg.0.10`)

The first line of the file is a header. The rest of the file is column-based, where the meaning of each column is:

    radius temperature RMS(V_horizontal) RMS(V_vertical)

C.6.9 Geoid Output (`test-case.geoid.10`)

The first line of the file is a header. The rest of the file is column-based, where the meaning of each column is:

col 1	spherical harmonic degrees (`l`)
col 2	spherical harmonic orders (m)
col 3	cosine coefficients of total geoid (S_{lm})
col 4	sine coefficients of total geoid (C_{lm})
col 5	cosine coefficients of the geoid due to surface topography
col 6	sine coefficents of the geoid due to surface topography
col 7	cosine coefficients of the geoid due to internal density variation
col 8	sine coefficients of the geoid due to internal density variation

The units of the geoid coefficients are meters. The geoid field can be reconstructed by

$$\sum \left(S_{lm}\sin(m\phi) + C_{lm}\cos(m\phi)\right) P_{lm}(\cos\theta)$$

where P_{lm} is the associated Legendre polynomials.

C.6.10 Tracer Output (`test-case.tracer.0.10`)

The first line of the file is a header. The second field in the header is the number of tracers in the file. The third field in the header is the number of columns in the file. The rest of the file is column-based, where the meaning of the columns is:

    theta phi radius [flavor]

C.6.11 Composition Output (`test-case.comp_el.0.10` and `test-case.comp_nd.0.10`)

These files contain the composition field either on the element (`comp_el`) or on the node (`comp_nd`). The format of the files is the same. The first two lines of the file are headers. The fourth field in the first line is the number of composition components. In the second line, the first field is the current bulk sum of composition 1. The second field is the initial bulk sum of composition 1. The third and fourth fields (if they exist) are the current and initial bulk sum of composition 2, etc. The rest of the file is column-based, where the meaning of the columns is:

    composition1 [composition2 ... compositionN]

C.6.12 Heating Output (`test-case.heating.0.10`)

These files contain various heating terms on the element. The first two lines of the file are the headers. The rest of the file is column-based, where the meaning of the columns is:

    adiabatic_heating viscous_heating latent_heating

C.7   HDF5 Output (`test-case.h5`)

The format and layout of HDF5 output is described in Section 4.4 on page 47.

C.8   Misc. Binary Output

C.8.1   Checkpoint Output (`test-case.checkpoint.0.10`)

These files are used for restarting the run. These files are not portable. You cannot run a model on machine A, copy the checkpoint files to machine B, and expect you can always restart the simulation on machine B. Their format is undocumented on purpose and will remain so.

C.8.2   Domain Output (`test-case.domain`)

This file is only outputted at the 0th time step. This file is output by rank-0 processor only. It contains the domain bounds of all processors in binary format. The file begins with four intergers: `nproc`, `ncolumns`, `const1`, `const2`, where `nproc` is the number of processors, `ncolumns` is 10, `const1` and `const2` are used to detect binary incompatibility. The rest of the file has `nproc`×`ncolumns` doubles, the columns contains the min/max of radius and the θ, ϕ coordinates of the four corners:

```
r_min r_max theta0 phi0 theta1 phi1 theta2 phi2 theta3 phi3
```

C.8.3   Coordinate Binary Output (`test-case.coord_bin.0`)

These files are only outputted at the 0th time step. These files contain the coordinates of nodes in binary format. The file begins with four intergers: `nodex`, `nodey`, `nodez`, `const`, then followed by the θ, ϕ, r coordinates of all nodes.

C.8.4   Seismic Output (`test-case.seismic.0.10`)

These files contain the density, P wave velocity and S wave velocity in binary format. The density of all nodes is stored in double, then followed by P wave velocity of all nodes, and finally S wave velocity of all nodes.

Appendix D

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