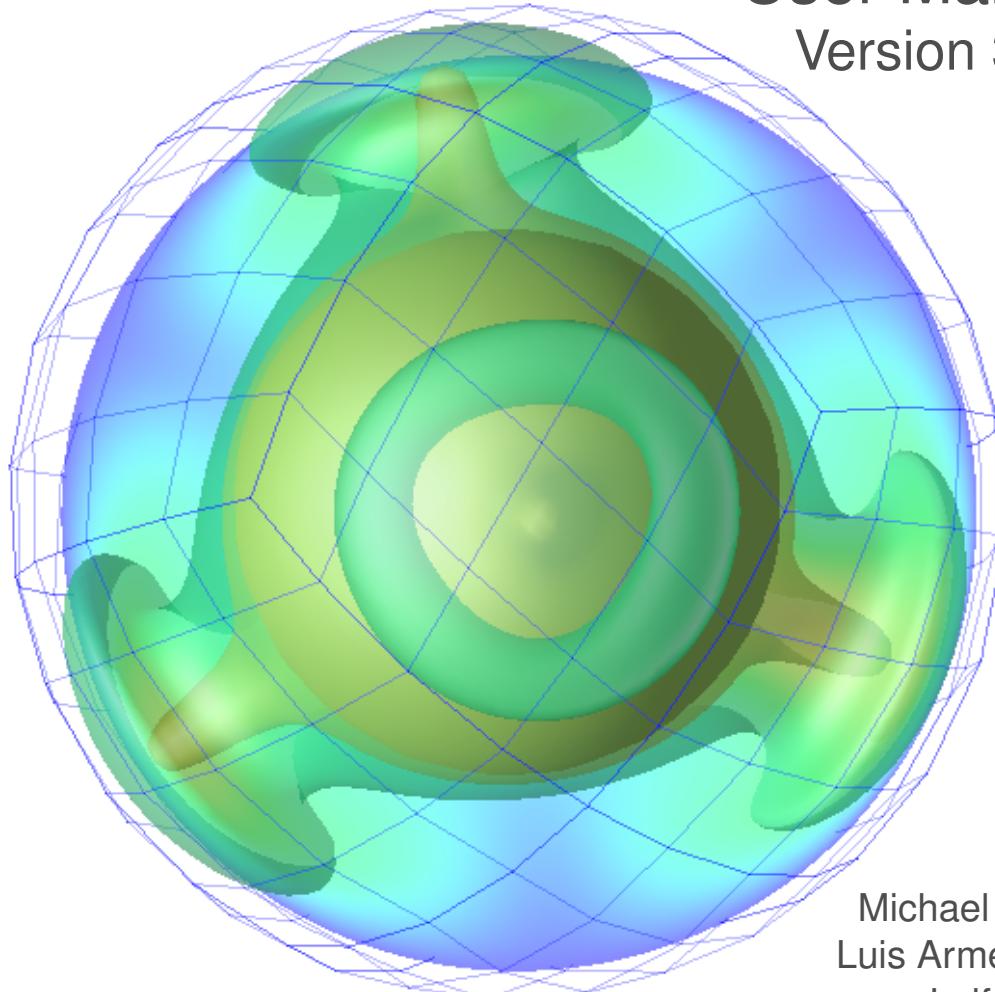


CitcomS

User Manual
Version 3.??



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CitcomS User Manual

June 25, 2014

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Part I

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 describes the capabilities of CitcomS and 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 L^AT_EX, 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

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 95). Written in C, the code runs on a variety of parallel processing computers, including shared and distributed memory platforms.

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 California Institute of Technology **Convection in the Mantle**) 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 35). 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-plasticity, 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. Other enhancements include:

- 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.
 - Replaced fixed accuracy setting. Bug reported by Rob Moucha.
 - Fixed temperature perturbation bug for multiple processors.

1.3 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:

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

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

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

where ρ is the density, u is the velocity, P is the dynamic pressure, η is the viscosity, δ_{ij} is the Kronecker 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:

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

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:

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

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

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:

$$\rho = \rho_0 \rho' \quad (1.7)$$

$$\alpha = \alpha_0 \alpha' \quad (1.8)$$

$$g = g_0 g' \quad (1.9)$$

$$\kappa = \kappa_0 \kappa' \quad (1.10)$$

$$\eta = \eta_0 \eta' \quad (1.11)$$

$$c_P = c_{P0} c'_P \quad (1.12)$$

$$x_i = R_0 x'_i \quad (1.13)$$

$$u_i = \frac{\kappa_0}{R_0} u'_i \quad (1.14)$$

$$T_0 = \Delta T T'_0 \quad (1.15)$$

$$T = \Delta T (T' + T'_0) \quad (1.16)$$

$$t = \frac{R_0^2}{\kappa_0} t' \quad (1.17)$$

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

$$P = \frac{\eta_0 \kappa_0}{R_0^2} P' \quad (1.19)$$

$$d_{ph} = R_0 d'_{ph} \quad (1.20)$$

$$\gamma_{ph} = \frac{\rho_0 g_0 R_0}{\Delta T} \gamma'_{ph} \quad (1.21)$$

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:

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

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

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

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

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

This is not the usual definition of the Rayleigh 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:

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

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

$$Ra_H = RaH \frac{R_0^3 - R_{CMB}^3}{3R_0^3} \quad (1.28)$$

$$Di = \frac{\alpha_0 g_0 R_0}{c_{P0}} \quad (1.29)$$

1.4 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 Stealine-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]:

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

$$\mathbf{A}u + \mathbf{B}p = f \quad (1.31)$$

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:

$$\mathbf{B}^T \mathbf{A}^{-1} \mathbf{B}p = \mathbf{B}^T \mathbf{A}^{-1} f \quad (1.32)$$

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.

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

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

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

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

1.5 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.

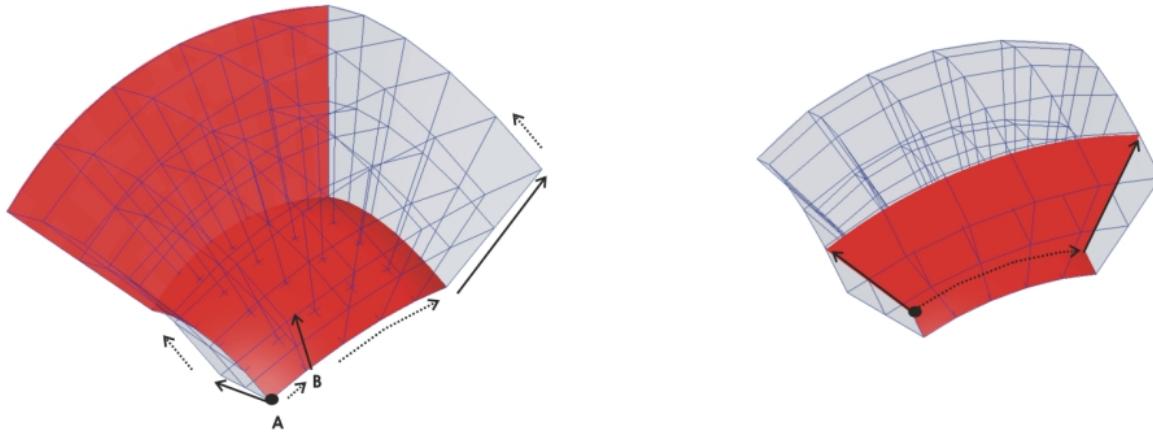


Figure 1.1: Global Node Numbering. Left: Global node numbering starts at the base of arrow A (θ_{\min} , ϕ_{\min} , r_{inner}), and advances from 1 at the base to $node_z$ at the tip. Upon reaching the tip, numbering continues from the base of arrow B ($node_z+1$) to its tip ($2 \cdot node_z$), and so on for all nodes on the plane $\phi = \phi_{\min}$. Right: After completing each theta radius plane, the ϕ index is incremented and numbering commences from $(\theta_{\min}, r_{\text{inner}})$ 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).

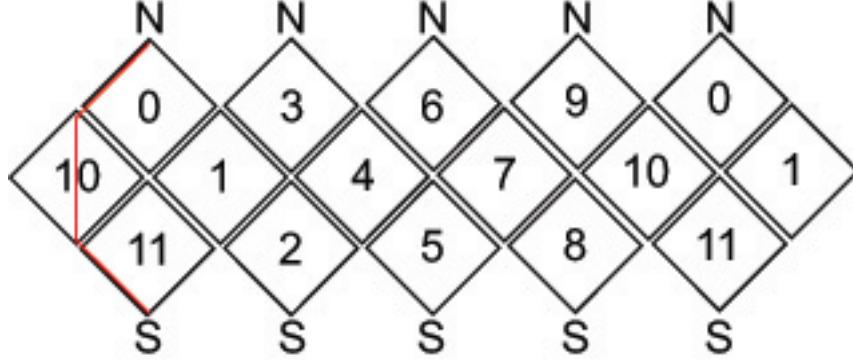


Figure 1.2: Topological connectivity of the 12 caps. N is the north pole and S is the south pole. The red line marks the 0 degree meridian.

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.

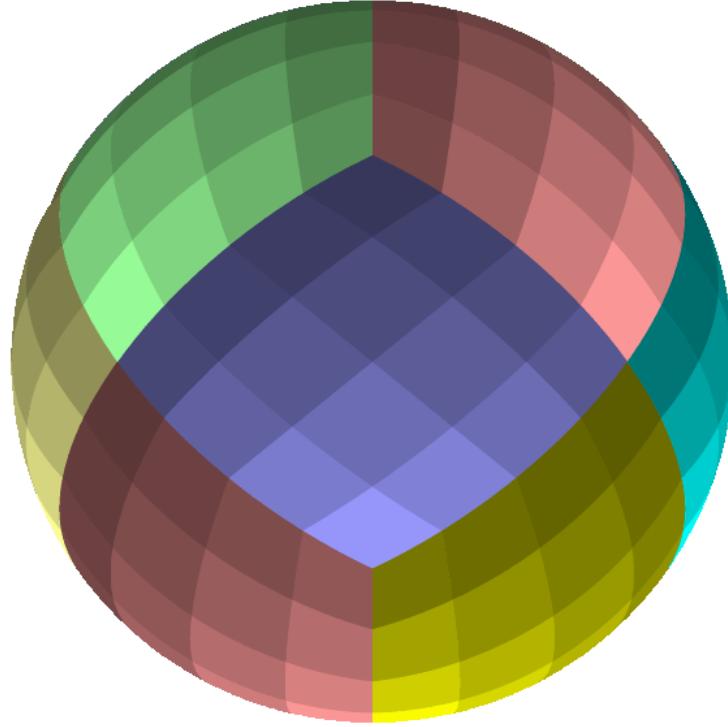


Figure 1.3: Orthographic projection of processors from a full CitcomS mesh in which there are 16 processors in map view for each cap. The CitcomS cap is shown as distinct colors while the processor domains within the caps are indicated by the intensity of the color. This example was produced for a run 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 2.9 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

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.

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 manager 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 compiler 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
```

2.4 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.

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
CC	C compiler command. This is usually set to the name of an MPI wrapper command, e.g., <code>./configure \</code> <code>CC=/opt/mpich-1.2.6/bin/mpicc</code> 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., <code>-I<dir></code> if you have headers in a nonstandard directory.
LDFLAGS	Linker flags; e.g., <code>-L<dir></code> if you have libraries in a nonstandard directory.
LIBS	Library flags; e.g., <code>-l<lib></code> 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 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 is 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
```

2.7.1 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.

2.7.1.1 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.

2.7.1.2 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.

2.7.1.3 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).

2.7.1.4 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.

2.8 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.

2.9 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.

2.9.1 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.

2.9.2 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.

2.9.3 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

Upon the completion of a successful build, 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 77.

3.2 Changing Parameters

A configuration file should be used to set the input parameters for CitcomS. A configuration file is a plain text file whose format is based on the Windows INI file. The format of a configuration file is as follows:

```
#CitcomS.component1.component2  
# this is a comment  
property1=value1  
property2=value2 ; this is another comment  
property3=val1,val2,val3 ; this property is specified by a list of values
```

Upon termination of each run, all of the parameters are logged in a `pidXXXXXX` file, where `XXXXXX` is the process id of the CitcomS application. Section names such as `#CitcomS.component1.component2` are optional, but are recommended for the purpose of organizing the contents of the configuration file

3.3 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. The CitcomS source package contains an `examples` directory (the `make install` command installs the examples under `PREFIX/share/CitcomS/examples`, where `PREFIX` is the CitcomS installation directory). In this directory, you will find the `example0` configuration file. Switch to the `examples` directory and execute the following on the command line:

```
$ CitcomSRegional example0
```

or, equivalently,

```
$ mpirun -np 1 CitcomSRegional example0
```

3.3.0.1 Example: Uniprocessor, `example0`

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=5

# CitcomS.controller
storage_spacing=1

# CitcomS.solver
datafile=example0
rayleigh=100000

# CitcomS.solver.mesh
fi_max=1
fi_min=0
node_x=17
node_y=17
node_z=9
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.ic
num_perturbations=1
perturbl=1
perturblayer=5
perturbm=1
perturbmag=0.05

# CitcomS.solver.visc
num_mat=4
```

3.4 Multiprocessor Example

In the `examples` directory, type the following at the command line:

```
$ mpirun -np 4 CitcomSRegional example1
```

3.4.0.2 Example: Multiprocessor, `example1`

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=70

# CitcomS.controller
storage_spacing=10

# CitcomS.solver
datafile=example1
rayleigh=100000

# CitcomS.solver.mesh
fi_max=1
fi_min=0
```

```

nodex=17
nodey=17
nodez=9
nprocx=2
nprocy=2
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.ic
num_perturbations=1
perturbl=1
perturblayer=5
perturbm=1
perturbmag=0.05

# CitcomS.solver.visc
num_mat=4

```

This example has:

- 2 processors in colatitude (x -coordinate), specified by the `nprocx=2` line in the configuration file
- 2 processors in longitude (y -direction), specified by the `nprocy=2` line
- 1 processor in the radial (z -direction). The default value for the `nprocx`, `nprocy`, `nprocz` parameters is 1. Hence the `nprocz=1` line is omitted from the configuration file.
- The total number of processors used is given by $nprocx \times nprocy \times nprocz$. Hence this model uses 4 processors in total.
- There are 17 nodes in x (theta) direction.
- There are 17 nodes in y (fi) direction.
- There are 9 nodes in z (radius_inner) direction.

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`, 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 cluster or supercomputer or the number of CPUs in a given computer. We run one “process” on each node. In the example script this is indicated with:

```

nprocx=2
nprocy=2

```

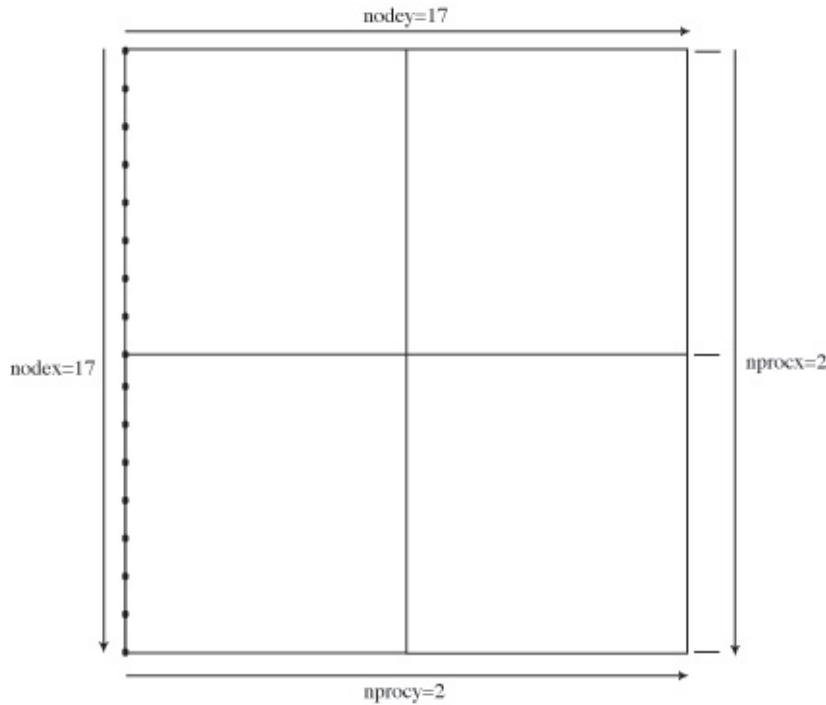


Figure 3.1: Computational Domain. Map view on the configuration of the top layer of the computational nodes and the processors.

3.4.1 Output Formats

The possible output formats in CitcomS are `ascii`, `ascii-gz`, `hdf5`, `vtk` with `ascii` being the default. The output format is specified by the `output_format` configuration parameter. 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:

```
output_format=ascii-gz
```

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

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 2.7 on page 27). You can run the example script with:

```
output_format=hdf5
```

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

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 41). 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
<code>/input</code>	N/A
<code>/coord</code>	(caps, nodex, nodey, nodez, 3)
<code>/connectivity</code>	(cap_elements, 8)

Table 4.1: Layout of the time-independent data file

Dataset	Shape
<code>/velocity</code>	(caps, nodex, nodey, nodez, 3)
<code>/temperature</code>	(caps, nodex, nodey, nodez)
<code>/viscosity</code>	(caps, nodex, nodey, nodez)
<code>/pressure</code>	(caps, nodex, nodey, nodez)
<code>/stress</code>	(caps, nodex, nodey, nodez, 6)
<code>/geoid</code>	(8) See Section C.6.9 on page 93 for details
<code>/surf/velocity</code>	(caps, nodex, nodey, 2)
<code>/surf/heatflux</code>	(caps, nodex, nodey)
<code>/surf/topography</code>	(caps, nodex, nodey)
<code>/botm/velocity</code>	(caps, nodex, nodey, 2)
<code>/botm/heatflux</code>	(caps, nodex, nodey)
<code>/botm/topography</code>	(caps, nodex, nodey)
<code>/horiz_avg/temperature</code>	(caps, nodez)
<code>/horiz_avg/velocity_xy</code>	(caps, nodez)
<code>/horiz_avg/velocity_z</code>	(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 92 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 49.

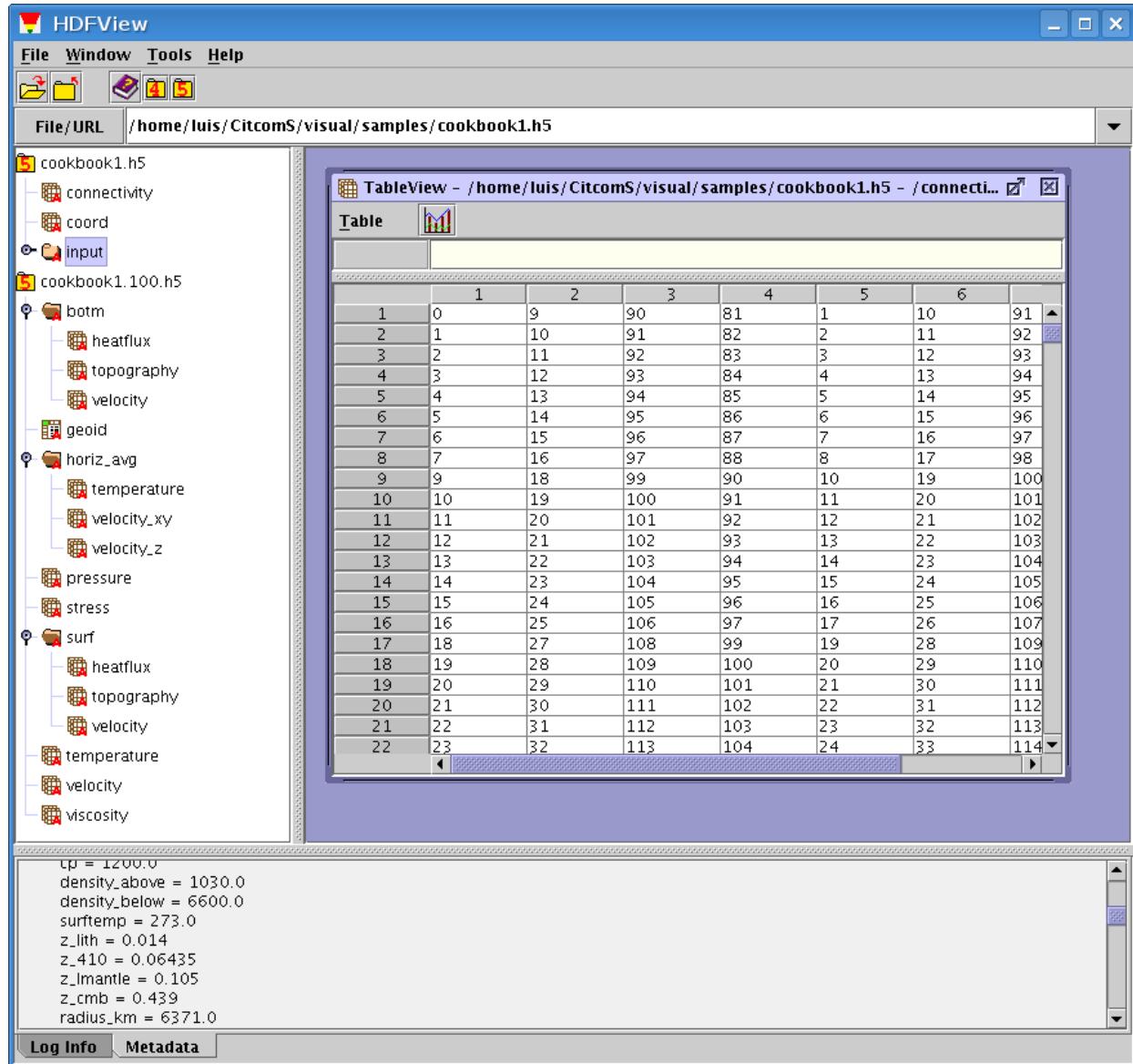


Figure 4.1: A screenshot of HDFView. The left panel shows the hierarchy of the groups and datasets. The right panel shows a 2D slice of a dataset. The bottom panel shows the metadata associated with the selected group or dataset.

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 45. Scripts using GMT commands to plot 2D cross sections of temperature field are also provided; see Section 5.8 on page 47.

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 44 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.

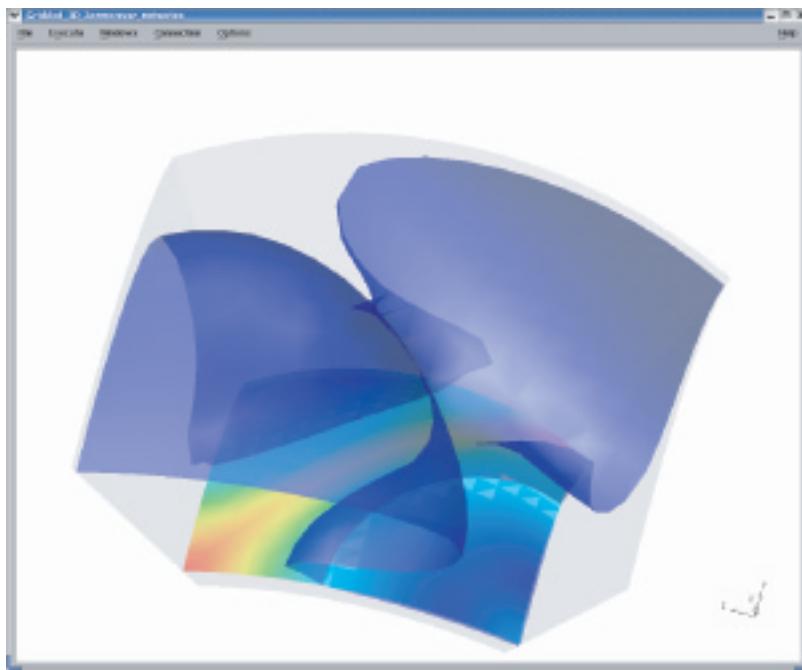


Figure 5.1: Regional Model Visualized with OpenDX. A snapshot of an upwelling (blue isosurface) with a slice of the temperature field (bisecting plane).

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 2.7.1.4 on page 28). 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`).

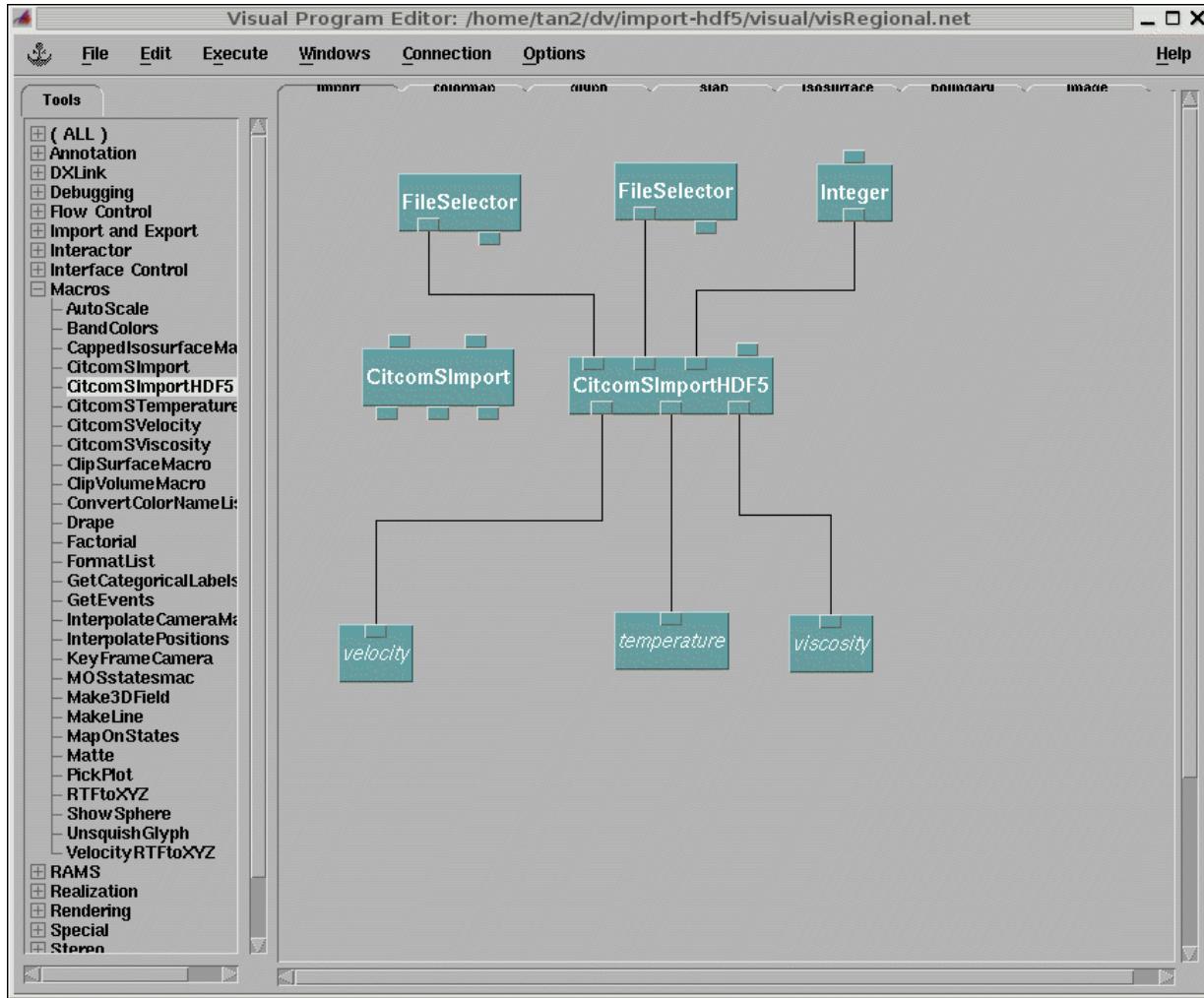


Figure 5.2: How to import CitcomS HDF5 data. The `CitcomSImportHDF5` module is highlighted in the Tools panel.

- (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 2.7.1.2 on page 27) 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).

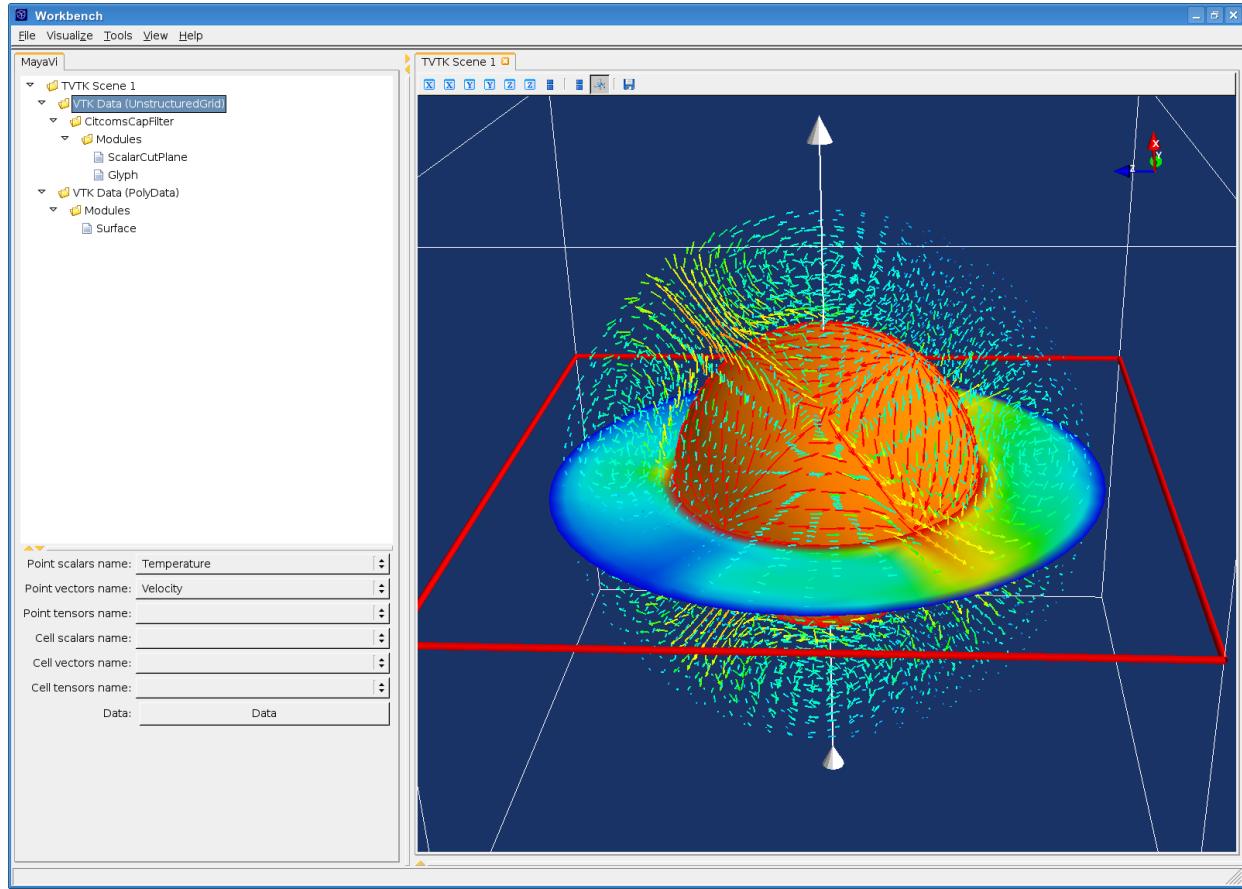


Figure 5.3: Example MayaVi2 visualization of `cookbook1.100.h5`. Here we display the velocity field as vectors, as well a slice of the temperature field. Note the visualization pipeline in the tree view on the left panel.

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.

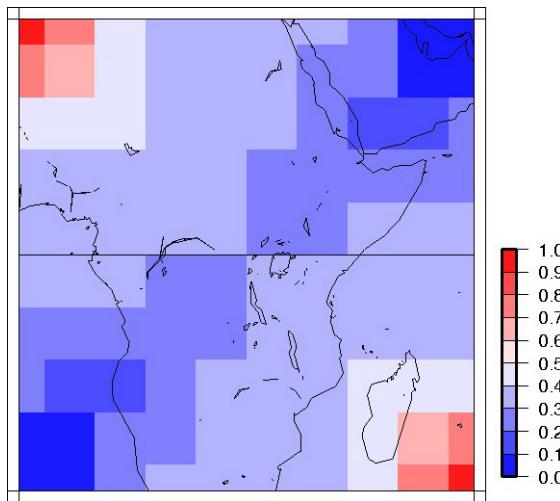


Figure 5.4: Temperature field generated by `plot_layer.py`. This image is the mid-layer (layer 5) of the sample data `visual/samples/regtest.cap00.100`. The resolution of the image is poor because the data has only $9 \times 9 \times 9$ nodes.

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.

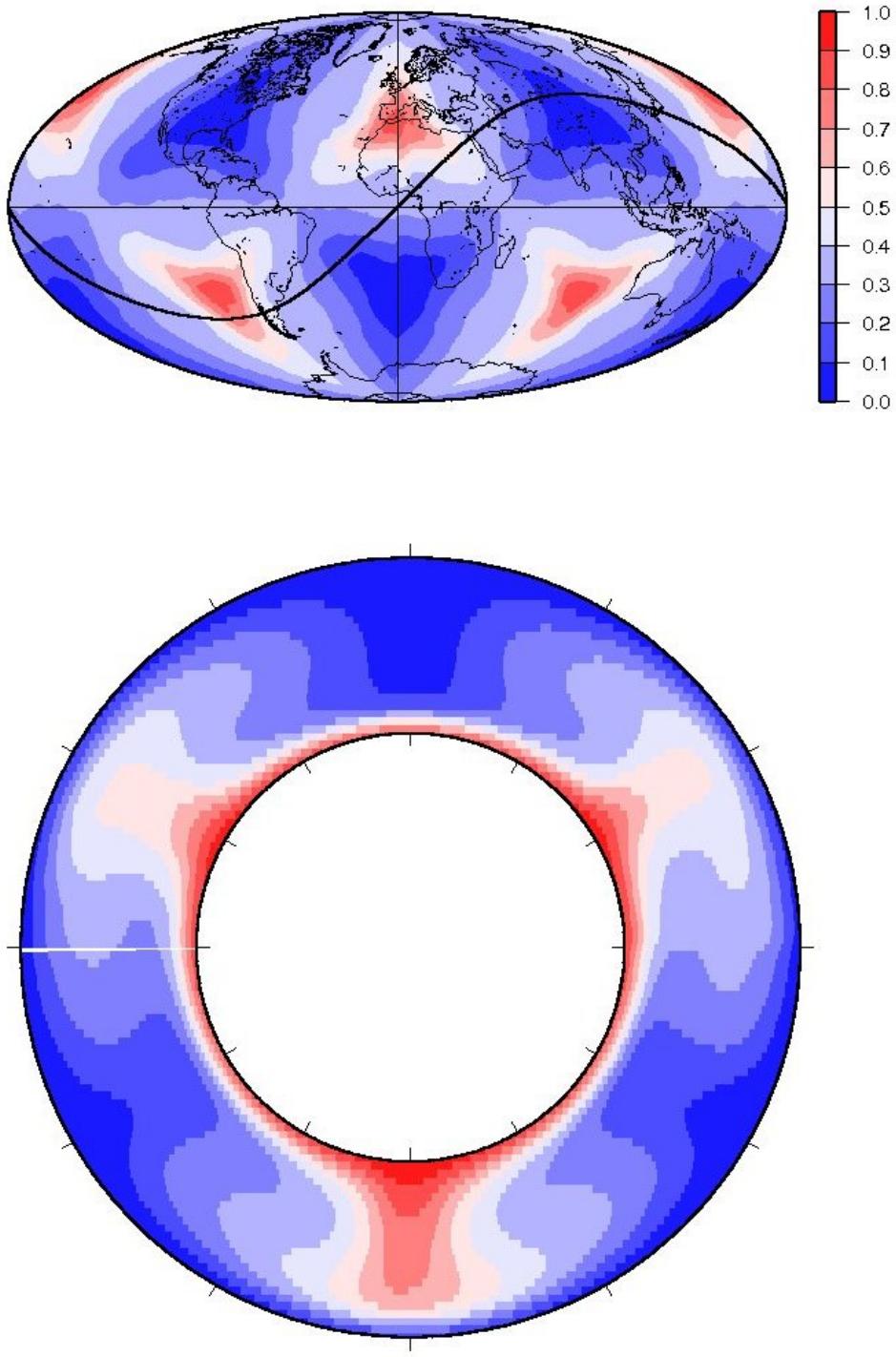


Figure 5.5: Temperature fields generated by `plot_annulus.py`. The top panel is the horizontal cross section at the mid layer in Hammer-Aitoff projection. The thick line marks the surface track of the radial cross section. The bottom panel is the radial cross section. The cross section starts at 0° latitude 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. 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 3.4 on page 32 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.

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.

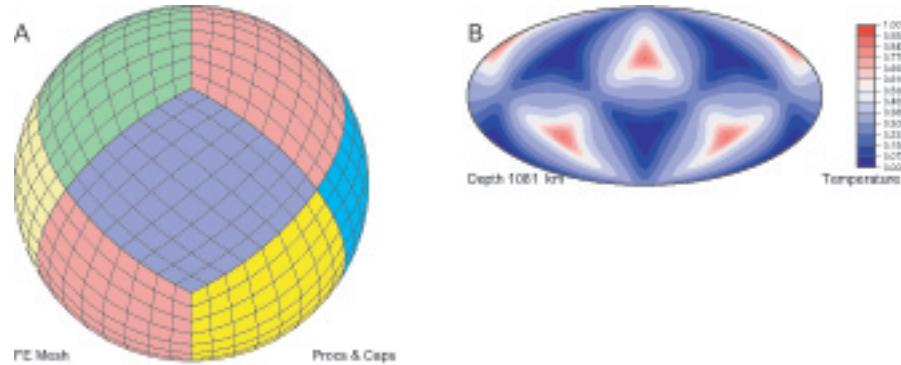


Figure 6.1: Global Model “Caps.” Left (A): Three-dimensional perspective image showing seven of the 12 spherical caps used in a full CitcomS run. Right (B): The temperature field at 1081 km depth from a Cookbook 1 run.

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`.

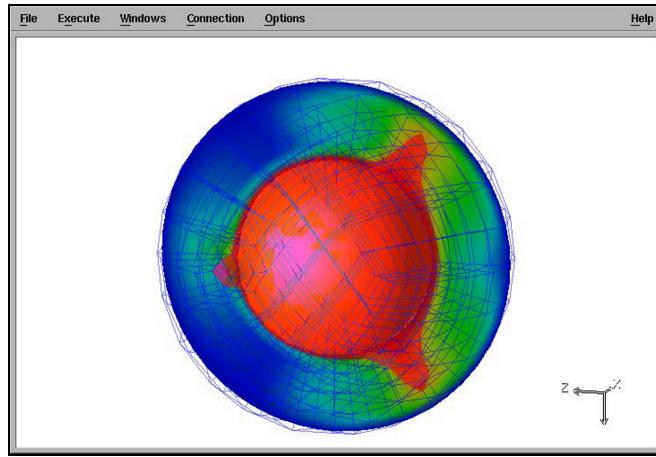


Figure 6.2: Cookbook 1: Global Model. This image, created by OpenDX, depicts a slice through a spherical model of convection, with warmer colors indicating upwelling and the cooler colors showing downwelling.

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]
```

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, longitudinal, 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 18 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.

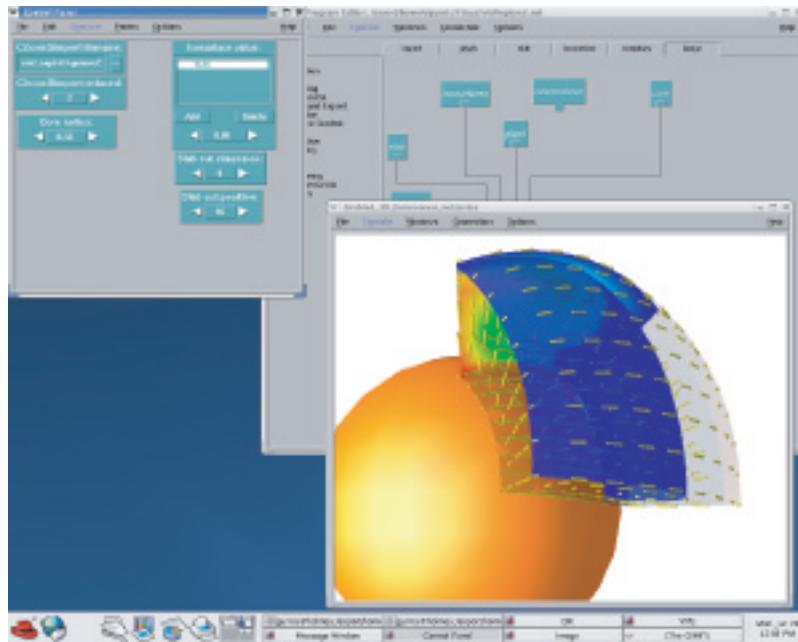


Figure 6.3: Cookbook 2: Velocity Boundary Conditions. This model, visualized with OpenDX, highlights a region of the sphere and the heated upwellings (warm colors), downwellings (cool colors), and the velocities (yellow arrows).

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:

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

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:

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

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 1.3, it is clear that

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

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

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

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
```

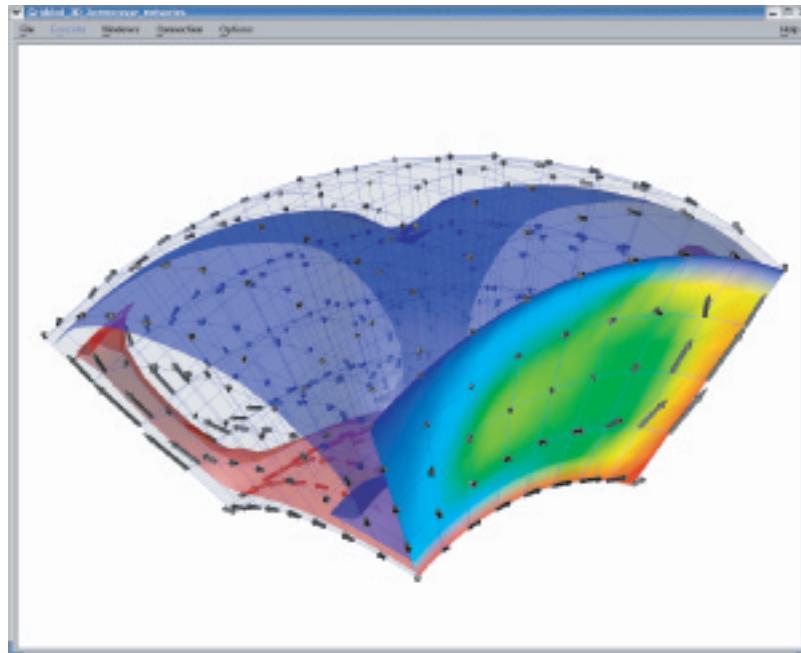


Figure 6.4: Cookbook 3: Temperature-Dependent Viscosity. This model, visualized with OpenDX, highlights a region that features both the heated upwelling (warm colors) and the even distribution of the velocities (arrows).

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 `coor`. Set it to 1 (`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 87.

```
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`

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=250

# CitcomS.controller
storage_spacing=50

# CitcomS.solver
datafile=cookbook4
rayleigh=1e6

# CitcomS.solver.mesher
coor=1
coor_file=coor.dat
fi_max=1
fi_min=0
nodex=33
nodey=17
nodez=17
nprocx=1
nprocy=1
nprocz=1
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.ic
num_perturbations=1
perturbl=1
perturblayer=10
perturbm=0
perturbmag=0.05
```

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

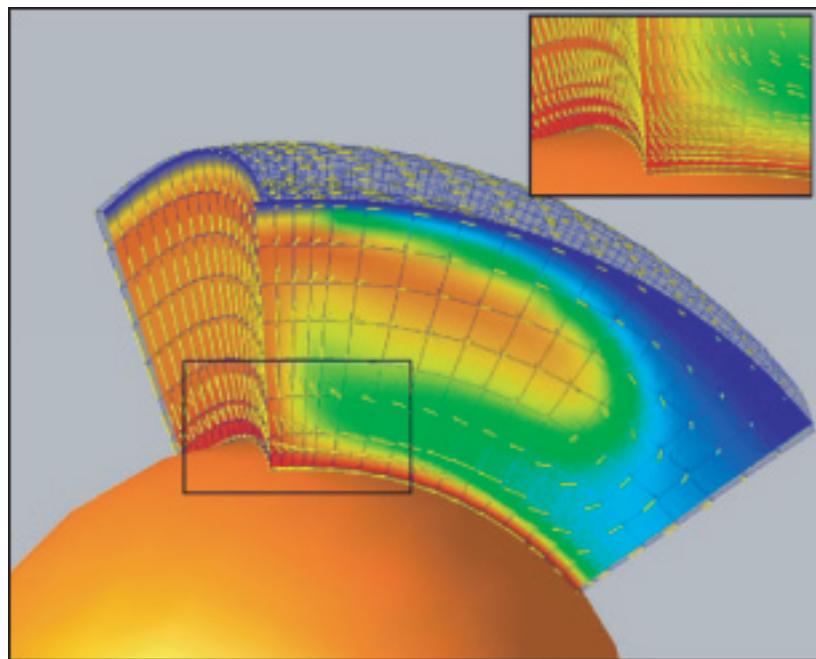


Figure 6.5: Cookbook 4: Regionally Refined Mesher. This model shows the temperature (upwelling – warm colors, downwelling – cool colors) and the uneven distribution of the velocities (yellow arrows). Note the refined mesh for the left and bottom regions of the model (inset).

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 88. 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 92. The location and prefix of the file is specified in `datadir_old` and `datafile_old`, and the time step of the velo file in `soltion_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
```

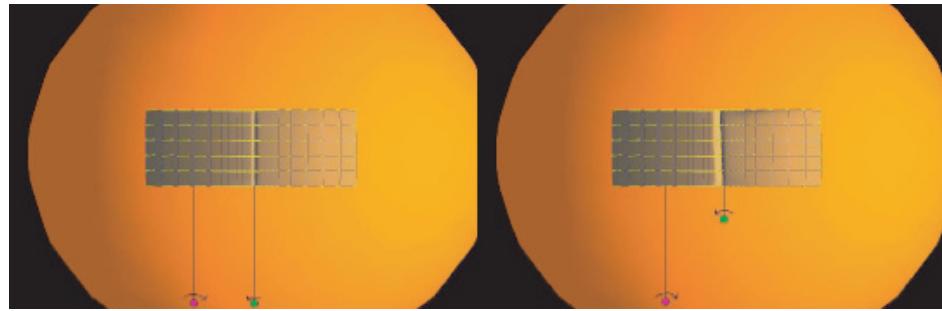


Figure 6.6: Cookbook 5: Left (A): Initially, both plates have Euler poles (magenta and green dots) situated far apart from the plate, so the velocities are approximately constant (about 5 cm/yr for the left plate and about 2 cm/yr for the right plate). Right (B): After 30 Ma a pole jump occurred for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

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

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=1100

# CitcomS.controller
storage_spacing=100

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

# CitcomS.solver.mesher
coor=1
coor_file=./coor.dat
fi_max=1
fi_min=0
nodex=17
nodey=65
nodez=33
nprocx=1
nprocy=2
nprocz=1
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.tsolver
finetunedt=0.75
monitor_max_T=on

# CitcomS.solver.bc
topvbc=1

# CitcomS.solver.ic
num_perturbations=1
perturbl=1
```

```

perturblayer=5
perturbm=1
perturbmag=0.05
solution_cycles_init=0
tic_method=-1

# CitcomS.solver.param
file_vbcss=on
start_age=55
vel_bound_file=./velocity/bvel.dat

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

```

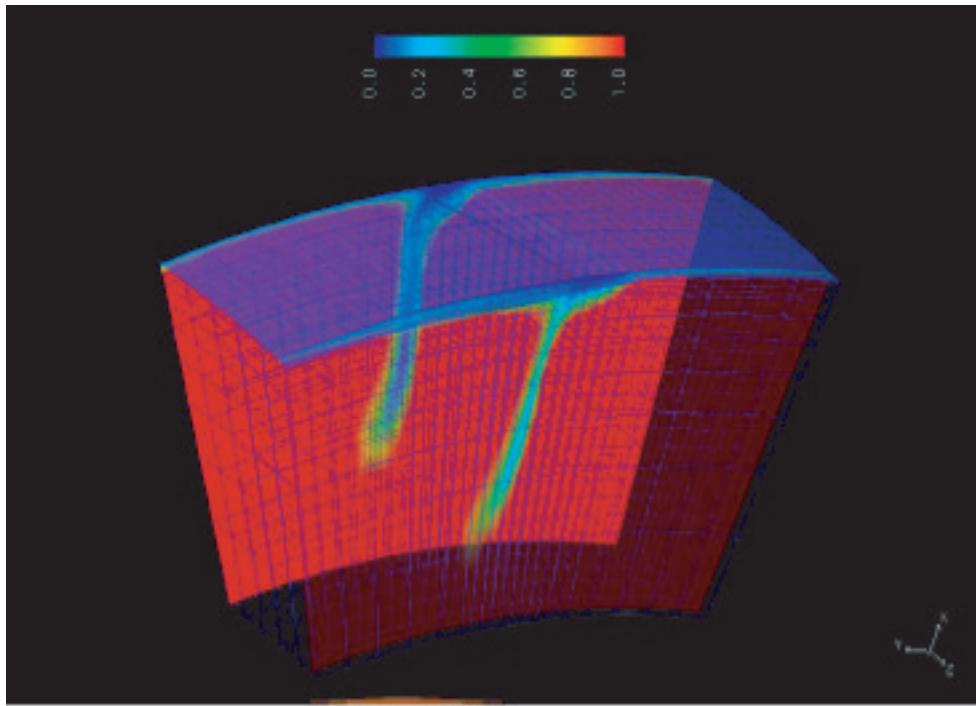


Figure 6.7: Cookbook 5: The pole jump after 30 Ma produced a flat slab on one side (fore side) and a steep slab on the other side (back side).

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.

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: $45^\circ \times 45^\circ \times 1200$ 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.

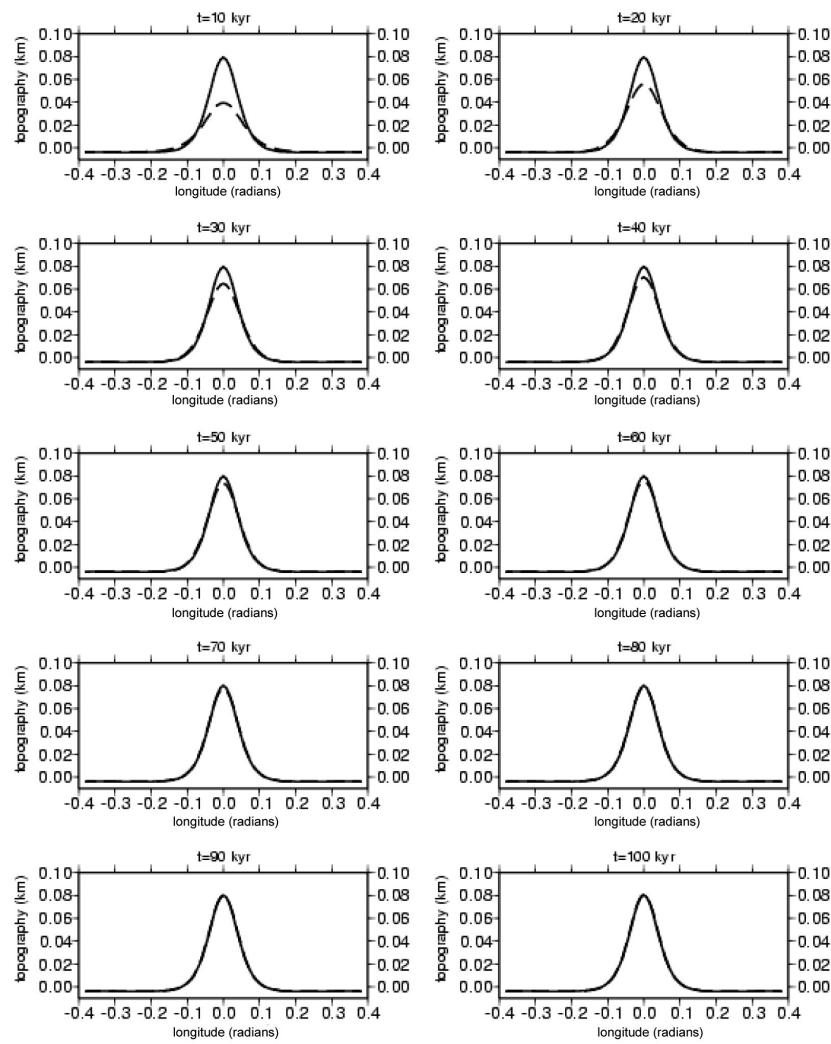


Figure 6.8: Cookbook 6: Graphs of topography profiles.

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`. 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 composition 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`

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=15
solver=full

# CitcomS.controller
storage_spacing=5

# CitcomS.solver
datadir=output
datafile=cookbook7
rayleigh=1e7

# CitcomS.solver.mesher
fi_max=1
fi_min=0
nodex=9
nodey=9
nodez=9
nproc_surf=12
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.vsolver
Solver=cgrad
accuracy=1e-04
piterations=1000
```

```

vlowstep=1000

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

# CitcomS.solver.output
output_optional=tracer,comp_nd

# CitcomS.solver.tracer

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

```

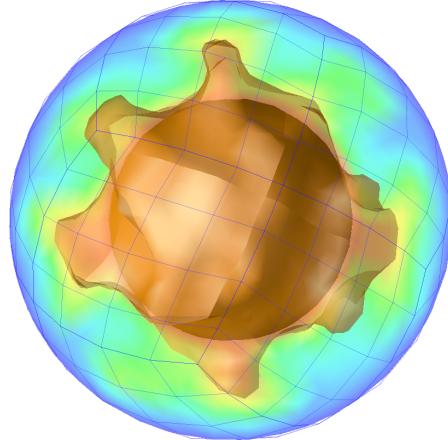


Figure 6.9: Cookbook 7: The composition and velocity field at the 15th step. The arrows are the velocity vectors. The composition field is shown in an isosurface of 0.7 and in a cross section.

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:

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

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 is provided in the `examples/Cookbook8/` directory. To restart the computation from this checkpoint, set these parameters:

```
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 $\gamma = \alpha_0 K_{S0} / \rho_0 c P_0$, and the non-dimensionalized absolute surface temperature, which are defined in Section 1.3. 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 ($= 7.68175583 \times 10^4 \times (r_{outer} - r_{inner})^3$). Similarly, 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:

$$\text{nodeX} = 1 + \text{nprocX} \times \text{mgunitX} \times 2^{levels-1} \quad (6.7)$$

where `mgunitX`, which **must be an integer**, 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`

```
# CitcomS
cpu_limits_in_seconds=360000000
minstep=10000
solver=full

# CitcomS.controller
checkpointFrequency=1000
storage_spacing=1000

# CitcomS.solver
datadir=output
datadir_old=restart
datafile=cookbook8
datafile_old=cookbook8
dissipation_number=0.5
gruneisen=1.25
rayleigh=7.68175583e4
```

```
surfaceT=0.1

# CitcomS.solver.mesher
coor=1
coor_file=coord.dat
fi_max=1
fi_min=0
levels=5
mgunitx=2
mgunity=2
mgunitz=2
nodex=33
nodey=33
nodez=33
nproc_surf=12
theta_max=2.0708
theta_min=1.0708

# CitcomS.solver.tsolver
finetunedt=0.75

# CitcomS.solver.vsolver
Solver=multigrid
accuracy=0.001
aug_lagr=on
aug_number=2.0e3
compress_iter_maxstep=100
down_heavy=2
max_mg_cycles=50
mg_cycle=1
piterations=375
precond=on
remove-angular_momentum=on
remove_rigid_rotation=off
up_heavy=2
uzawa=cg
vhighstep=2
vlowstep=20

# CitcomS.solver.ic
num_perturbations=1
perturbl=3
perturblayer=17
perturbm=2
perturbmag=0.01
restart=off
solution_cycles_init=9000
tic_method=3

# CitcomS.solver.output
output_ll_max=20
output_optional=geoid,surf,botm
self_gravitation=on
use_cbf_topo=on
```

```
# CitcomS.solver.param
reference_state=1
refstate_file=ref.dat

# CitcomS.solver.visc
TDEPV=on
VISC_UPDATE=on
VMAX=on
VMIN=on
num_mat=4
rheol=1
visc0=1,1,1,1
viscE=2.99573,2.99573,2.99573,2.99573
viscT=0.5,0.5,0.5,0.5
visc_max=1e+06
visc_min=0.001
visc_smooth_method=1
```

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 Nusselt 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.

```
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
```

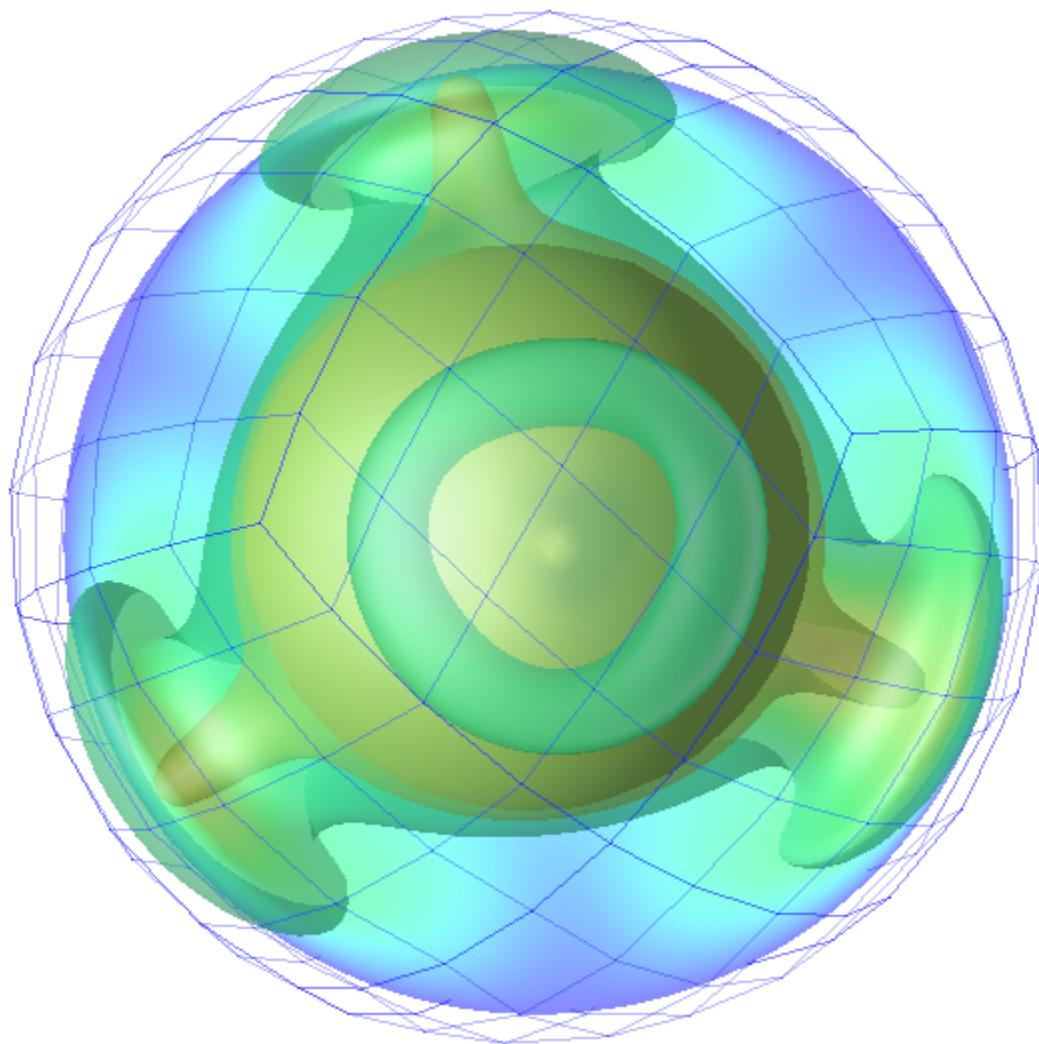


Figure 6.10: Cookbook 8: The steady state temperature field at the 10,000th time step. A tetrahedral symmetric convection pattern is developed. Two temperature isosurfaces of 0.4 and 0.8 are shown.

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

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

A.1.2 Parameters that Control Output Files

<code>output_format=ascii</code>	Choose the format and layout of the output files. Can be either <code>ascii</code> , <code>ascii-gz</code> or <code>hdf5</code> . If <code>ascii-gz</code> is chosen, the code places gzipped files into <code>data_dir</code> , and will put all time-step output into subdirectories of <code>data_dir</code> . The same naming logic holds for reading old velo files.
<code>output_optional="surf, botm, tracer"</code>	Choose additional output, including <code>surf</code> , <code>botm</code> , <code>geoid</code> , <code>seismic</code> , <code>stress</code> , <code>pressure</code> , <code>connectivity</code> , <code>horiz_avg</code> , <code>tracer</code> , <code>heating</code> , <code>comp_el</code> and <code>comp_nd</code> .
<code>datadir=". "</code>	Controls the location of output files.
<code>datafile="regtest"</code>	Controls the prefix of output file names such as <code>regtest.xxx</code> . Cannot contain the “/” character if <code>output_format=ascii</code> .
<code>storage_spacing=10</code> (in non-Pyre version) or <code>monitoringFrequency=100</code> (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.
<code>checkpointFrequency=100</code>	The time-step interval between checkpoint output, which can be used later to resume the computation.
<code>output_ll_max=20</code>	This parameter controls the maximum degree of spherical harmonics coefficients for geoid output.
<code>self_gravitation=off</code>	Considering the effect the self gravitation on the geoid or not.
<code>use_cbf_topo=off</code>	Using the Consistent Boundary Flux (CBF) method to compute the dynamic topography or not.

A.1.3 Mesh and Processors Setup

<code>nproc_surf=1</code>	This specifies the number of spherical caps of the mesh; must be <code>1</code> for regional spherical model and <code>12</code> for full spherical model.
<code>nprocx=1</code> <code>nprocy=1</code> <code>nprocz=1</code>	These specify the number of processors in each spherical cap. For a full spherical model, <code>nprocx</code> must be equal to <code>nprocy</code>
<code>nodex=9</code> <code>nodey=9</code> <code>nodez=9</code>	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, <code>nodex</code> must be equal to <code>nodey</code>
<code>mgunitx=8</code> <code>mgunity=8</code> <code>mgunitz=8</code> <code>levels=1</code>	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 <code>conjgrad</code> solver is used. For a full spherical model, <code>mgunitx</code> must be equal to <code>mgunity</code>

A.1.4 Domain Size

<code>theta_min=1.0708 theta_max=2.0708 fi_min=0 fi_max=1</code>	These parameters specify the horizontal extent of the computational domain. <code>theta_min</code> and <code>theta_max</code> are the colatitude measured in radians from the north pole. <code>fi_min</code> and <code>fi_max</code> are the longitudes measured from the prime meridian eastward in radians. Only in regional CitcomS.
<code>radius_inner=0.55 radius_outer=1.0</code>	These parameters specify the radial extent of the computational domain. <code>radius_inner</code> and <code>radius_outer</code> 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.
<code>coor=0 coor_file="coor.dat" coor_refine=0.1,0.15,0.1</code>	If <code>coor=0</code> , there will be uniform mesh in the latitudinal, longitudinal, and radial directions. If <code>coor=1</code> , the coordinate is reading from the file specified by <code>coor_file</code> . This is used to have a regular but uneven spacing between elements. If <code>coor=2</code> , there will be uniform mesh in the latitudinal and longitudinal directions. The mesh in the radial direction is generated according to <code>coor_refine</code> , which is a vector of 4 numbers. The 1st value of <code>coor_refine</code> 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

<code>restart=off</code>	If <code>restart</code> is <code>on</code> , each processor will resume the computation from the checkpoint files.
<code>post_p=off</code>	Similar to <code>restart</code> , 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.
<code>datadir_old=". " datafile_old="regtest" solution_cycles_init=0</code>	If <code>restart</code> is <code>on</code> , for example, processor #5 will read its initial conditions from checkpoint file <code>regtest.chkpt.5.0</code> in this case.

A.1.6 Run Length

<code>minstep=1 maxtotstep=1000000 (only in pure C version) or steps=1 (only in Pyre version)</code>	The maximum and minimum number of time steps for the model, including the 0th time step.
<code>cpu_limits_in_seconds=360000000</code>	Controls the termination of the code based on total wall clock time used. Available only in pure C version.

A.1.7 Initial Conditions

<code>tic_method=0</code>	Which method to use to generate the initial temperature field.
---------------------------	--

<pre>datadir_old=." datafile_old="regtest" solution_cycles_init=0 zero_elapsed_time=on</pre>	<p>If <code>tic_method=-1</code>, the initial temperature is read from files. For example, processor #5 will read its initial temperature from old velo file <code>regtest.velo.5.0</code> in this case. If <code>zero_elapsed_time</code> is <code>on</code>, the initial time is set to zero. If it is <code>off</code> and <code>tic_method=-1</code>, the initial time is read in from the old velo files. Note that this option has no effect when <code>restart=on</code>.</p>
<pre>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</pre>	<p>If <code>tic_method=0</code>. The initial temperature is a linear temperature gradient with perturbations at specific layers, where <code>num_perturbations</code> specifies the number of perturbations, and <code>perturblayer</code> specifies the layers to be perturbed, representing the number of the mesh node in radial direction. There must be as many entries as <code>num_perturbations</code> in a comma-separated list. The perturbation added to each layer is given by:</p> $mag \times \cos(m\phi) \times P_{lm}(\cos \theta)$ <p>for the full sphere, and by:</p> $mag \times \cos\left(\frac{(\theta - \theta_{min}) l\pi}{\theta_{max} - \theta_{min}}\right) \times \cos\left(\frac{(\phi - \phi_{min}) m\pi}{\phi_{max} - \phi_{min}}\right)$ <p>for the regional sphere.</p> <p>If <code>tic_method=1</code>, T is 1 everywhere, except a cold thermal boundary layer at the top, whose temperature is determined by the half-space cooling model and <code>half_space_age</code> (in million of years, Myrs).</p> <p>If <code>tic_method=2</code>, T is <code>mantle_temp</code> 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 <code>half_space_age</code> (in Myrs). The location of the blob is default to the center of the computational domain.</p> <p>If <code>tic_method=3</code>, the initial temperature is a conductive profile with perturbations to all layers. The perturbation is given by:</p> $mag \times \sin\left(\frac{(r - r_{in})\pi}{r_{out} - r_{in}}\right) (\sin(m\phi) + \cos(m\phi)) P_{lm}(\cos \theta)$ <p>for the full sphere, and by:</p> $mag \times \sin\left(\frac{(r - r_{in})\pi}{r_{out} - r_{in}}\right) \times \cos\left(\frac{(\theta - \theta_{min}) l\pi}{\theta_{max} - \theta_{min}}\right) \times \cos\left(\frac{(\phi - \phi_{min}) m\pi}{\phi_{max} - \phi_{min}}\right)$ <p>for the regional sphere.</p> <p>If <code>tic_method=4</code>, the initial temperature is read from grd files.</p> <p>If <code>tic_method=10</code>, T is <code>mantle_temp</code> everywhere, except for a cold thermal boundary layer at the top and perturbations at all layers, similar to <code>tic_method=3</code>.</p> <p>If <code>tic_method=11</code>, T is <code>mantle_temp</code> everywhere, except for a hot thermal boundary layer at the bottom and perturbations at all layers, similar to <code>tic_method=3</code>.</p> <p>If <code>tic_method=12</code>, T is <code>mantle_temp</code> everywhere, except for a cold thermal boundary layer, a hot thermal boundary layer at the bottom and perturbations at all layers, similar to <code>tic_method=3</code>.</p> <p>If <code>tic_method=90</code>, T is 0 everywhere, except for a single perturbation at the middle layer. This initial temperature is good for comparison with analytical solutions.</p>

A.1.8 Boundary Conditions

<code>topvbc=0</code> <code>topvbxval=0.0</code> <code>topvbyval=0.0</code>	Surface velocity boundary condition parameters. If <code>topvbc</code> is 0, <code>topvbxval</code> and <code>topvbyval</code> specify the tangential surface stress (stress BC). If <code>topvbc</code> is 1, <code>topvbxval</code> and <code>topvbyval</code> specify the tangential surface velocity (velocity BC). The surface normal velocity is zero in these two cases (impermeable BC).
<code>botvbc=0</code> <code>botvbxval=0.0</code> <code>botvbyval=0.0</code>	As above, but for bottom velocity boundary conditions.
<code>side_sbcs=off</code>	Enable traction boundary condition for the sidewalls or not. Must be <code>on</code> for coupled model.
<code>pseudo_free_surf=off</code>	Enable pseudo free surface or not.
<code>toptbc=1</code> <code>toptbcval=0.0</code>	Surface temperature boundary conditions. If <code>toptbc</code> is 0, <code>toptbcval</code> specifies the surface heat flux (not working in this version). If <code>toptbc</code> is 1, the <code>toptbcval</code> specifies the surface temperature.
<code>bottbc=1</code> <code>bottbcval=1.0</code>	As above, but for bottom temperature boundary conditions.
<code>temperature_bound_adj=off</code> <code>depth_bound_adj=0.157</code> <code>width_bound_adj=0.08727</code> <code>lith_age_depth=0.0314</code>	Additional parameters for temperature boundary conditions when <code>lith_age</code> is <code>on</code> .

A.1.9 Non-Dimensional Numbers

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

A.1.10 Depth Information

<code>z_lith=0.014</code> <code>z_410=0.06435</code> <code>z_lmantle=0.105</code> <code>z_cmb=0.439</code>	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 <code>z_lith</code> to an arbitrary depth, for example.
---	--

A.1.11 Viscosity

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

<code>num_mat=4</code>	This specifies the number of material layers. Material 1 is at depth between 0 and <code>z_lith</code> , material 2 between <code>z_lith</code> and <code>z_410</code> , material 3 between <code>z_410</code> and <code>z_lmantle</code> , and material 4 between <code>z_lmantle</code> and the bottom. If <code>mat_control</code> is on, then a multiplicative factor is applied to the viscosity, as defined below.
<code>visc0=1,1,1,1</code>	The pre-exponent factor of layered viscosity structure (η_0 in the equations below). There must be as many entries as <code>num_mat</code> in a comma-separated list.
<code>TDEPV=off</code>	Enable temperature dependence or not.
<code>rheol=3</code>	When <code>rheol=1</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(E_\eta(T_\eta - T))$ When <code>rheol=2</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(-T/T_\eta)$ When <code>rheol=3</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp\left(\frac{E_\eta}{T^*+T_\eta} - \frac{E_\eta}{1+T_\eta}\right)$, where $T^* = \min(\max(T, 0), 1)$. When <code>rheol=4</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp\left(\frac{E_\eta + Z_\eta(1-r)}{T^*+T_\eta}\right)$ When <code>rheol=5</code> , same as <code>rheol=3</code> , except the viscosity cut-off is applied before <code>mat_control</code> . When <code>rheol=6</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp(E_\eta(T_\eta - T^*) + Z_\eta(1-r))$ When <code>rheol=7</code> , temperature-dependent viscosity is computed by $\eta = \eta_0 \times \exp\left(\frac{E_\eta + Z_\eta(1-r)}{T+T_\eta} - \frac{E_\eta + Z_\eta(1-r_{inner})}{1+T_\eta}\right)$, where r_{inner} is the inner radius of the mesh. When <code>rheol=8</code> , same as <code>rheol=3</code> , except viscosity reduction is applied when the temperature exceeds the solidus. When <code>rheol=9</code> , same as <code>rheol=3</code> , except using T , not T^* . When <code>rheol=10</code> , same as <code>rheol=8</code> , except using T , not T^* .
<code>viscE=1,1,1,1</code> <code>viscT=1,1,1,1</code> <code>viscZ=1,1,1,1</code>	Parameters defining viscosity law (E_η , T_η , and Z_η in the equations above, respectively). There must be as many entries as <code>num_mat</code> in a comma-separated list.
<code>SDEPV=off</code>	Enable stress dependence (non-Newtonian) or not.
<code>sdepv_expt=1,1,1,1</code> <code>sdepv_misfit=0.001</code>	If <code>SDEPV</code> is on, these specify the exponent in the viscosity law and the criterion of convergence test. There must be as many entries as <code>num_mat</code> in a comma-separated list.
<code>PDEPV=off</code>	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 $\sigma_y = \min(a + b(1-z), y)$ 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 $\eta' = \frac{\eta_p \eta}{(\eta + \eta_p)}$ (<code>pdepv_eff=on</code>) or $\eta' = \min(\eta, \eta_p)$ (<code>pdepv_eff=off</code>).
<code>pdepv_a=1e20,1e20,1e20,1e20</code> <code>pdepv_b=0,0,0,0</code> <code>pdepv_y=1e20,1e20,1e20,1e20</code>	Parameters for σ_y .
<code>pdepv_eff=on</code>	Effective or minimum viscosity “plasticity” (see above).
<code>pdepv_offset=0</code>	Offset for plastic viscosity η_p^0 .
<code>CDEPV=off</code>	Compositionally dependent viscosity pre-factor (only for <code>tracer=on</code>). 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].
<code>cdepv_ff=1,1</code>	Flavor-wise viscosity pre-factors for C = 0 and C = 1, respectively.
<code>low_visc_channel=off</code> <code>low_visc_wedge=off</code>	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

<code>tracer=off</code>	If on, enables the tracers.
<code>tracer_ic_method=0</code> <code>tracers_per_element=10</code> <code>tracer_file="tracer.dat"</code>	Specify the initial location of the tracers. If <code>tracer_ic_method=0</code> , the tracers are generated randomly, with the number of tracers per element specified by <code>tracers_per_element</code> . If <code>tracer_ic_method=1</code> , the location of the tracers is read from a file specified in <code>tracer_file</code> . If <code>tracer_ic_method=2</code> , the location of the tracers is read from the old tracer output, similar to <code>tic_method=-1</code> .
<code>tracer_flavors=0</code>	The number of flavors among the tracers. If set to 0, flavor counting is turned off.
<code>ic_method_for_flavors=0</code> <code>z_interface=0.7</code>	Specify the initial flavors of the tracers. Used only when <code>tracer_ic_method=0</code> . Currently only <code>ic_method_for_flavors=0</code> is supported. A layered structure is generated. <code>z_interface</code> must be a comma-separated list with <code>(tracer_flavors-1)</code> entries. Tracers above the 1st radius in <code>z_interface</code> are of flavor 0, between the 1st and 2nd radii are of flavor 1, ... etc.
<code>regular_grid_deltheta=1.0</code> <code>regular_grid_delphi=1.0</code>	The grid spacing of the regular grid. The regular grid is an auxiliary grid to help locate the tracers.
<code>chemical_buoyancy=on</code>	If on, enables thermo-chemical convection.
<code>buoy_type=1</code>	If <code>buoy_type=1</code> , the composition field is determined by the ratio method [19]. (No other methods are implemented yet.)
<code>buoyancy_ratio=1.0</code>	The ratio of chemical density anomaly to the reference density, must be a comma-separated list with <code>(tracer_flavors-1)</code> entries.
<code>itracer_warnings=on</code>	The warning level of the tracer module.
<code>tracer_enriched=off</code> <code>Q0_enriched=0.0</code>	Whether the composition anomaly is associated with radioactive heating anomaly. If <code>on</code> , specifies the internal heating number inside the composition anomaly.

A.1.19 Dimensional Information

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

A.1.20 Required Information

<code>Problem=convection</code> <code>Geometry=sphere</code>	For this version of CitcomS, all of these parameters must be set as indicated.
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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
...
...
nodey 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:

$$\begin{bmatrix} S_{\theta\theta} & S_{\theta\phi} & S_{\theta r} \\ S_{\phi\theta} & S_{\phi\phi} & S_{\phi r} \\ S_{r\theta} & S_{r\phi} & S_{rr} \end{bmatrix} \quad (\text{C.1})$$

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 coefficients 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

$$\sum (S_{lm} \sin(m\phi) + C_{lm} \cos(m\phi)) P_{lm}(\cos \theta)$$

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 37.

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 integers: `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 $nproc \times ncolumns$ 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 integers: `node_x`, `node_y`, `node_z`, `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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