CitcomS

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at

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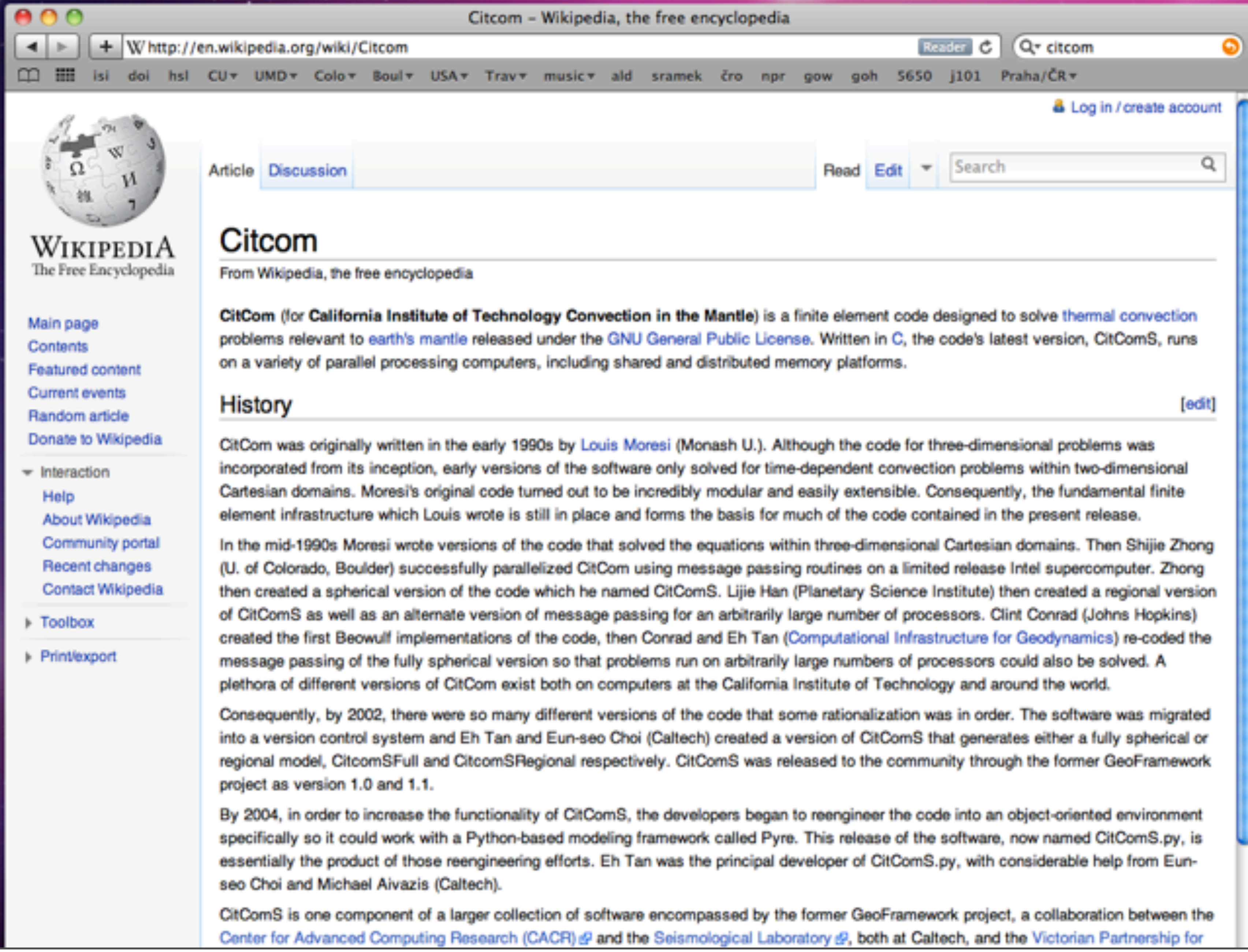
CitcomS

- 3-D spherical global finite element highly parallel convection code
- written by geophysicist(s) specifically for convection in planetary mantles
- variable viscosity, tracers & compositions, phase transitions, dynamic topography, geoid
- open source
- maintained, documented, supported (CIG)

http://en.wikipedia.org/wiki/Citcom



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Citcom

From Wikipedia, the free encyclopedia

CitCom (for **California Institute of Technology Convection in the Mantle**) is a finite element code designed to solve thermal convection problems relevant to earth's mantle released under the GNU General Public License. Written in C, the code's latest version, CitComS, runs on a variety of parallel processing computers, including shared and distributed memory platforms.

History [edit]

CitCom was originally written in the early 1990s by Louis Moresi (Monash U.). 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 (U. of Colorado, Boulder) 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 (Planetary Science Institute) 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 (Johns Hopkins) created the first Beowulf implementations of the code, then Conrad and Eh Tan (Computational Infrastructure for Geodynamics) 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 (Caltech) created a version of CitComS that generates either a fully spherical or regional model, CitcomSFull and CitcomSRegional respectively. 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, now named CitComS.py, is essentially the product of those reengineering efforts. Eh Tan was the principal developer of CitComS.py, with considerable help from Eun-seo Choi and Michael Aivazis (Caltech).

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) and the Seismological Laboratory, both at Caltech, and the Victorian Partnership for

Citcom = **C**alifornia **I**nstitute of **T**echnology **Co**nvection in the **M**antle

Citcom ... 2-D then 3-D cartesian serial [Moresi & Solomatov 1995, Moresi & Gurnis 1996]

+ spherical geometry
+ new grid design
+ parallel computing
+ full multigrid algorithm
→ **CitcomS** [Zhong & Zuber 2000]

+ tracers (chemical components) [McNamara & Zhong 2004]

In early 2000's Shijie Zhong provided the code to "CIG" or Computational Infrastructure in Geodynamics www.geodynamics.org where it has been maintained, documented and supported, messed with (i.e., Pyre framework...)

open source version
You will use this one

Shijie's version
I am familiar with this one

The "guts" are the same but the "skin" is different
(Pyre, file structure, ...)

Can solve

- classical Boussinesq
- extended Boussinesq
- compressible, anelastic (i.e, TALA or truncated anelastic liquid approximation)

- global spherical shell
- regional spherical shell domain

Governing equations – dimensional

TALA (truncated anelastic liquid approximation)

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

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

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

$$\frac{\partial C}{\partial t} + (\mathbf{u} \cdot \nabla) C = 0$$

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

thermal expansion, phase change, compositional buoyancy

[from CIG manual]

Governing equations – non-dimensional

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

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

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

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

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

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

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

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

[from CIG manual]

Viscosity

Obviously, user can define various viscosity options. I will use the following setting in '*inputTC10*':

`Viscosity=system`	viscosity depends on system state (temperature, ...)
`rheol=3  TDEPV=on`	option 3 is defined in function `visc_from_T` in file '*Viscosity_Structure.c*'
`VISC_UPDATE=on`	viscosity is updated (every other timestep)
`visc_smooth_method=1`	??

In option 3, the viscosity is calculated based on dimensional equation

$$\eta=\eta_{ref}(r)\exp\left[\frac{E'+PV'}{RT}\right]=\eta_{ref}(r)\exp\left[\frac{E'+V'\rho_0 g(1-r)}{RT}\right],$$

that is temperature- and pressure/depth-dependent viscosity (through activation energy E' and activation volume V') superimposed on a prescribed radial profle $\eta_{ref}(r)$ (viscosity layering). Taking the CMB value as the reference viscosity and performing non-dimensionalization, one gets

$$\eta=\eta_r\exp\left[\frac{E+V(1-r)}{T_s+T}-\frac{E+V(1-r_c)}{T_s+1}\right],$$

where

$E = E'/(R\,\Delta T)$, $V = \rho_0\, g\, R_0\, V'/(R\,\Delta T)$, $\eta_r(r) = \eta_{ref}(r)/\eta_{ref}(r_{CMB})$, $T_s = T_{surf}/\Delta T$

(see *Roberts & Zhong 2006 JGR*; note that different formulations were used in other CitcomS papers, e.g. *Zhong et al. 2000 JGR, Zhong et al. 2008 G3*)

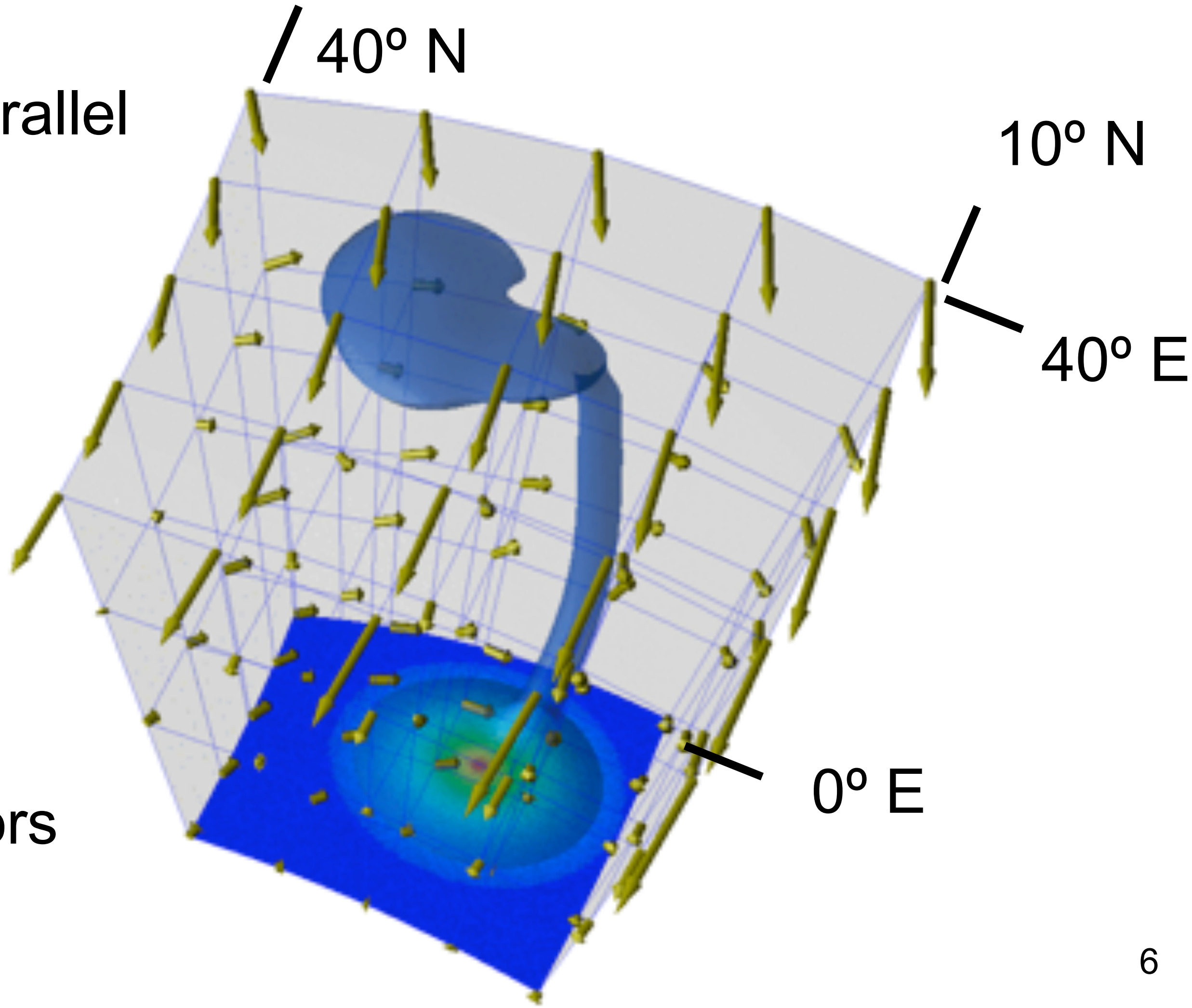
[This relates to CU Boulder version]

Many different options – see CIG Manual, Sec. A.1.11
(or you can code your own...)

Regional Mesh

Grid lines are parallel to longitude and latitude

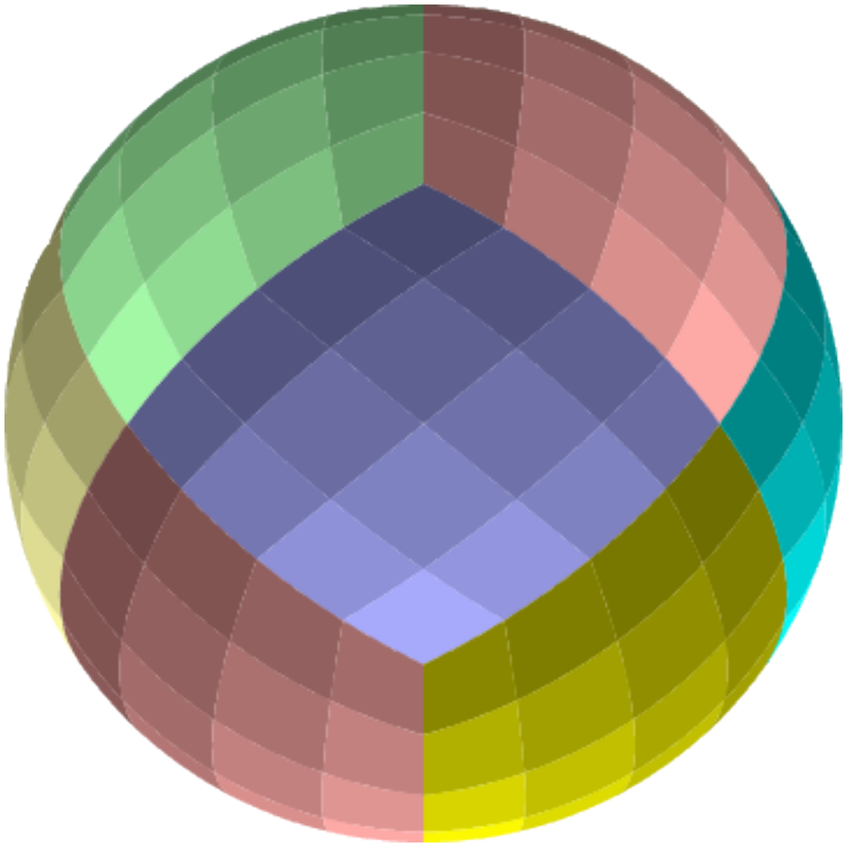
The whole domain can be partitioned into NxMxL processors



Computational Infrastructur
Geodynami

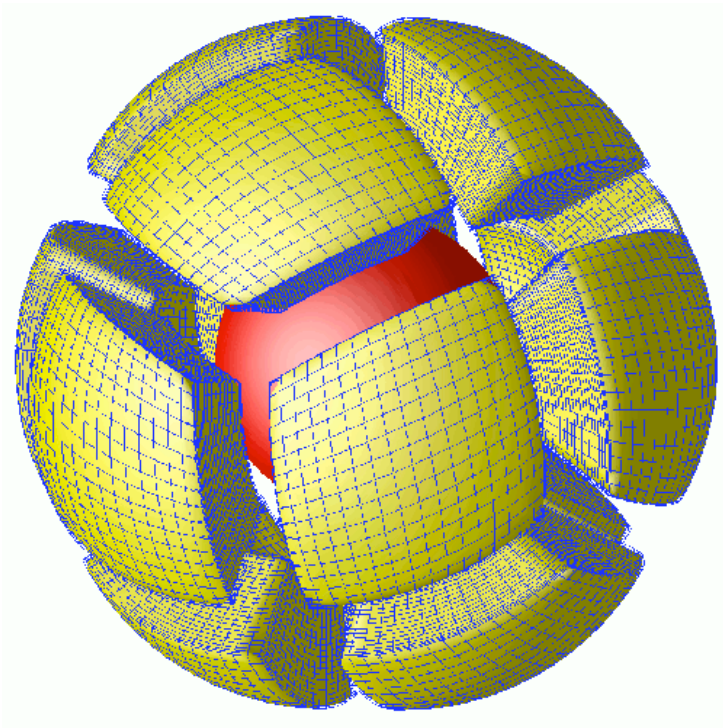
Global Mesh

- 12 caps
- Each cap extends from the surface to the CMB
- Each cap can be partitioned into NxNxM processors
- 12xNxNxM processors in total (N=4 in this figure)

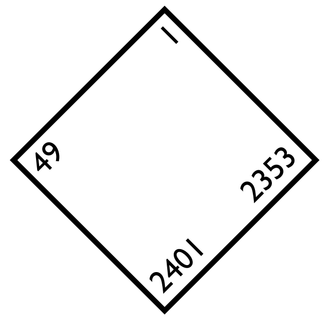


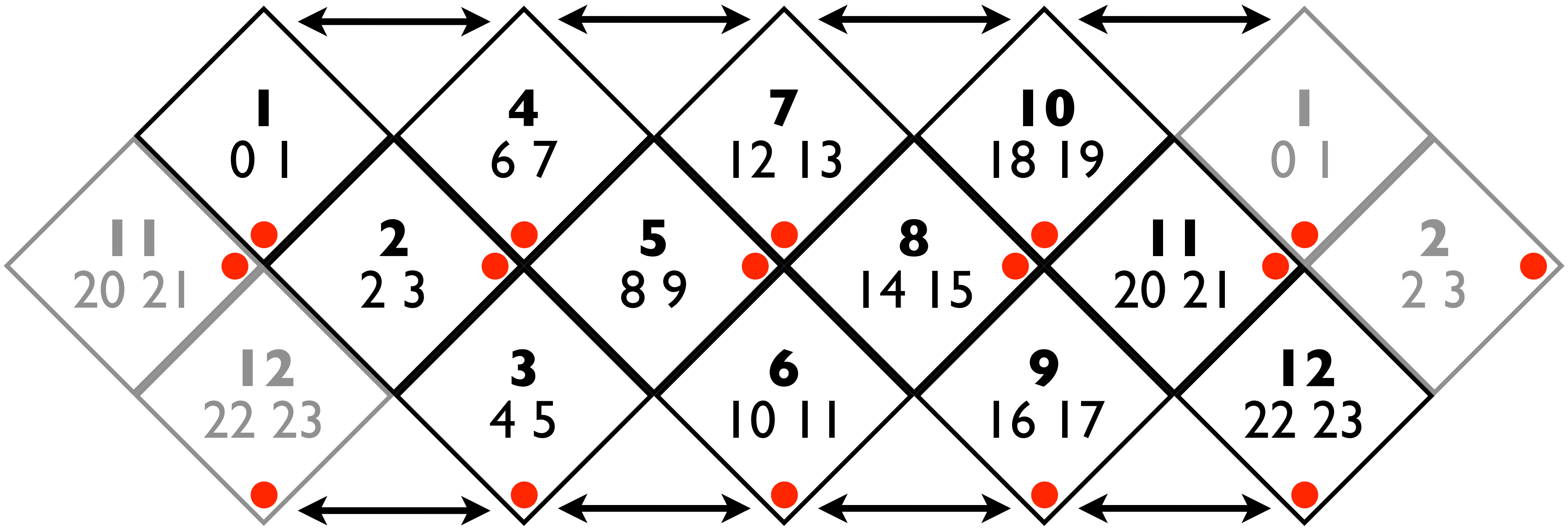
Computational Infrastructure for Geodynamics

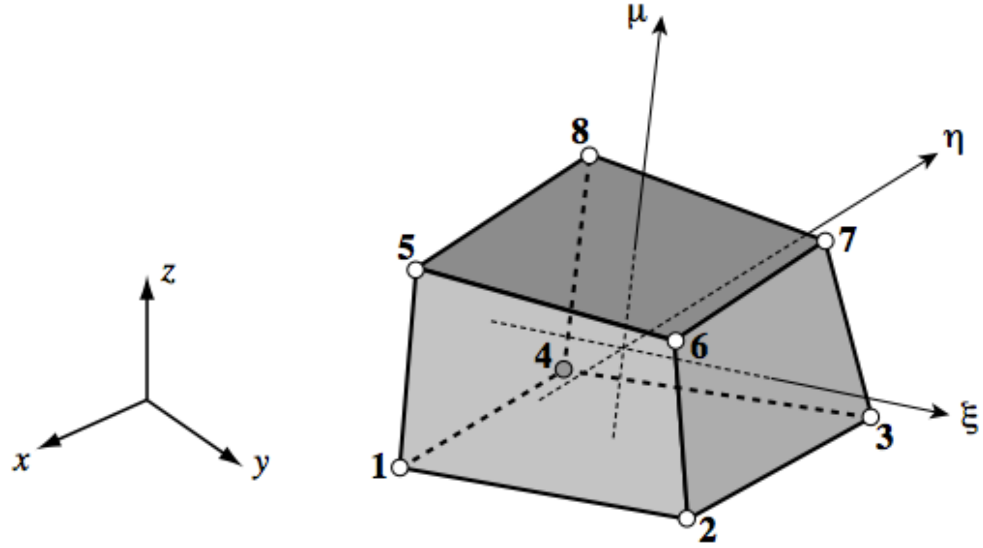
12 caps



need at least 12 cores for full spherical shell





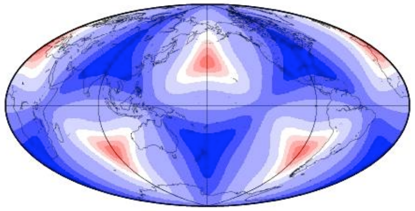


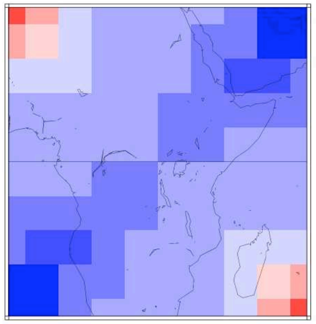
- trilinear hexahedral elements
  - brick elements – only approximate sphericity
  - 8 velocity nodes, trilinear approximation
  - 1 pressure node, constant

Visualization in GMT

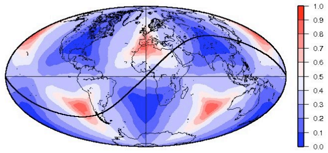
- plot_layer.py
  - plot horizontal cross section, for both regional and global versions
- plot_annulus.py
  - plot radial cross section, for global version only
- sample data files in *visual/samples/*

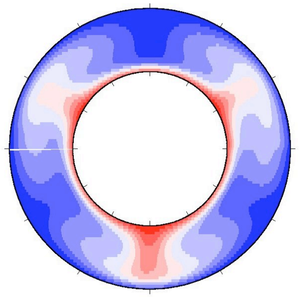
plot_layer.py



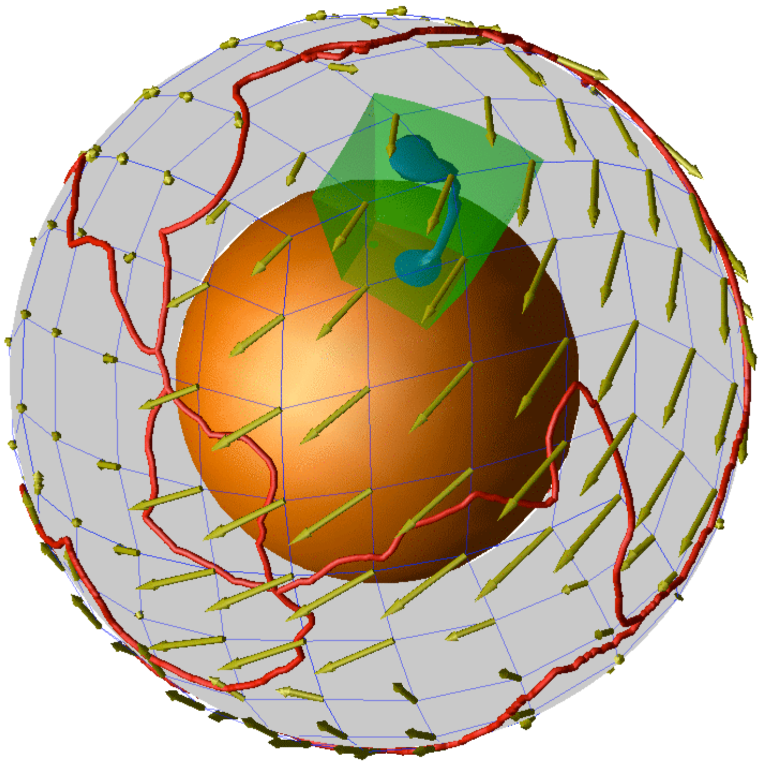


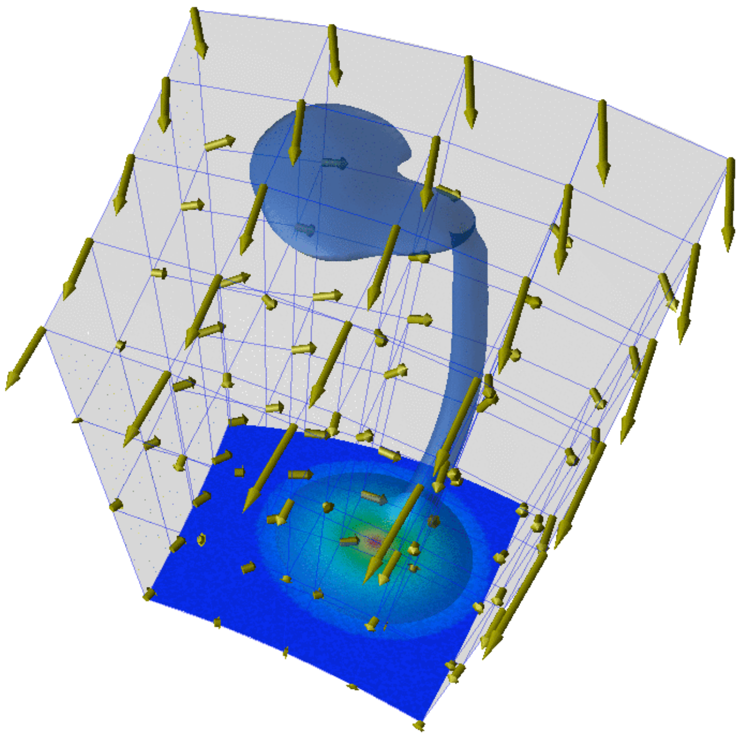
plot_annulus.py



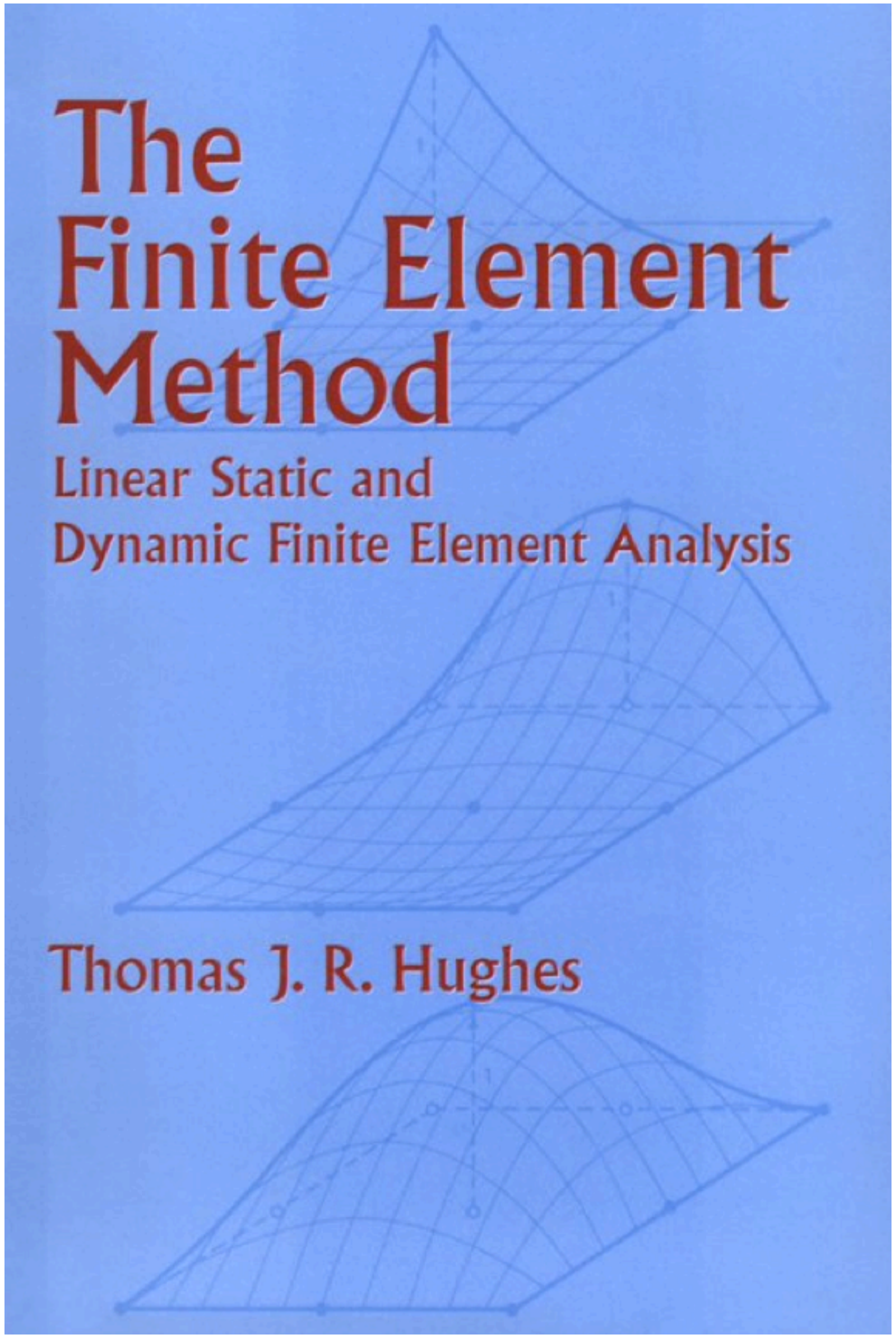


Visualization in OpenDX





Computational Infrastructure for Geodynamics

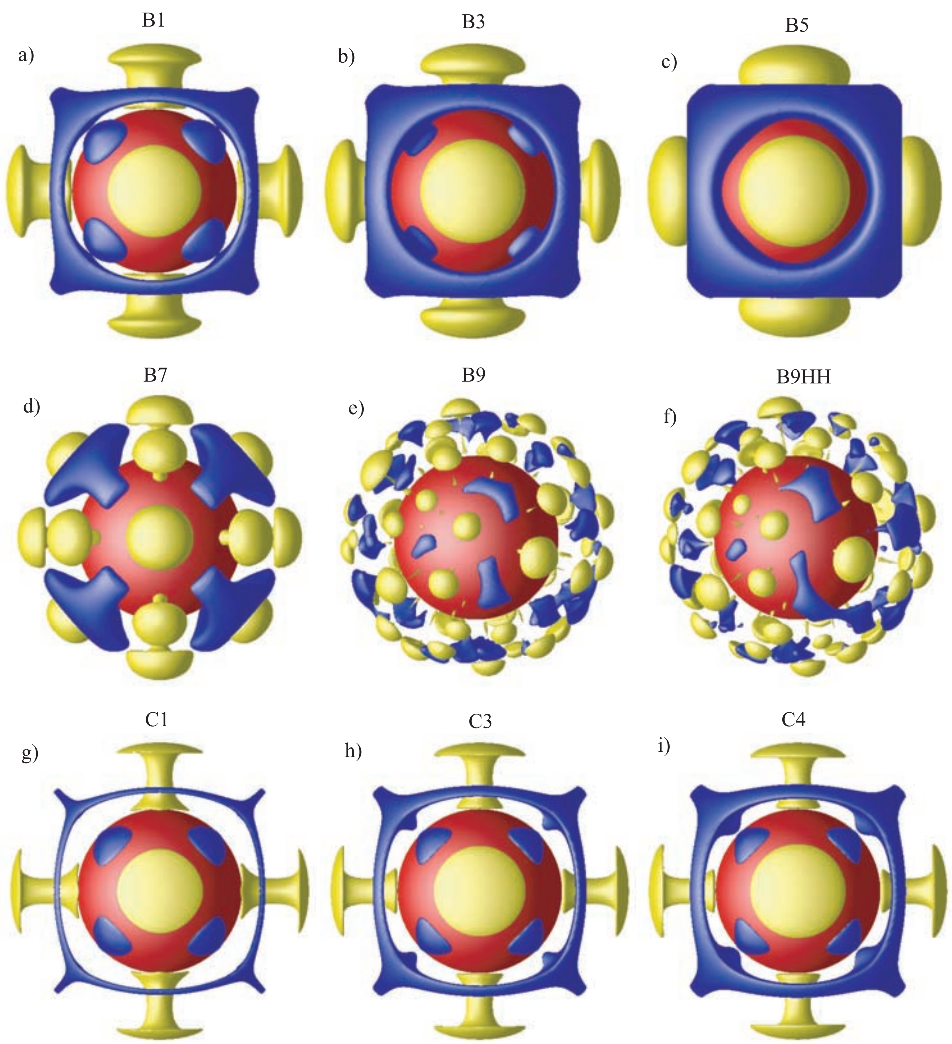

The Finite Element Method
Linear Static and
Dynamic Finite Element Analysis
Thomas J. R. Hughes

Major ingredients of the mathematical & numerical model

- streamline upwind Petrov-Galerkin approx (SUPG) for the energy equation
- mixed formulation in primitive variables (P,v) and Uzawa algorithm with two-loop iterations for Stokes problem
- Uzawa: outer loop (P) – preconditioned conjugate gradient method; inner loop (v) – full multigrid methods
- Gauss-Seidel iteration for inner nodes, Jacobi iteration for shared nodes
- predictor–corrector and 2nd order Runge-Kutta to advect tracers, ratio method used to map tracers to composition
- Poisson equation for gravitational potential solved with a spectral method

Benchmarks

Geochemistry Geophysics Geosystems G3 ZHONG ET AL.: BENCHMARKS OF 3-D SPHERICAL CONVECTION MODELS 10.1029/2008GC002048



Zhong et al. 2008 G^3

Parallel efficiency

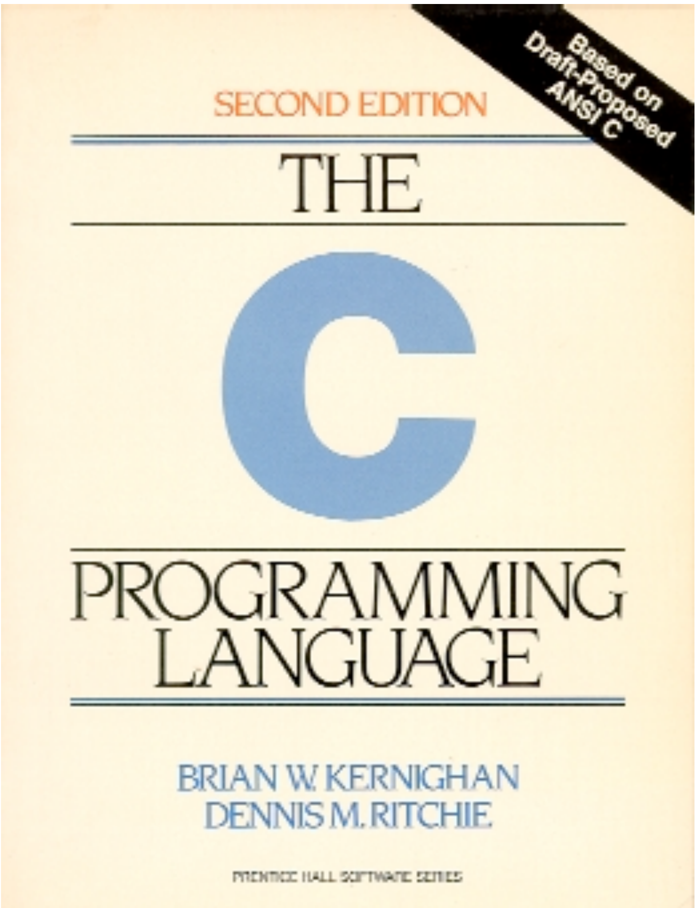
Geochemistry Geophysics Geosystems G3 ZHONG ET AL.: BENCHMARKS OF 3-D SPHERICAL CONVECTION MODELS 10.1029/2008GC002048

Table 1. CPU Time With Different Number of Cores

N_c[a]	Total Time (s)	Time for Zeroth Step (s)	Iterations[b]	Time Per v Iteration (s)	Efficiency (%)
12(1 × 1 × 1)	69.8	9.3	112(118)	0.59	100
24(1 × 1 × 2)	64.1	9.8	95(103)	0.62	95
48(2 × 2 × 1)	53.7	9.7	73(78)	0.69	86
96(2 × 2 × 2)	53.9	8.8	74(79)	0.68	87
192(4 × 4 × 1)	47.2	11.3	55(63)	0.75	79
384(4 × 4 × 2)	46.8	8.2	55(58)	0.81	73
768(4 × 4 × 4)	52.4	10.0	58(61)	0.86	69
1536(8 × 8 × 2)	58.2	16.0	60(70)	0.83	71
3072(8 × 8 × 8)	59.1	17.5	54(57)	1.04	57

[a] N_c stands for the number of core. The numbers in the parentheses represent the domain decomposition in each of 12 spherical caps for CitcomS. For example, 2 × 2 × 2 indicates that each cap is further divided into two in each of the three directions with the last number for the radial direction.
[b] The numbers in and out of the parentheses represent the numbers of inner loop velocity iteration and of outer loop pressure iteration, respectively.

C

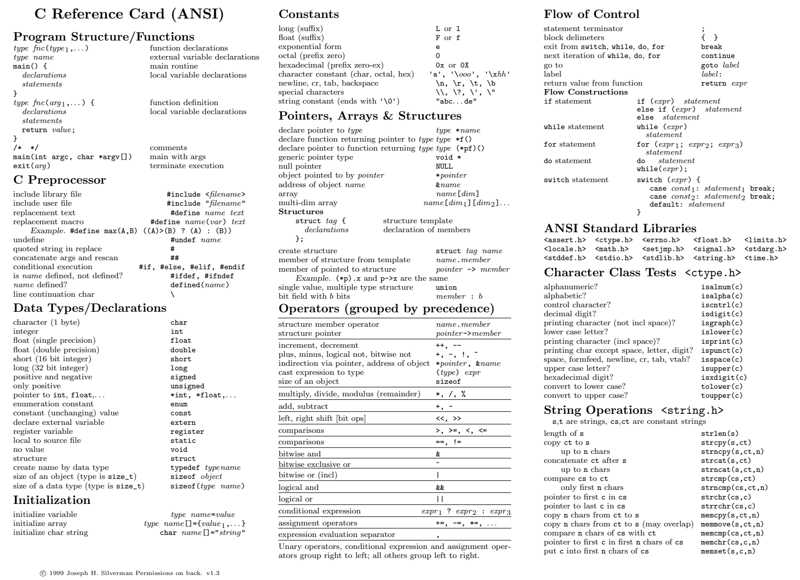


The C Book — Table of Contents

This is the online version of *The C Book*, second edition by Mike Banahan, Declan Brady and Mark Doran, originally published by Addison Wesley in 1991. This version is made freely available.

http://publications.gbdirect.co.uk/c_book/

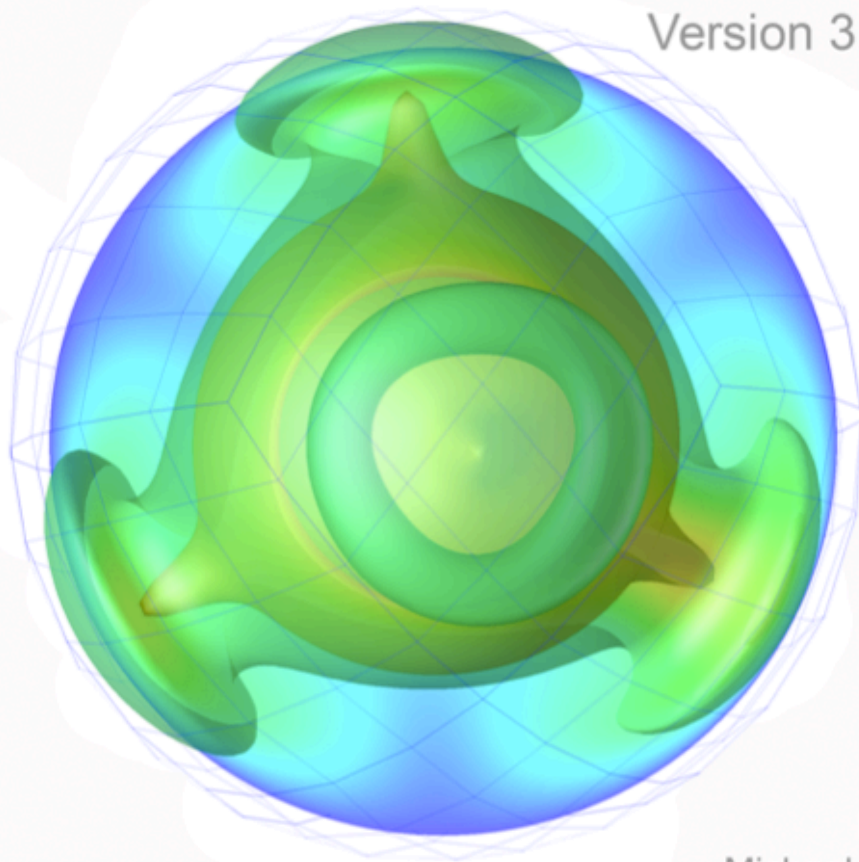
C Reference Card (ANSI)



COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)

CitcomS

User Manual
Version 3.1.1.1



Eh Tan
Michael Gurnis
Luis Armendariz
Leif Strand
Susan Kientz

www.geodynamics.org

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