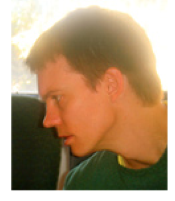
3-D Spherical Mantle Convection with Radial Basis Functions


Grady B. Wright
Boise State University


Natasha Flyer
NCAR


David Yuen
University of Minnesota

Brief History: Numerical Methods for Mantle Convection

Late 60s: Turcotte & Torrance, 2nd order finite-difference(FD) with 20x20 nodes for variable depth-dependent viscosity with the steady-state approach

Mid 70s: Weiss & McKenzie, time-dependent convection with staggered FDs

Late 70s: Woidt & Christiansen, Bi-cubic splines were introduced

Mid 80s: French school-Toulouse, 3-D spherical convection using spherical harmonics (SH) and 2nd order FD in the radial direction

Late 80s: Glatzmaier, 3-D spherical convection problem with Chebyshev polynomials in the radial direction and SH for the angular portion.

Early 90s: Tackley, used a 2nd order finite-volume method (FV) with multigrid in 3-D Cartesian geometry for variable viscosity

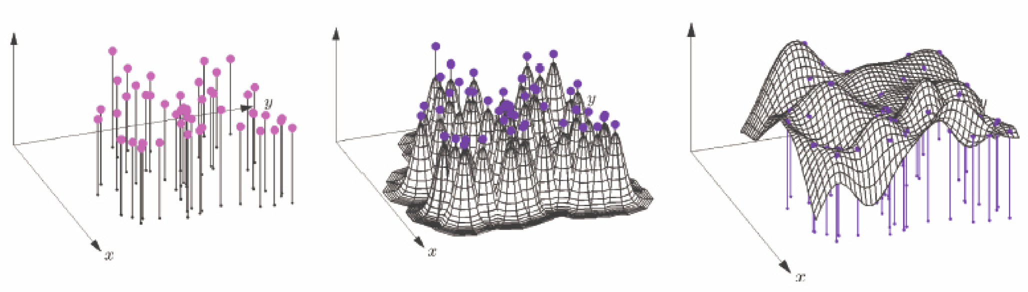
Mid 90s: Moresi, 2nd order finite-elements using a weak variational formulation

Late 90s: Extending Moresi's work to 3-D, resulting in CITCOM code-mainstay in the mantle convection community in this millenium.

Mid 00s: Kageyama, Yin-Yang grid for 3-D spherical problems with 2nd order FV

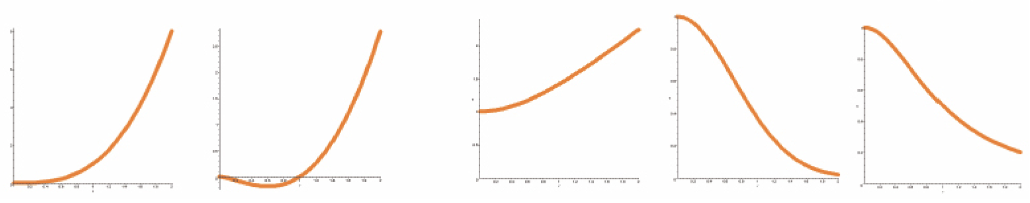
Introduction to Radial Basis Functions via Interpolation

In pictures:



Types: Piecewise smooth $\phi(r)$ — Infinitely smooth $\phi(r)$

Cubics	TP splines	Multiquadric	Gaussian	Inverse quadratic
r^3	$r^2 \log r$	$\sqrt{1+(\varepsilon r)^2}$	$e^{-(\varepsilon r)^2}$	$\frac{1}{1+(\varepsilon r)^2}$



In Formulas:

Given scattered data $(\underline{x}_k, f_k)$, $k = 1, 2, \dots, N$, the coefficients λ_k in

$$s(\underline{x}) = \sum_{k=1}^{N} \lambda_k \, \phi(\|\underline{x} - \underline{x}_k\|)$$

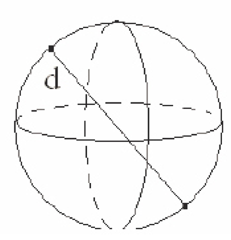
are found by collocation: $s(\underline{x}_k) = f_k$, $k = 1, 2, \dots, N$:

$$\begin{bmatrix} \phi(\|\underline{x}_1-\underline{x}_1\|) & \phi(\|\underline{x}_1-\underline{x}_2\|) & \cdots & \phi(\|\underline{x}_1-\underline{x}_N\|) \\ \phi(\|\underline{x}_2-\underline{x}_1\|) & \phi(\|\underline{x}_2-\underline{x}_2\|) & \cdots & \phi(\|\underline{x}_2-\underline{x}_N\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|\underline{x}_N-\underline{x}_1\|) & \phi(\|\underline{x}_N-\underline{x}_2\|) & \cdots & \phi(\|\underline{x}_N-\underline{x}_N\|) \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \vdots \\ \vdots \\ \lambda_N \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ \vdots \\ f_N \end{bmatrix}$$

where $\|\bullet\|$ is the Euclidean distance between 2 nodes

For spheres:

$$\mathrm{d} = \|\underline{x} - \underline{x}_k\| = \sqrt{(x-x_k)^2 + (y-y_k)^2 + (z-z_k)^2}$$
$$= \sqrt{2}\,\sqrt{1 - \cos\theta\cos\theta_k\cos(\varphi-\varphi_k) - \sin\theta\sin\theta_k}$$



Advantages:

- Algorithmic *Simplicity*

  Example: $\triangle_{surface} = \frac{1}{4}((4-d^2)\phi''(d) + \frac{4-3d^2}{d}\phi'(d))$

  $\triangle_{surface}$ Code using Gaussian RBFs (**2 lines**)

```
dsq = max(2-2*(x*x' + y*y' + z*z'),0);
L_sfc = 1/4*((4-dsq)*(-2*eps^2*exp(-eps^2*dsq) + ...
         2*eps^4*dsq*exp(-eps^2*dsq)) + ...
        (4-3dsq)/sqrt(dsq)*(-2*eps^2*sqrt(d)*exp(-eps^2*dsq));
```

- Simplicity of Algorithm *Independent of Dimension*

  d is a scalar measure between nodes that exist in n-dimensional space

- Handles Completely *Irregular Geometries* due to No Grids
- Gives *Spectral Accuracy* with Local Node *Refinement*

Thermal Convection Model in 3-D Spherical Shell

- Infinite Prandtl Number
- Constant Viscosity
- Incompressible
- Boussinesq Approximation

Momentum equation in terms of a polodial potential Φ:

$$\underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]}_{\triangle_{surface}}\Phi + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\Phi = r^2\Omega \qquad (1)$$

$$\triangle_{surface}\,\Omega + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\Omega = r^2 Ra\mathrm{T} \qquad (2)$$

Impermeable and shear-stress free boundary conditions at $r = 0.55/0.45,\ 1/0.45$

$$\vec{v} = \frac{1}{r^2}\triangle_{surface}\Phi\boldsymbol{e}_r + \frac{1}{r}\frac{\partial^2}{\partial r\partial\theta}\Phi\boldsymbol{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial^2}{\partial r\partial\theta}\Phi\boldsymbol{e}_\varphi$$

Energy equation

$$\frac{\partial \mathrm{T}}{\partial t} + \vec{v}\bullet\left(\frac{\partial}{\partial r}\boldsymbol{e}_r + \frac{1}{r}\frac{\partial}{\partial\theta}\boldsymbol{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\boldsymbol{e}_\varphi\right)\mathrm{T} = \frac{1}{r^2}\left[\triangle_{surface} + \frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]\mathrm{T}$$

$\mathrm{T} = 1$ at $r = 0.55/0.45$, $\mathrm{T} = 0$ at $r = 1/0.45$

Algorithm:

1) Discretize $\triangle_{surface}$, $\frac{\partial}{\partial\theta}$, $\frac{\partial}{\partial\varphi}$ using RBFs
2) Discretize $\frac{\partial}{\partial r}$, $\frac{\partial^2}{\partial r^2}$ using Chebyshev polynomials
3) Discretize time using a *time-splitting* scheme
   - 2nd order Adams-Moulton (AM2) in radial direction (implicit)
   - 3rd order Adams-Bashforth (AB3) in angular portion (explicit)
4) Time-step energy equation to get T^{n+1} - solution at time step $n+1$
5) Use T^{n+1} solution to solve for Ω^{n+1} in (2)
6) Use Ω^{n+1} solution to solve for Φ^{n+1} in (1)
7) Use Φ^{n+1} solution to calculate $\vec{v}^{\,n+1}$
8) Use $\vec{v}^{\,n+1}$ in energy equation to calculate T at next time step

Poisson Solver

Continuous: $\left(\underbrace{\triangle_{surface}}_{\downarrow\ \mathbf{S}\ \text{(RBF)}} + \underbrace{\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)}_{\downarrow\ \mathbf{R}\ \text{(Chebyshev)}}\right)\underbrace{\Omega}_{\downarrow\ \vec{\Omega}} = \underbrace{r^2 Ra\mathrm{T}}_{\downarrow\ \vec{\mathrm{T}}}$

Discrete: **S** (RBF), **R** (Chebyshev), $\vec{\Omega}$, $\vec{\mathrm{T}}$

Do not directly invert Laplace operator, use eigenvector decomposition of matrix

$$\mathbf{S} = \mathbf{P}\,\Lambda_\mathbf{S}\,\mathbf{P}^{-1}\ ,\quad \mathbf{R} = \mathbf{Q}\,\Lambda_\mathbf{R}\,\mathbf{Q}^{-1}$$

After some matrix algebra:

$$\underbrace{(\mathbf{I_M}\otimes\Lambda_\mathbf{S} + \Lambda_\mathbf{R}\otimes\mathbf{I_N})}_{\text{Diagonal}}\mathbf{P}^{-1}\vec{\Omega}\mathbf{Q} = \mathbf{P}^{-1}\vec{\mathrm{T}}\mathbf{Q}$$

Likewise,

$$(\mathbf{I_M}\otimes\Lambda_\mathbf{S} + \Lambda_\mathbf{R}\otimes\mathbf{I_N})\mathbf{P}^{-1}\vec{\Phi}\mathbf{Q} = \mathbf{P}^{-1}\vec{\Omega}\mathbf{Q}$$

Operation Count: $O(N^2M + M^2N)$ instead of $O(N^3M^3)$

Time-Stepping Scheme

$$\frac{\partial \mathrm{T}}{\partial t} = \underbrace{-\vec{v}\bullet\left(\frac{\partial}{\partial r}\boldsymbol{e}_r + \frac{1}{r}\frac{\partial}{\partial\theta}\boldsymbol{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\boldsymbol{e}_\varphi\right)\mathrm{T} + \frac{1}{r^2}\triangle_{surface}\mathrm{T}}_{f(\mathrm{T},t)\ \text{- explicit}} + \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\mathrm{T}}_{g(\mathrm{T},t)\ \text{- implicit}}$$

In discrete form:

$$\mathrm{T}^{n+1} = \mathrm{T}^n + \underbrace{\tfrac{\Delta t}{12}[23f(\mathrm{T}^n,t^n) - 16f(\mathrm{T}^{n-1},t^{n-1}) + 5f(\mathrm{T}^{n-2},t^{n-2})]}_{\text{AB3 - explicit}} + \underbrace{\tfrac{\Delta t}{2}[g(\mathrm{T}^{n+1},t^{n+1}) + g(\mathrm{T}^n,t^n)]}_{\text{AM2 - implicit}}$$

Or as implemented

$$\mathrm{T}^{n+1} = \left[\mathrm{T}^n + \tfrac{\Delta t}{12}[23f(\mathrm{T}^n,t^n) - 16f(\mathrm{T}^{n-1},t^{n-1}) + 5f(\mathrm{T}^{n-2},t^{n-2})] + \tfrac{\Delta t}{2}g(\mathrm{T}^n,t^n)\right]\left(\mathrm{I} - \tfrac{\Delta t}{2}g(\mathrm{T}^n,t^n)\right)^{-1}$$

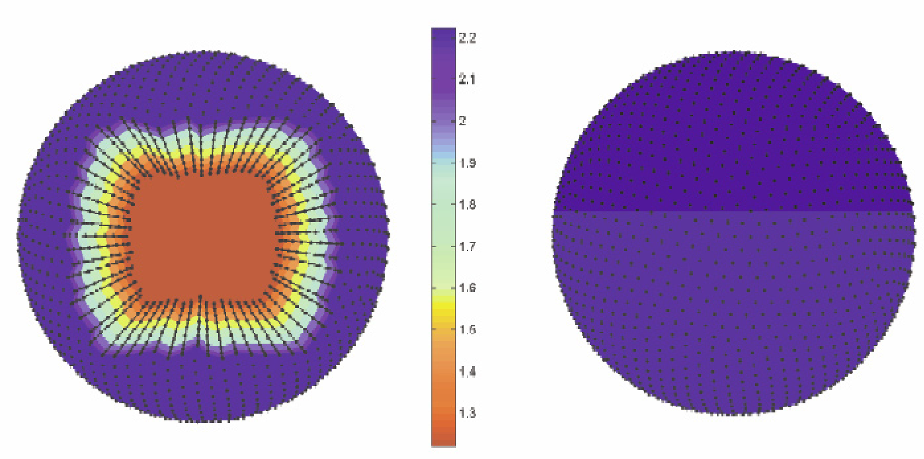
where $(\mathrm{I} - \frac{\Delta t}{2}g(\mathrm{T}^n,t^n))$ has been LU decomposed as a pre-processing step. The operators in r (such as in $g(\mathrm{T}^n,t^n)$) have been spatially discretized with Chebyshev polynomials and those in θ, φ with RBFs,

Total Cost per time step: $O(N^2M) + O(M^2N) + O(N^2)$

Node Layout

N = Number of RBF nodes on each spherical shell (θ and φ directions)

M = Number of Chebyshev nodes in radial direction

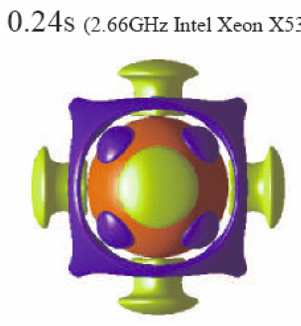


3-D Node Layout — **RBF nodes on a shell**

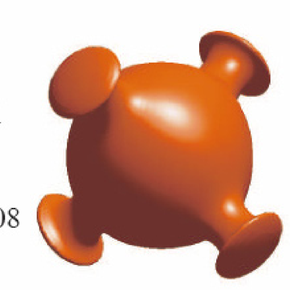
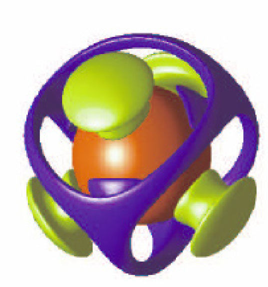
Numerical Results

Ra = 7000 N=1849 M=31 time/Δt = 0.24s (2.66GHz Intel Xeon X5335 6 cores)

Cubic Symmetry
Nu=3.496
RMS v=32.64

Tetrahedral Symmetry
Nu=3.609
RMS v=31.08

Isosurface T=0.5 — Isosurface of residual temperature δT Blue (-0.15), Yellow (0.15), Red (T=1)

Comparison with Other Numerical Methods for Ra = 7000

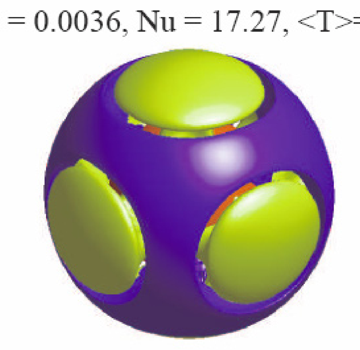
Model	Type	No. of Nodes	Nu_{outer}	$< V_{rms} >$	$< T >$
Tetrahedral					
Zhong [1]	FE	393,216	3.5126	32.66	0.2171
Kameyama [2]	FD	12,582,912	3.4945	32.6308	0.21597
Stemmer [3]	FV	663,552	3.4864	32.5894	0.21564
Harder [3]	SP-FD	552,960	3.4955	32.6375	0.21561
Harder [3]	SP-FD	Extrapolated*	3.4962	32.6424	0.21556
RBF	Pure SP	57,319	3.4962	32.6425	0.21556
Cubic					
Zhong [1]	FE	393,216	3.6254	31.09	0.2176
Kameyama [2]	FD	12,582,912	3.4945	32.6308	0.21597
Stemmer [3]	FV	663,552	3.5983	31.0226	0.21594
Harder [3]	SP-FD	552,960	3.6086	31.0765	0.21582
Harder [3]	SP-FD	Extrapolated*	3.6096	31.0821	0.21578
RBF	Pure SP	57,319	3.6096	31.0823	0.21578

SP=Spectral, FD=Finite Difference, FV = Finite Volume, FE = Finite Element
* Results extrapolated from the 552,960 SP-FD Harder model, based on the known convergence rate of the scheme

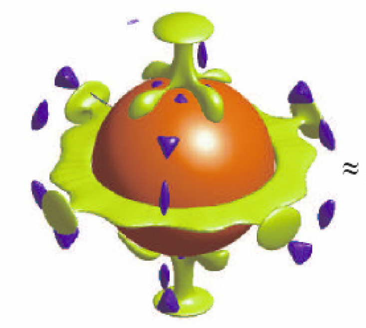
Numerical Results for Ra=70000

N=4096 M=51 time/Δt = 0.60s

T = 0.0036, Nu = 17.27, <T>= 0.31

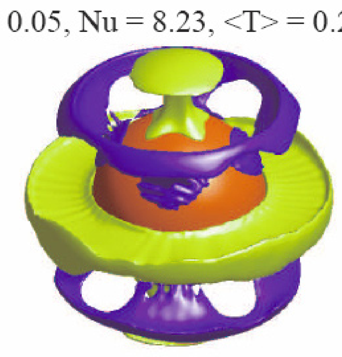


t = 0.0172, Nu = 4.91, <T> = 0.26

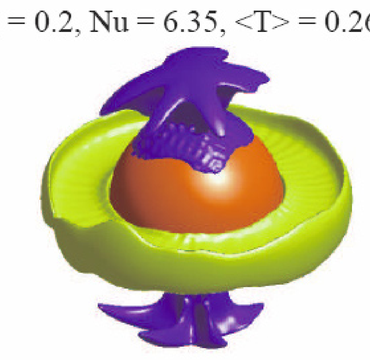


≈ age of Earth

t = 0.05, Nu = 8.23, <T> = 0.24

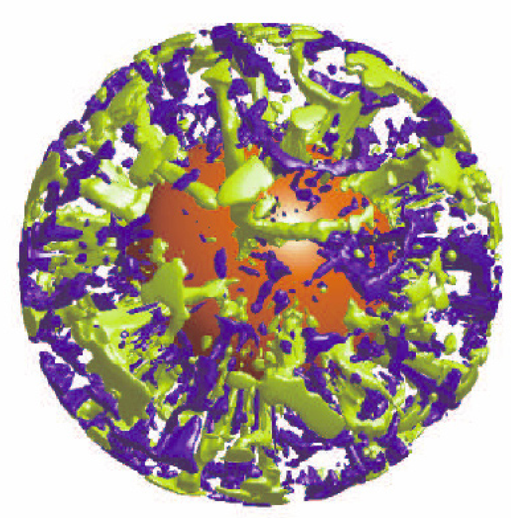


t = 0.2, Nu = 6.35, <T> = 0.26



Numerical Results for Ra=500,000

Nu = 14.46 , RMS v = 251



Isosurface of residual temperature δT
Blue (-0.15), Yellow (0.15), Red (T=1)

References:

[1] S. Zhong, A. McNamara, E. Tan, L. Moresi, M. Gurnis, A benchmark study on mantle convection in a 3-D spherical shell using CitComS, Geochem. Geophys. Geosyst., 9 (2008), no. 10.

[2] M.C. Kameyama, A. Kageyama, and T. Sato, Multigrid based simluation code for mantle convection in spherical shell using Yin-Yang grid, Phys. Earth Planet. Interiors, 171 (2008), 19-32.

[3] K. Stemmer, H. Harder, and U. Hansen, A new method to simulate convection with strongly temperature-dependent and pressure-dependent viscosity in spherical shell, Phys. Earth Plant. Inter., 157 (2006), 223-249