Towards Mantle Convection Simulations in the Exa-scale Era: Real World Models

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Processes deep beneath our feet...

Software requirements

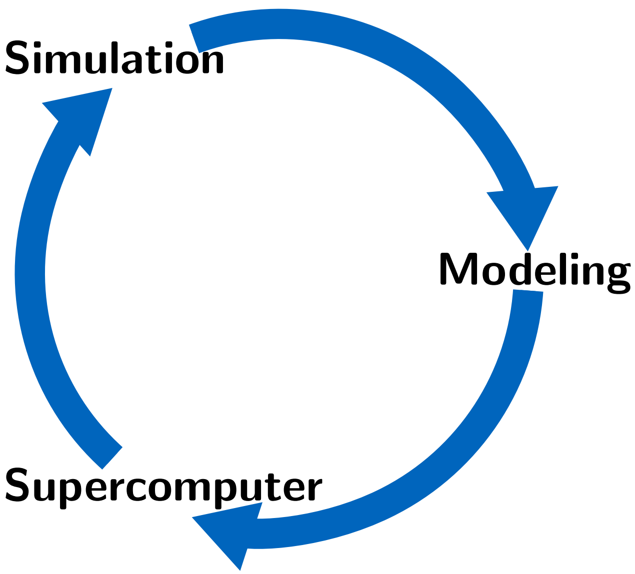
What are the requirements of the application to our software?

- **Many time steps** (one overturn 60 Myr) and **fine resolution** of 1 km (systems with $\mathcal{O}(10^{12})$ DOF)

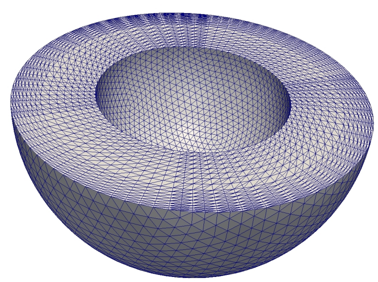
$\Longrightarrow$ Necessity of **supercomputers**

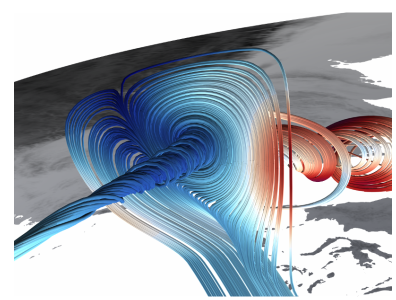
- **Complex models** (jumping viscosity of orders of magnitude)

$\Longrightarrow$ **Modern** and **efficient algorithms** and **architecture-aware optimization**



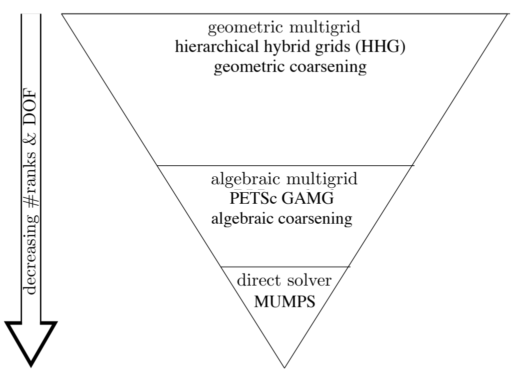
$$
\begin{aligned}
-\operatorname{div}\left(2\nu\dot{\varepsilon}(\mathbf{u})\right) + \nabla p &= \mathrm{Ra}\, T \frac{x}{\|x\|} && \text{in } \Omega \times I,\\
\operatorname{div} \mathbf{u} &= 0 && \text{in } \Omega \times I,\\
\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T &= \Delta T && \text{in } \Omega \times I.
\end{aligned}
$$

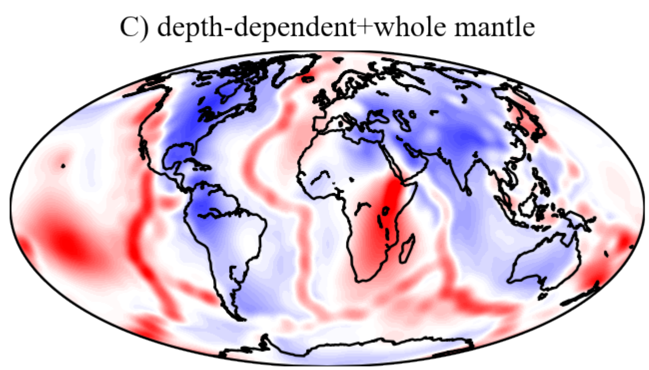


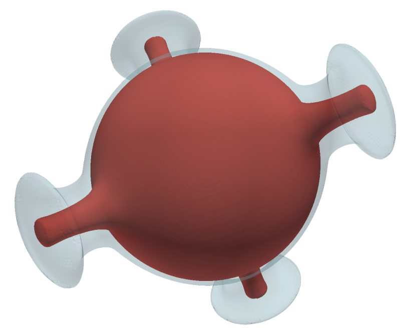


What are our achievements?

- **Fast matrix-free assembly** routines
- **Efficient solver for the Stokes problem** ⇒ Fast solving time for problems with fine resolution of 1.5 km (systems with $\mathcal{O}(10^{12})$ DOF)
- Investigation in **complex viscosity models** and the **Earth's topography**
- **Mantle convection benchmarks**







Model problems for geophysics: Stokes problem

Goal: Reduce the model to develop efficient software.

Let $\Omega \subset \mathbb{R}^3$

$$\begin{aligned} -\operatorname{div}(2\nu\dot{\varepsilon}(\mathbf{u})) + \nabla p &= \mathbf{f} \quad \text{in } \Omega, \\ \operatorname{div}\mathbf{u} &= 0 \quad \text{in } \Omega, \end{aligned} \qquad + \text{BC}$$

with positive scalar viscosity ν and $\dot{\varepsilon}(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^\top\right)$.
Equal-order $\mathbf{P}_1 - P_1$ FE- discretization with PSPG-stabilization[1]

$$\begin{pmatrix} \mathbf{A}_L & B_L^\top \\ B_L & -C_L \end{pmatrix} \begin{pmatrix} \underline{\mathbf{u}}_L \\ \underline{p}_L \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{f}}_L \\ \underline{g}_L \end{pmatrix}.$$

Winner in a large scale comparison: Uzawa-type multigrid solver [2]

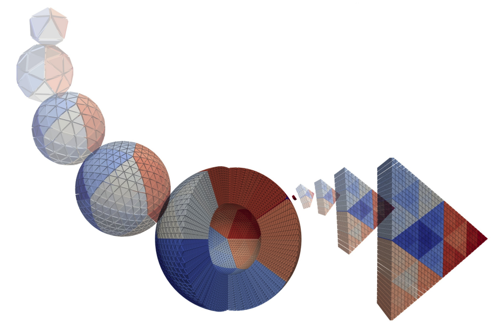
[1] T. J. R Hughes et al.: *A new finite element formulation for computational fluid dynamics: V. circumventing the Babuška-Brezzi condition: A stable Petrov-Galerkin formulation of the Stokes problem accommodating equal-order interpolations* Comput. Methods Appl. Mech. Eng., 1986.

[2] M. Huber et al.: *A quantitative performance study for Stokes solvers at the extreme scale.* J. Comput. Sci., 2016.

The high-performance geometric multigrid framework: Hierarchical Hybrid Grids [3,4]

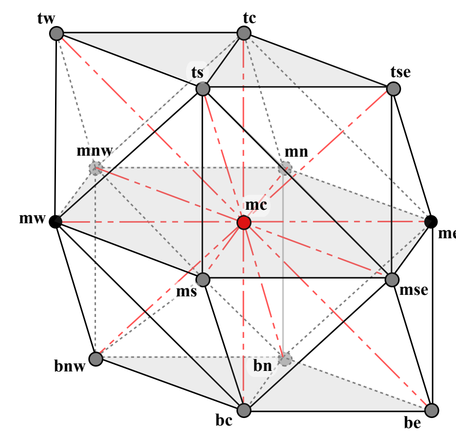
Multigrid hierarchy

- unstructured tetrahedral input grid $\mathcal{T}_0$
- structural refinement $\mathcal{T}_\ell, \ell = 1, \ldots, L$



Data-structure

- geometric classification of DOF
- hierarchical data organization



MPI parallelization

ghost layer enrichment

Matrix storage format

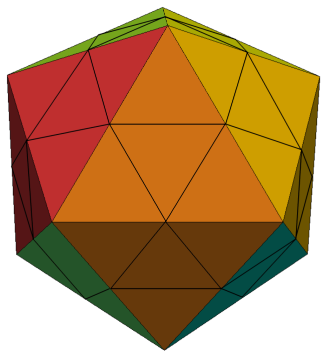
compression technique

[3] Bergen: *Hierarchical Hybrid Grids: Data structures and core algorithms for efficient finite element simulations on supercomputers.* SCS Publishing House eV, 2006.

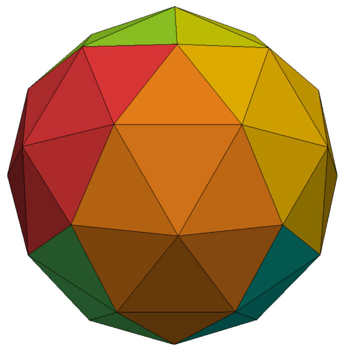
[4] Gmeiner: *Design and Analysis of Hierarchical Hybrid Multigrid Methods for Peta-Scale Systems and Beyond.* PhD thesis, University of Erlangen-Nuremberg, 2013.

Towards geophysical simulations: framework adjustments

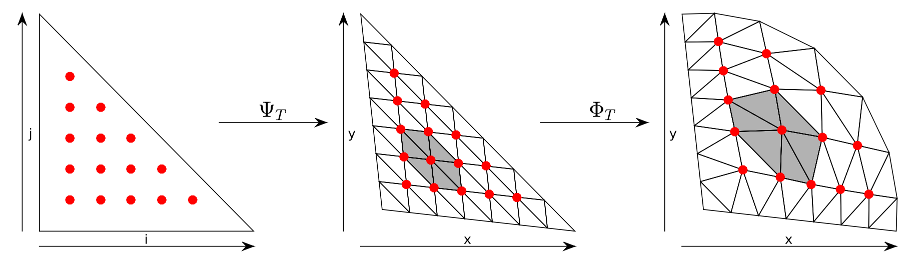
Multigrid hierarchy adjustment to the curved domain[5]



non-projected



projected



Matrix-free assembly adjustment[6]

- Compression technique fails $\Longrightarrow$ classical FEM assembly
- classical FEM assembly fails (too much memory $> 1\,000$ TByte) $\Longrightarrow$ on-the-fly assembly
- on-the-fly assembly fails (computational too expensive (factor > 20)) $\Longrightarrow$ surrogate on-the-fly assembly by low order polynomial approximations

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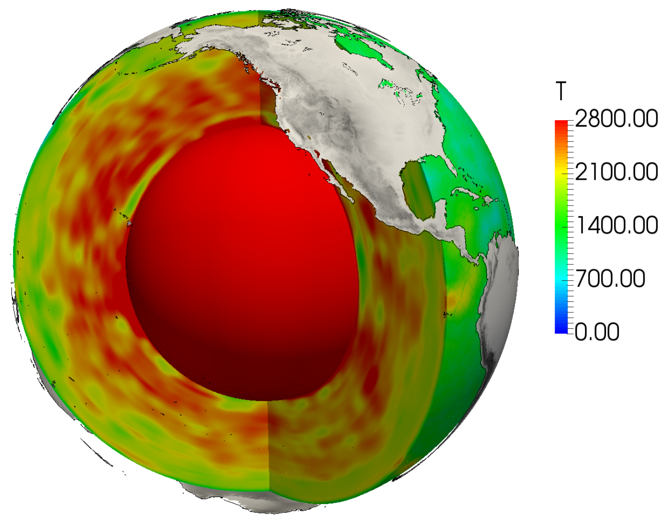
[5] Bauer et al: *A two-scale approach for efficient on-the-fly operator assembly in massively parallel high performance multigrid codes*, App. Num. Math. 2017.

[6] Bauer, Huber, et al: *Large-scale Simulation of Mantle Convection Based on a New Matrix-Free Approach*, J. Comp. Sci., 2019.

Towards geophysical simulations: the model

Stokes equation with different viscosity models with radial and lateral variations and right-hand side $\mathbf{f} = \mathrm{Ra}\,\tau\mathbf{x}/\|\mathbf{x}\|_2$ using real-world temperature data[7]

Real world measurements of the temperature data:



Boundary conditions:

- surface: plate velocity data[8]
- core-mantle-boundary: free-slip conditions

[7] N. A. Simmons et al.: *Evidence for long-lived subduction of an ancient tectonic plate beneath the southern Indian Ocean.* Geophys. Res. Lett. 2015.

[8] S. Williams et al.: *An open-source software environment for visualizing and refining plate tectonic reconstructions using high resolution geological and geophysical data sets.* GSA Today, 22(4), 2012.

Towards geophysical simulations: extended model

Viscosity model: temperature-dependent lateral and radial variations ($d_a = 0.0635$ (410 km)) [9]

$$\nu(\mathbf{x}, \tau) = \exp\left(2.99\frac{1 - \|\mathbf{x}\|_2}{1 - r_{\text{cmb}}} - 4.61\tau\right) \begin{cases} 1/10 \cdot 6.371^3\, d_a^3 & \text{for } d_a > 1 - \|\mathbf{x}\|_2, \\ 1 & \text{else.} \end{cases}$$

Solver structure: Uzawa multigrid method with a block-low-rank coarse level solver [10]

Weak scaling experiments on Hazel Hen (Stuttgart, position 30 on TOP500):

proc.	DOF	iter	time (s)		BLR ϵ	time (s)		
	fine		total	fine		coarse	ana. & fac.	par. eff.
1 920	$2.10 \cdot 10^{10}$	15	78.1	77.9	10^{-3}	0.03	2.7	1.00
15 360	$4.30 \cdot 10^{10}$	13	88.9	86.8	10^{-3}	0.22	25.0	0.93
43 200	$1.70 \cdot 10^{11}$	14	95.5	87.0	10^{-8}	0.59	111.6	0.82

[9] Huber et al.: *A New Matrix-Free Approach for Large-Scale Geodynamic Simulations and its Performance.* Computational Science – ICCS 2018. pages 17-30. 2018.

[10] Huber et al.: *Extreme scale multigrid with block-low-rank coarse grid solver* submitted. 2019.

Dynamic topography

Earth's topography is by means not constants. It changes by

- erosion,
- sedimentation,
- global isostatic adjustment,
- deflection $\Rightarrow$ dynamic topography (viscous stresses in the mantle)

Dynamic topography = normal component of the surfaces traction:

$$\sigma^s_{nn} = \mathbf{n}^T \boldsymbol{\sigma} \mathbf{n}$$

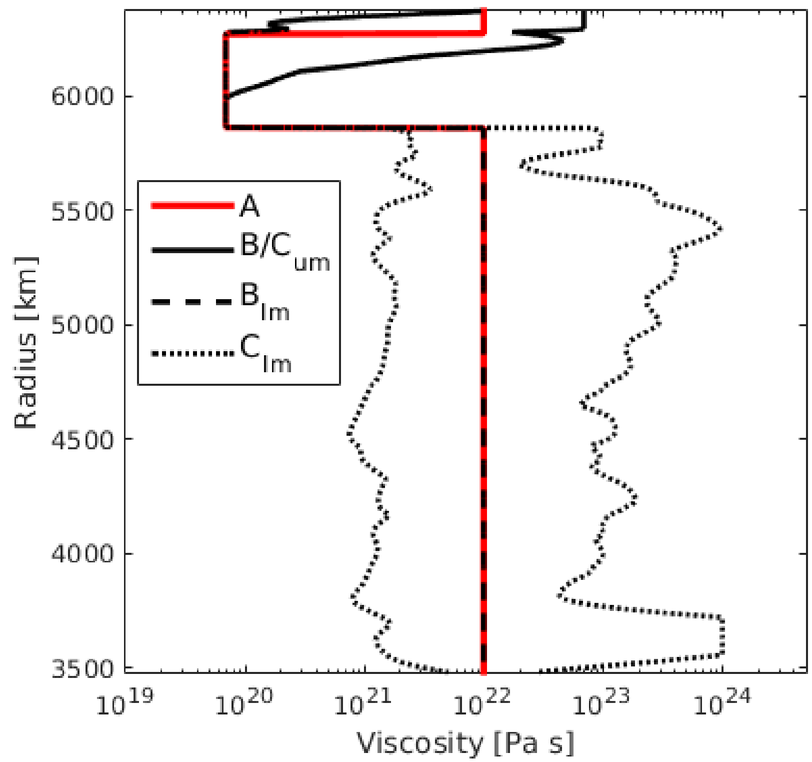
$$\boldsymbol{\sigma} = 2\nu\dot{\varepsilon}(\mathbf{u}) - p\mathbf{I}$$

Goal: Study the influence of the viscous stresses by using the Stokes model with different viscosity profiles.

Dynamic topography: viscosity profiles

Three viscosity models with asthenosphere thickness of 410km:

- ν_A: pure radial variations
- ν_B: lateral variations > 300km
- ν_C: lateral whole mantle

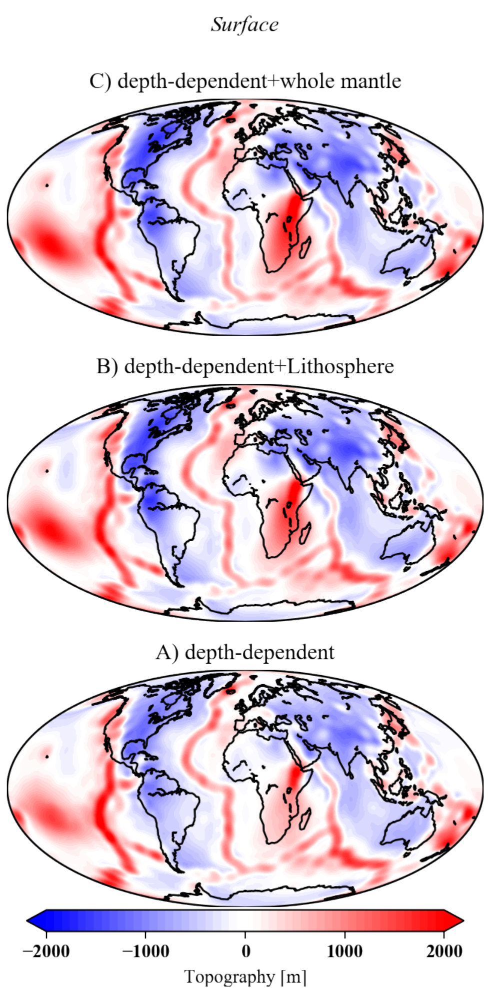


Further setup:

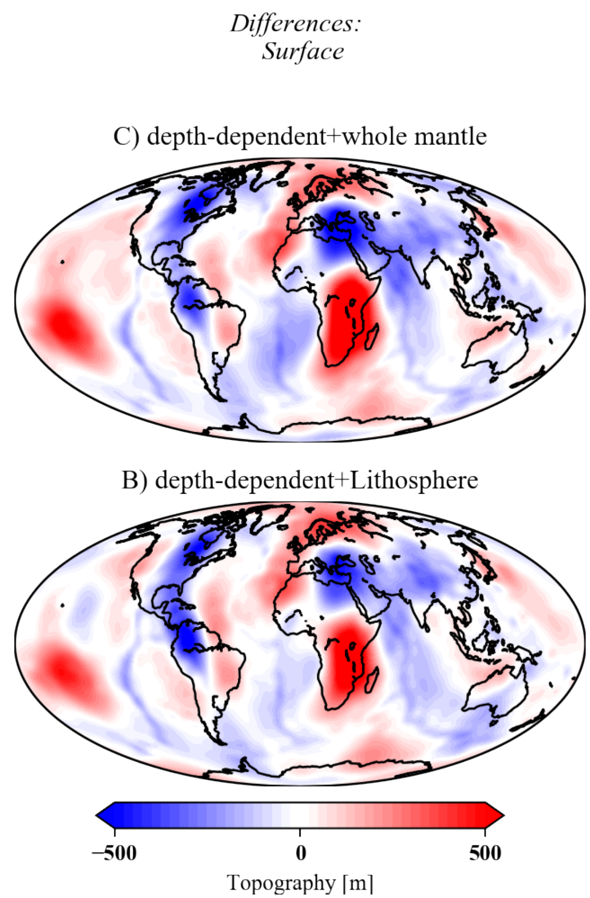
- Tomography model: real-world density and temperature data,
- Resolution: ≈ 1.5km surfaces resolution $(1.6 \cdot 10^{12}$ DOF),
- Uzawa multigrid solver executed on the Hazel Hen supercomputer (75 810 compute cores).

Dynamic topography: results[11]

Dynamic topography



Difference



11 Ghelichkhan, Huber, et al: *Large-scale Simulation of Mantle Convection Based on a New Matrix-Free Approach*, J. Comp. Sci., 2019.

Towards mantle convection simulations: benchmark setup

Software benchmarking for the coupled system[12]

$$\begin{aligned} -\operatorname{div}(2\nu\dot{\varepsilon}(\mathbf{u})) + \nabla p &= \mathsf{Ra}\, T \frac{x}{\|x\|} && \text{in } \Omega \times I, \\ \operatorname{div} \mathbf{u} &= 0 && \text{in } \Omega \times I, \\ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T &= \Delta T && \text{in } \Omega \times I. \end{aligned}$$

Benchmark settings:

- $\mathsf{Ra} = 7.6818 \cdot 10^4$, pure free-slip boundary conditions
- initial temperature spherical harmonics $(l, m) = (3, 2)$

$$T_0(r, \phi, \theta) = \frac{r_{\mathsf{cmb}}(r - r_{\mathsf{srf}})}{r(r_{\mathsf{cmb}} - r_{\mathsf{srf}})} + \varepsilon(\cos(m\,\theta) + \sin(m\,\theta))\, p_{lm}(\theta) \sin\left(\frac{\pi(r - r_{\mathsf{cmb}})}{(r_{\mathsf{srf}} - r_{\mathsf{cmb}})}\right)$$

  with $\varepsilon = 0.01$ and Lagrange polynomial $p_{lm}(\theta)$.
- temperature-dependent viscosity (with $\Delta\eta = 0, 20$):

$$\eta = exp(\eta_0(0.5 - T)).$$

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[12] Zhong et al: *A benchmark study on mantle convection in a 3-D spherical shell using CitcomS*, Geochem. Geophys., 2008.

Towards mantle convection simulations: Zhong's benchmarks (I)

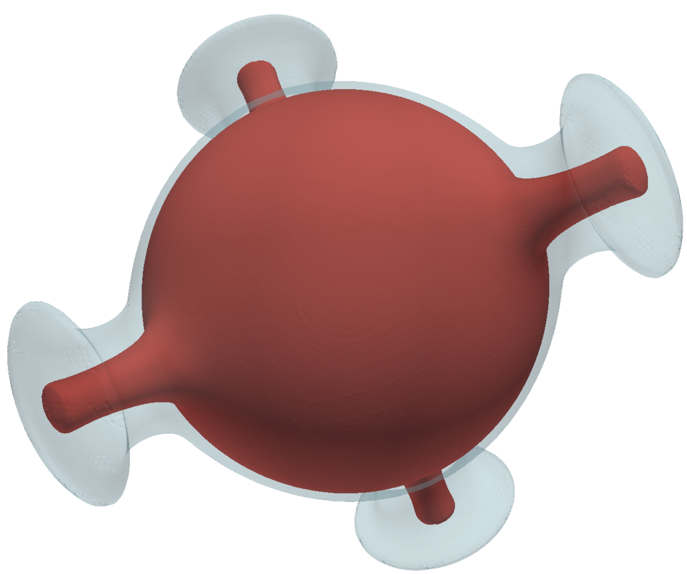
Discretization and solver setup:

FEM for Stokes and temperature equation (SUPG not necessary: diffusive problems).

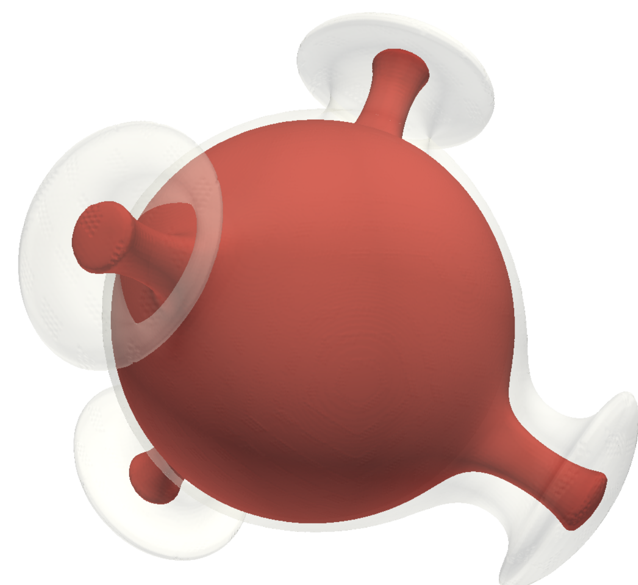
Decouple Stokes and temperature equation and solve iteratively.

Uzawa multigrid method and θ-scheme for time integration.

Setting $\Delta\eta = 0$:

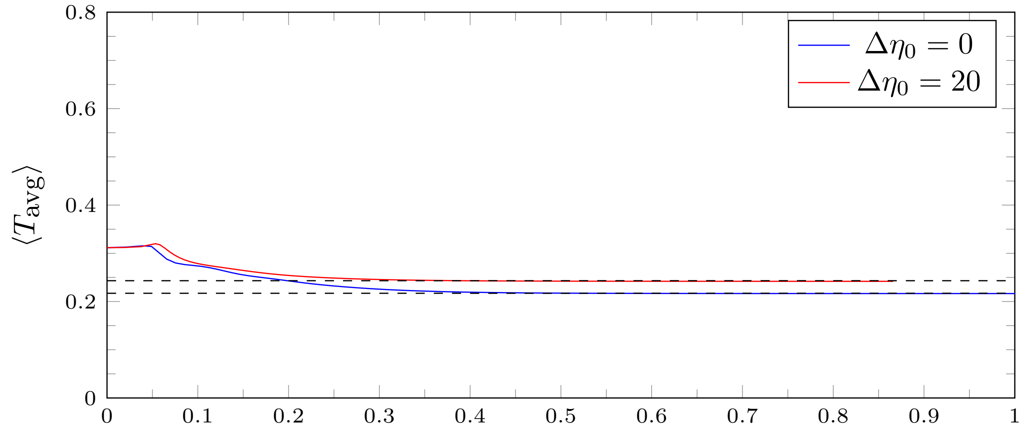


Setting $\Delta\eta = 20$:

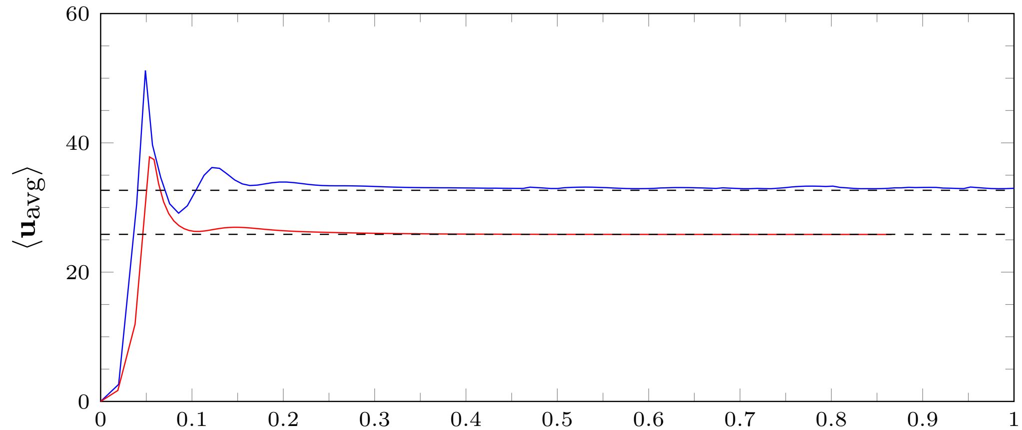


Towards mantle convection simulations: Zhong's benchmarks (II)

Time-average:



Velocity-average:



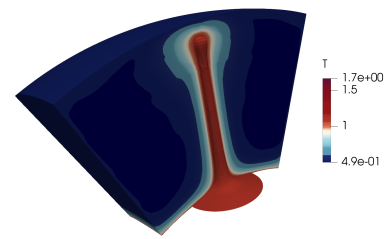
Similar results for other reference parameters: Nusselt numbers at surfaces and CMB

Conclusion

- Efficient **matrix-free assembly** approach for curved boundary domaisn
- **Excellent weak scaling** results for a multigrid method with BLR coarse level solver
- **Viscosity model influence** on the Earth's dynamic topography
- **Verification of the coupled solver** through benchmark test

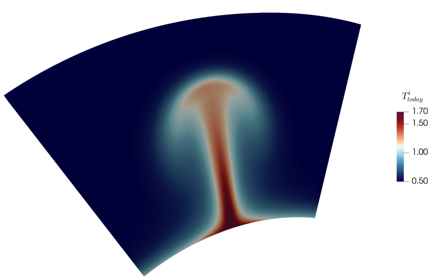
Future work:

Ra $= 10^7$

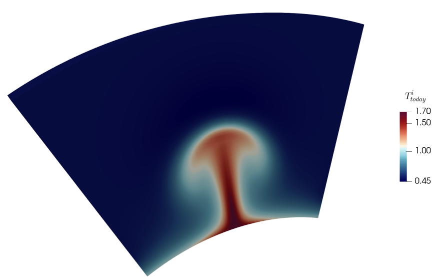


- **high Rayleigh number** simulations $\rightarrow$ SUPG stabilzation
- **adjointed mantle convection** simulations $\rightarrow$ relate today's observation with past

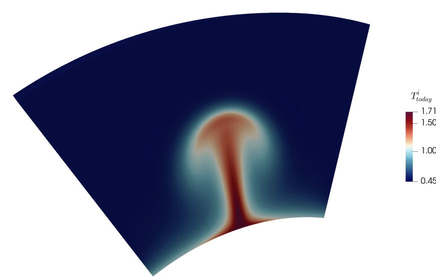
Iteration 0



Iteration 1



Iteration 5



Reference