Towards Sensitivity Analysis of 3D Subduction Zone Thermal Structure via Model Order Reduction

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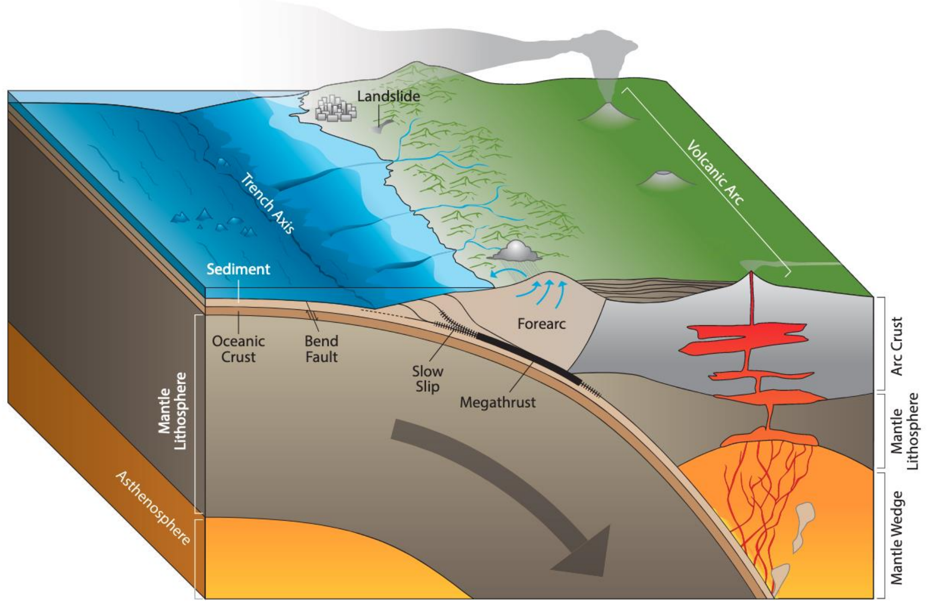
MTMOD: Megathrust Modeling Framework
A collaborative effort to advance our understanding of megathrust earthquakes
https://sites.utexas.edu/mtmod/
NSF FRES, grant EAR-2121568

The challenge: quantifying uncertainty in subduction zone temperature

Models are used to investigate subduction zone temperatures and to predict the potential extent of rupture, but they are naturally subject to uncertainty.

Quantifying uncertainty in subduction zone temperature is challenging due to the combination of:

- Multiple sources of uncertainty
- Computationally expensive physical models
- Large parameter space to explore



Modified from Fig S1-1 of SZ4D Implementation plan (2022).

Hyndman & Wang (1993); Tichelaar & Ruff (1993); Oleskevich et al., (1999); van Keken et al. (2002); Currie et al. (2004); Syracuse et al. (2010); Wada & Wang (2009); Peacock (2020); Penniston-Dorland et al. (2015)

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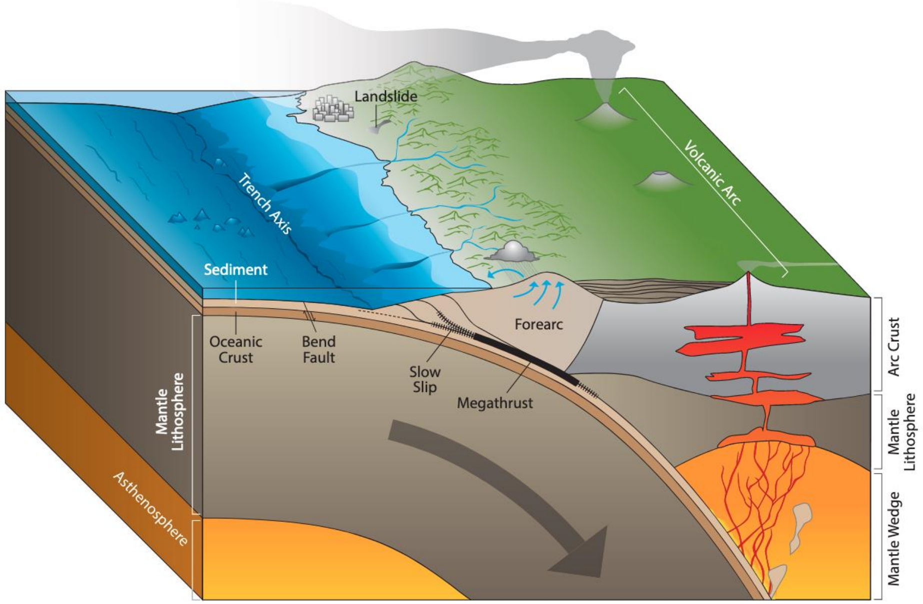
We used reduced-order modeling to accurately approximate temperature within 2D thermo-mechanical subduction zone models.



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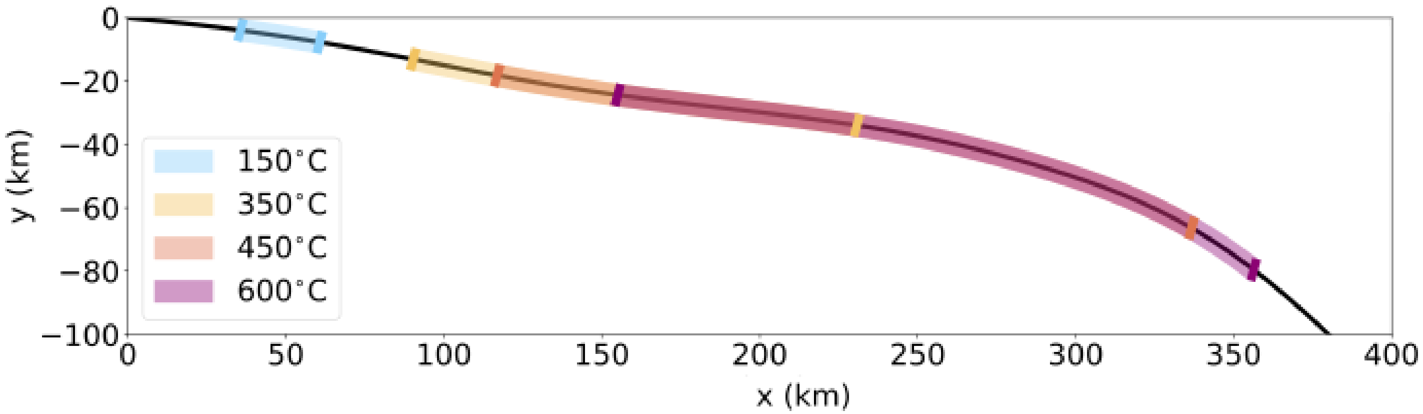

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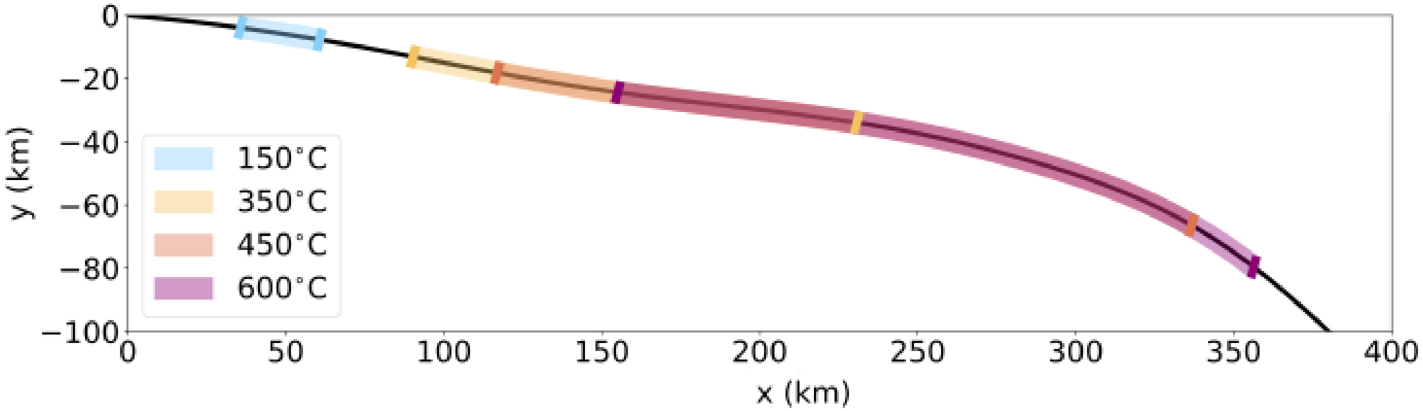

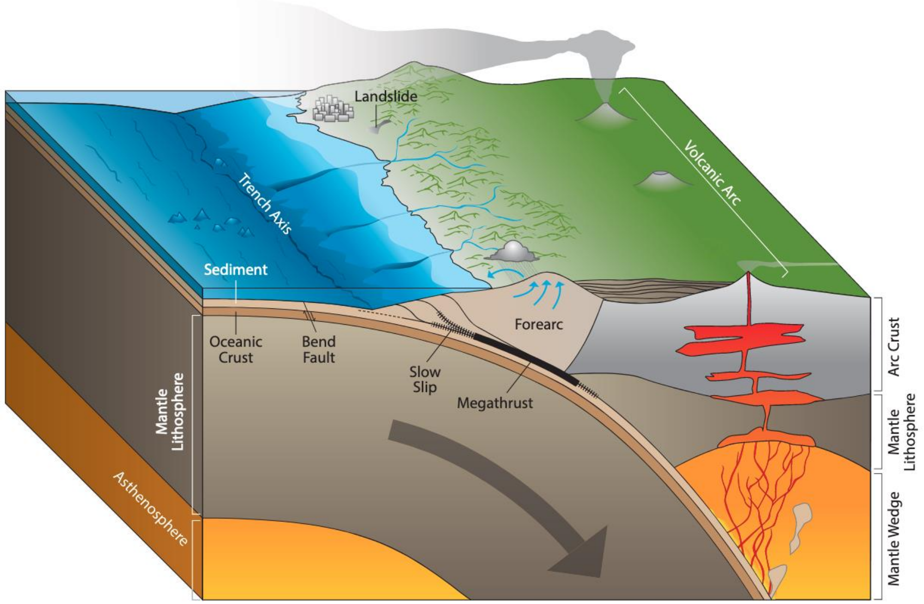

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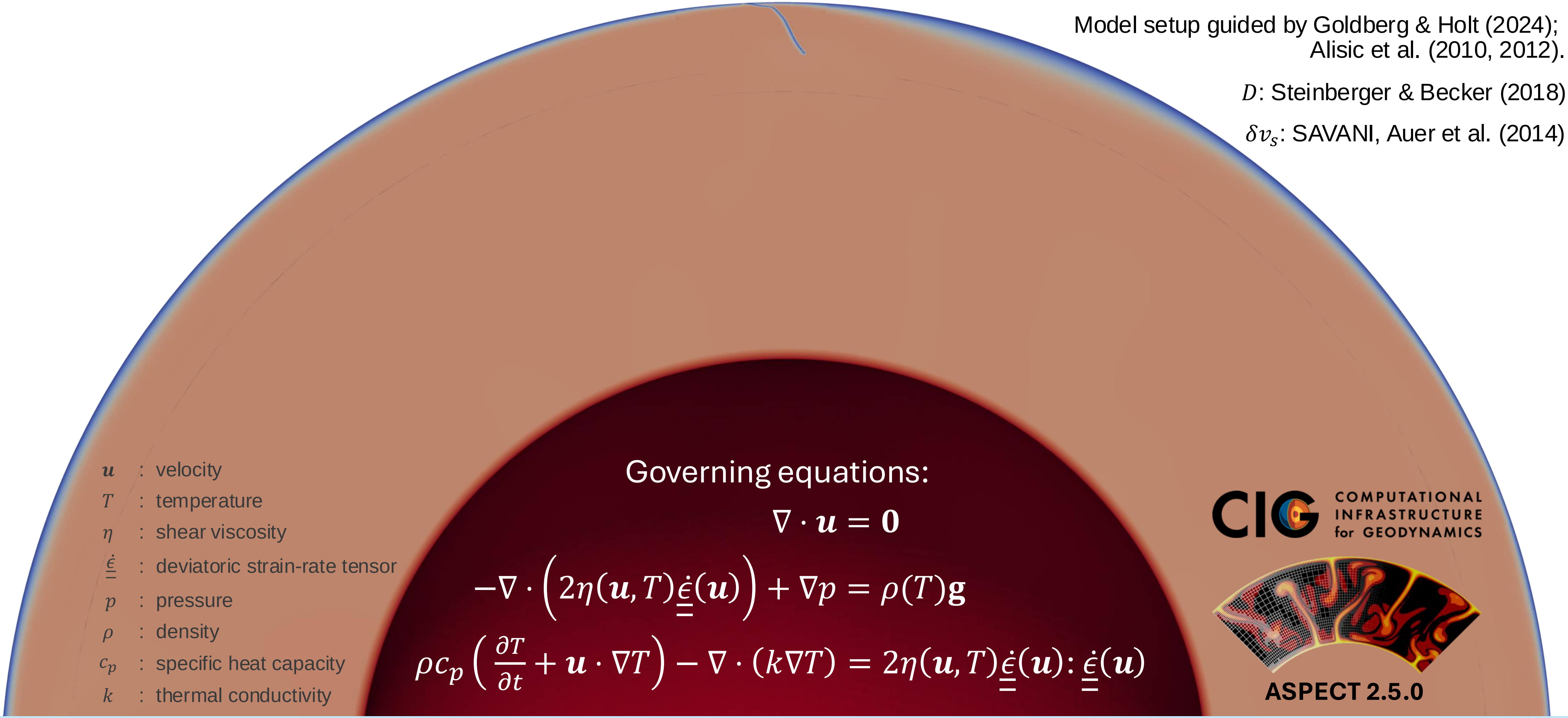
2D thermal models cannot capture certain 3D effects. We build ROMs for global 3D models of temperature in Cascadia.

- What is the uncertainty in the 3D subduction zone temperature given uncertainty in model inputs?
- Are ROMs feasible for 3D geodynamic models such as this?

Global 3D model of temperature at Cascadia



Model setup guided by Goldberg & Holt (2024);
Alisic et al. (2010, 2012).

D: Steinberger & Becker (2018)

δv_s: SAVANI, Auer et al. (2014)

Governing equations:

$$\nabla \cdot \boldsymbol{u} = \mathbf{0}$$

$$-\nabla \cdot \left(2\eta(\boldsymbol{u}, T)\underline{\dot{\epsilon}}(\boldsymbol{u})\right) + \nabla p = \rho(T)\mathbf{g}$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T\right) - \nabla \cdot (k \nabla T) = 2\eta(\boldsymbol{u}, T)\underline{\dot{\epsilon}}(\boldsymbol{u}) : \underline{\dot{\epsilon}}(\boldsymbol{u})$$

$\boldsymbol{u}$: velocity
T : temperature
η : shear viscosity
$\underline{\dot{\epsilon}}$: deviatoric strain-rate tensor
p : pressure
ρ : density
c_p : specific heat capacity
k : thermal conductivity

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

ASPECT 2.5.0

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Initial conditions

$$T(d) = T_b + (T_s - T_b)\,\mathrm{erfc}\left(\frac{d}{0.8621\,D}\right)$$

Linear transition

$$\frac{\rho - \rho_{\mathrm{ref}}}{\rho_{\mathrm{ref}}} = \omega \delta v_s\,, \qquad T = T_{\mathrm{b}} - \frac{1}{\alpha}\frac{\rho - \rho_{\mathrm{ref}}}{\rho_{\mathrm{ref}}}$$

d : depth from surface
T_{b} : interior mantle temperature
T_s : surface temperature
D : lithospheric thickness
ρ_{ref} : reference density
ω : scaling factor
δv_s : shear wave vel. anomaly

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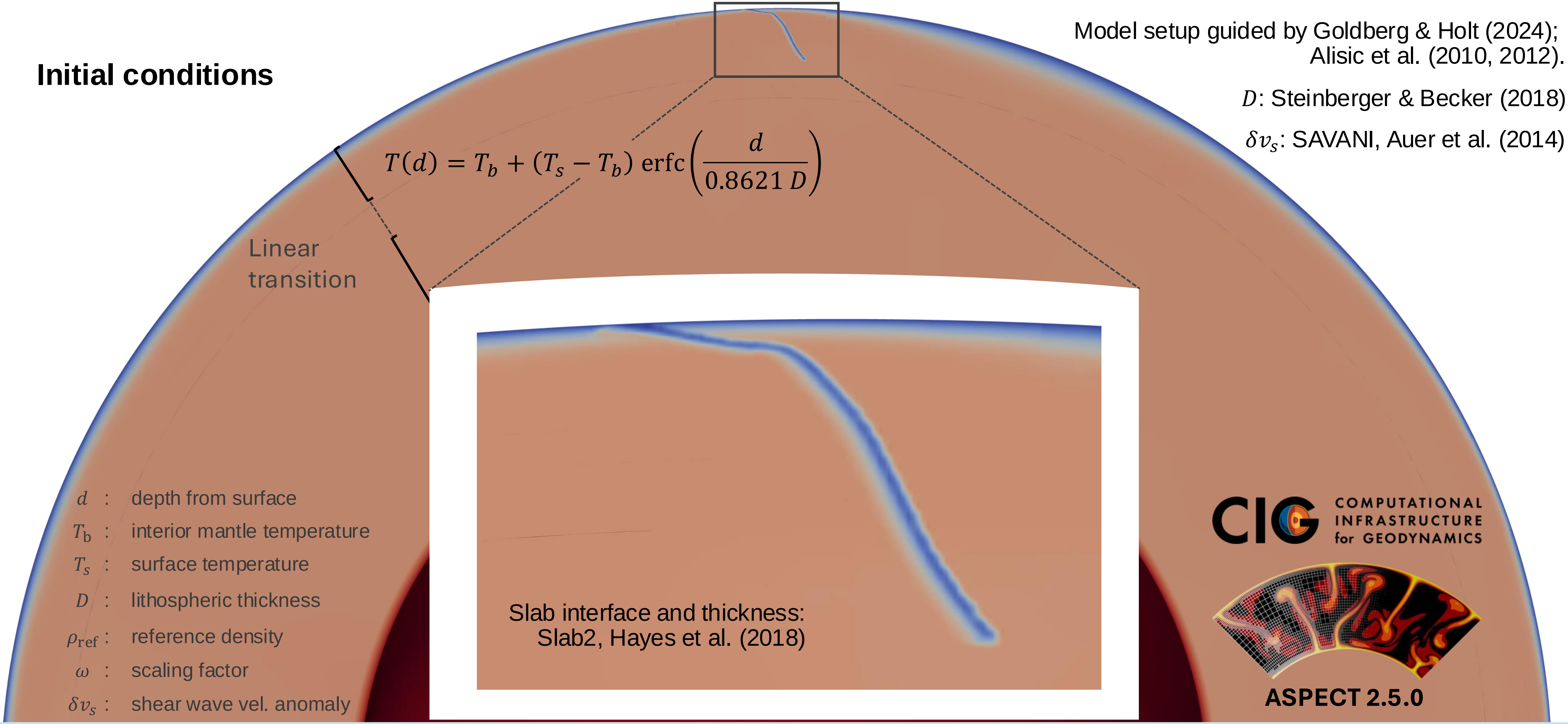

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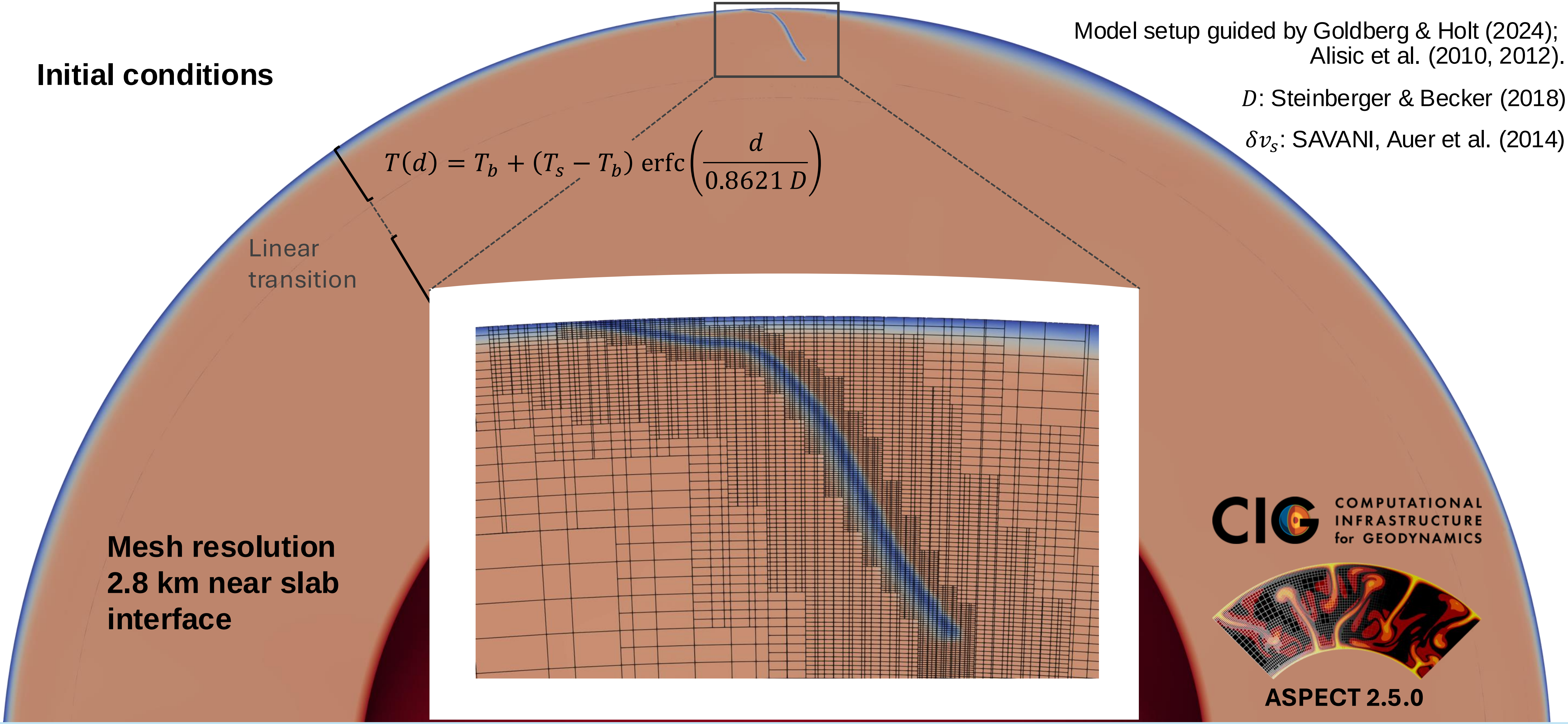

Mesh resolution 2.8 km near slab interface

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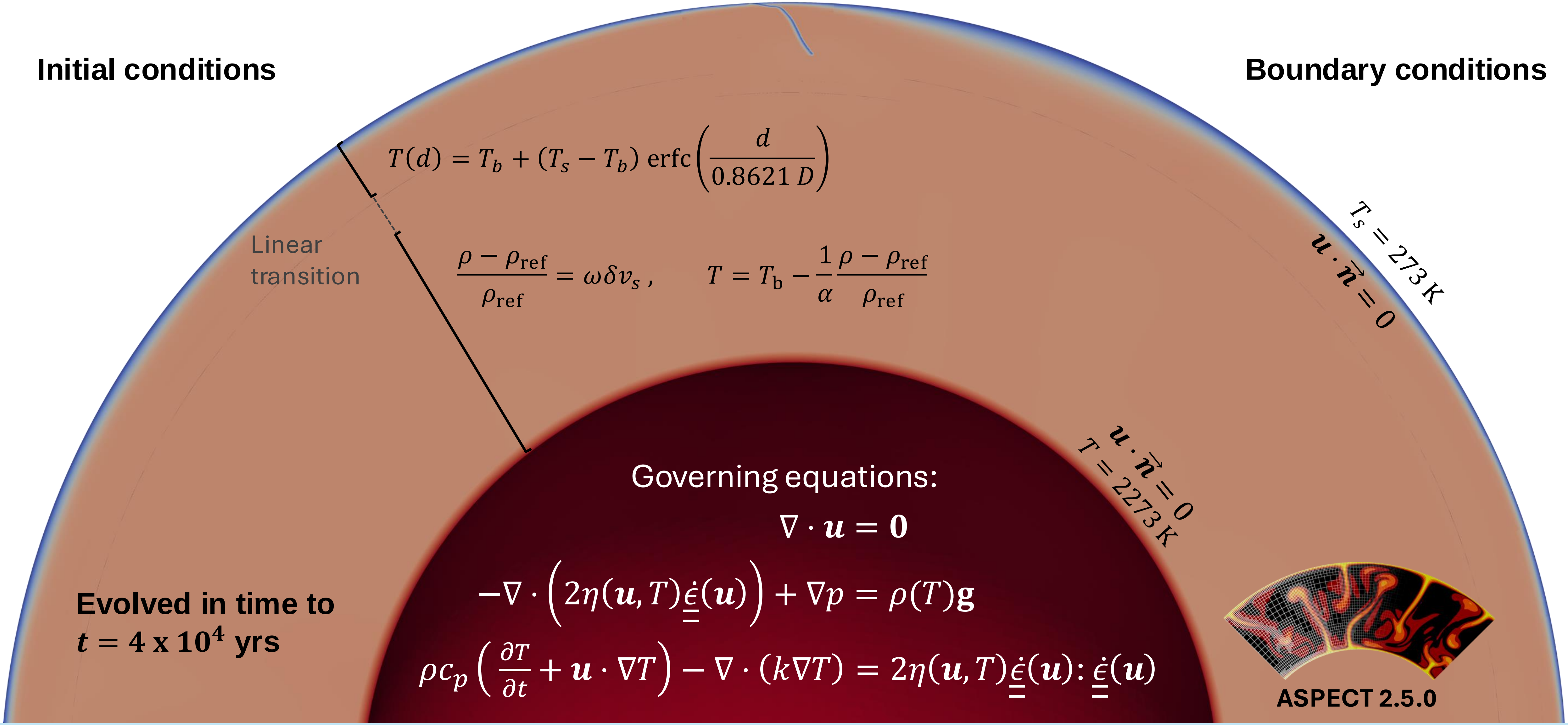

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Evolved in time to
$\boldsymbol{t = 4 \times 10^4}$ **yrs**

Boundary conditions

$T_s = 273\,\mathrm{K}$

$\boldsymbol{u} \cdot \vec{\boldsymbol{n}} = 0$

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$T = 2273\,\mathrm{K}$

Governing equations:

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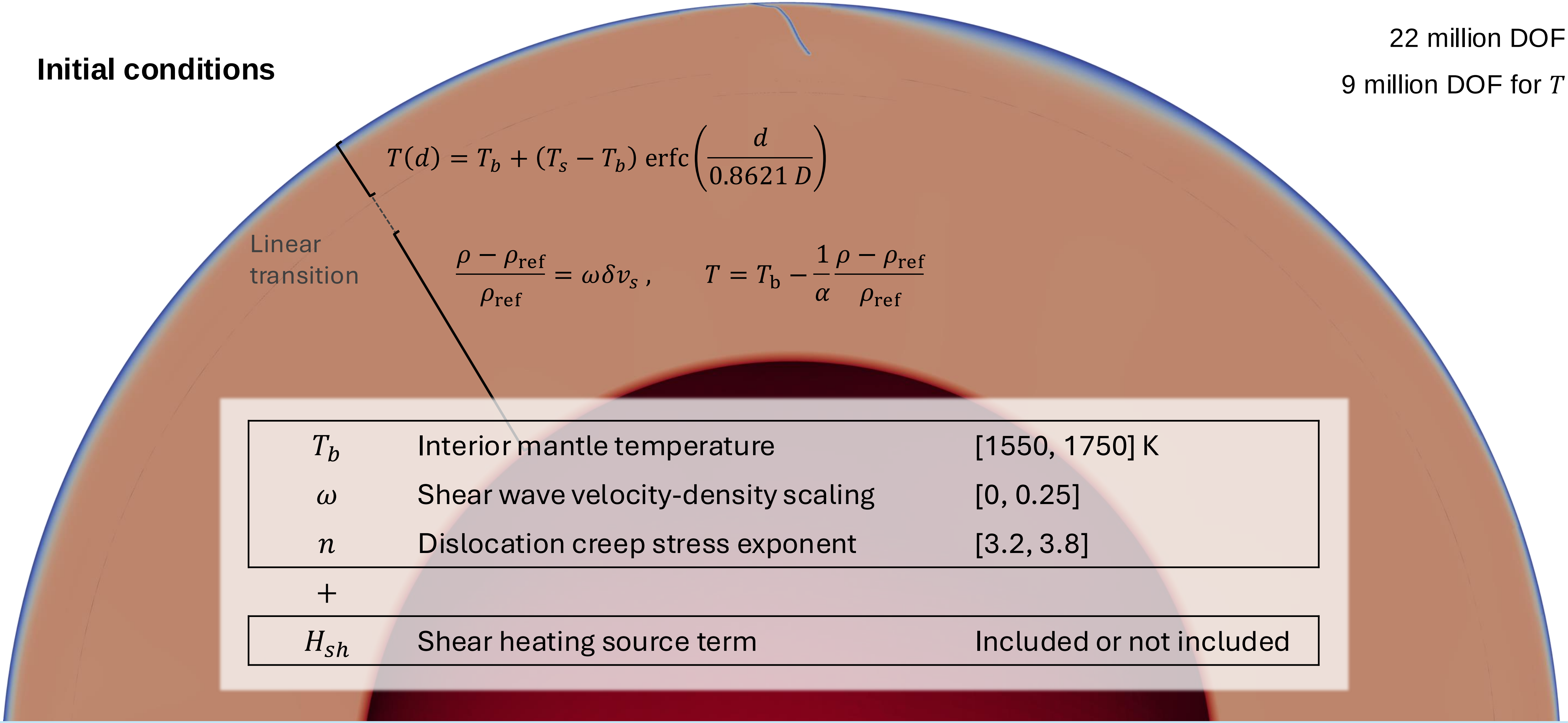

22 million DOF

9 million DOF for T

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T_b	Interior mantle temperature	[1550, 1750] K
ω	Shear wave velocity-density scaling	[0, 0.25]
n	Dislocation creep stress exponent	[3.2, 3.8]

$+$

H_{sh}	Shear heating source term	Included or not included

Heister et al. (2017); Kronbichler et al. (2012); Bangerth et al. (2023).

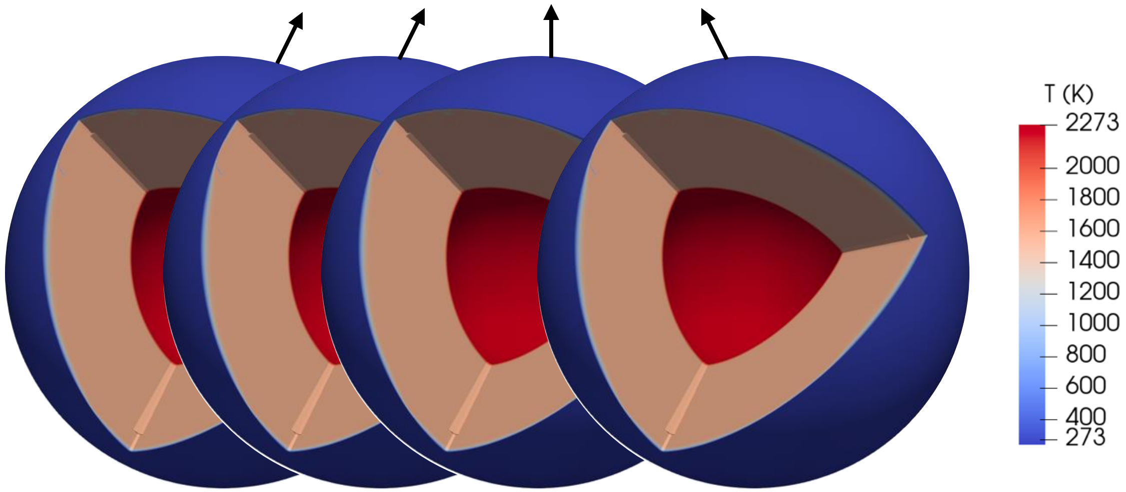
Building accurate, efficient reduced-order models for temperature

The interpolated Proper Orthogonal Decomposition (iPOD) process:

- Assemble model solutions into columns of snapshot matrix $\mathbf{X}$, with corresponding parameter vector :

$$\mathbf{X}_{\mathrm{M\,x\,N}} = \begin{bmatrix} | & | & | & & | \\ \mathbf{X}_1 & \mathbf{X}_2 & \mathbf{X}_3 & \dots & \mathbf{X}_{\mathrm{N}} \\ | & | & | & & | \end{bmatrix}, \qquad \mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \dots \mathbf{q}_{\mathrm{N}}].$$

$\mathbf{q}_{\mathrm{i}}$ is a vector in parameter space,
e.g. $\mathbf{q}_{\mathrm{i}} = (T_b,\ \omega,\ n)$.
$\mathbf{X}_{\mathrm{M\,x\,N}}$ has $M \gg N$
$M = \sim$ 9 million,
$N = 550$.



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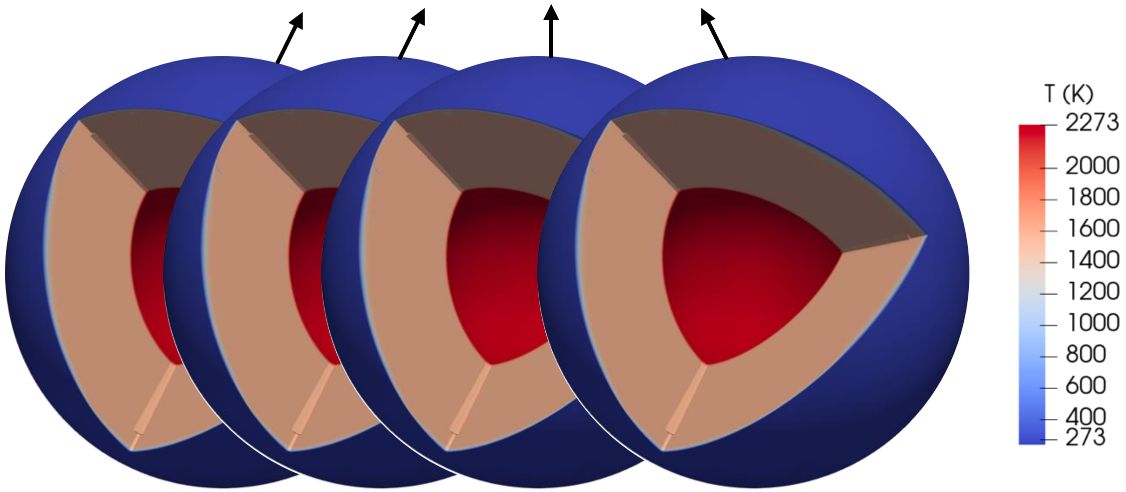

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- Take the Singular Value Decomposition (SVD):

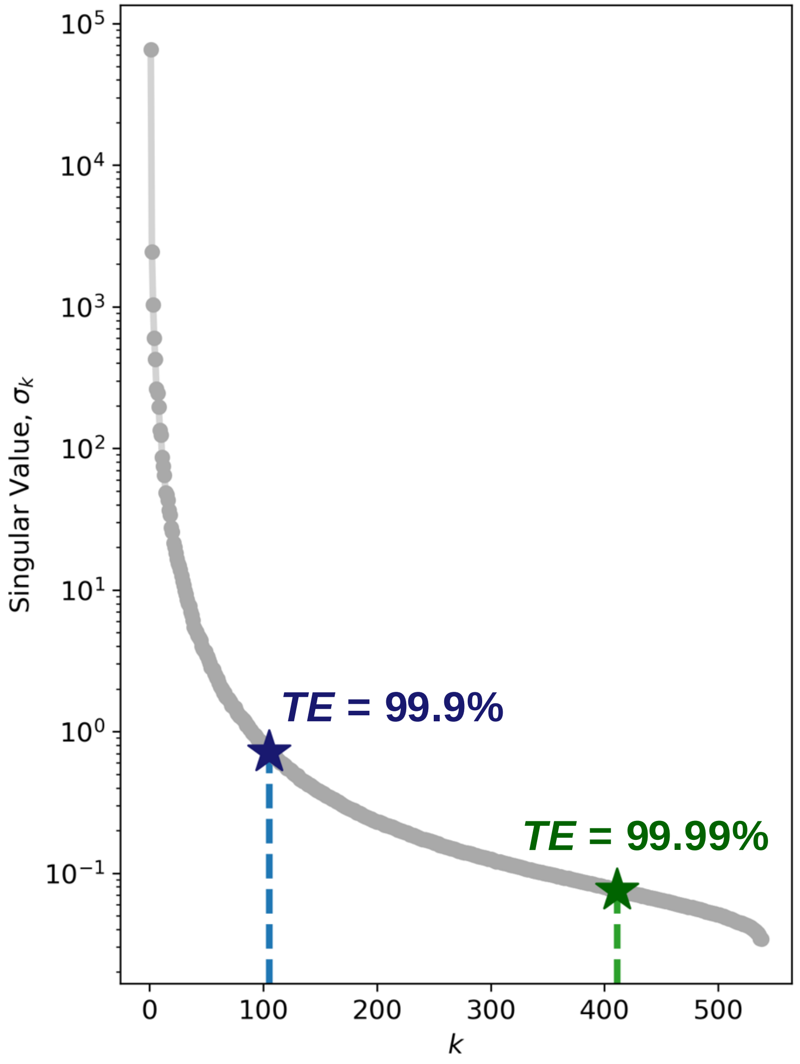
$$\mathbf{X} = \mathbf{U}\,\mathbf{\Sigma}\,\mathbf{V}^\mathbf{T}.$$

- Interpolate POD coefficients $\boldsymbol{\alpha} = \mathbf{\Sigma}\mathbf{V}^\mathbf{T}$ at a new $\hat{\mathbf{q}} \notin \mathbf{Q}$ using Radial Basis Function (RBF) interpolation.
- Approximate $\mathbf{X}(\hat{\mathbf{q}})$ using an optimal orthogonal basis $\mathbf{U}$ and interpolated coefficients $\hat{\boldsymbol{\alpha}}$:

$$\hat{\mathbf{X}}(\hat{\mathbf{q}}) = \mathbf{U}\,\hat{\boldsymbol{\alpha}}.$$

Bui-Thanh, Damodaran & Willcox (2003)
My-Ha, Lim, Khoo, & Willcox (2007)
Walton, Hassan & Morgan (2013)
Holmes et al. (2012)
Sirovich (1987)
Ly & Tran (2001)

Building accurate, efficient reduced-order models for temperature

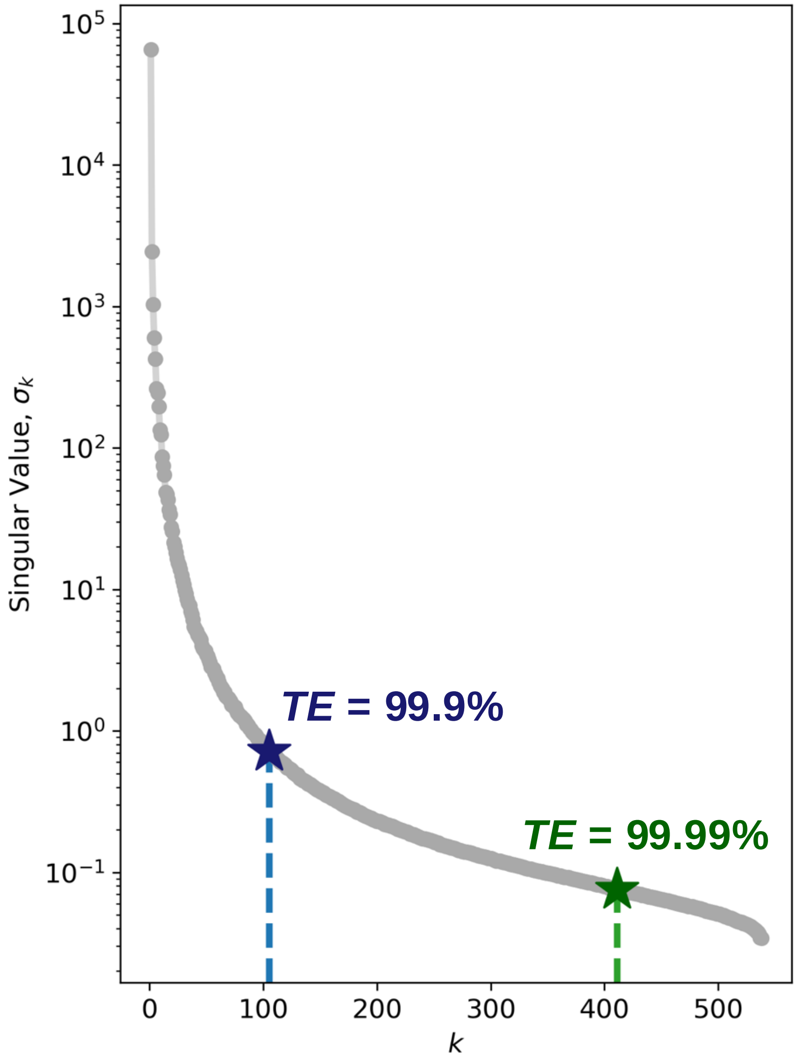


Truncation

Total energy retained in r POD modes: $TE(r) = \frac{\sum_{i=1}^{r} \sigma_i}{\sum_{i=1}^{N} \sigma_i}$

σ_i: ith singular value of $\mathbf{X}$

Building accurate, efficient reduced-order models for temperature



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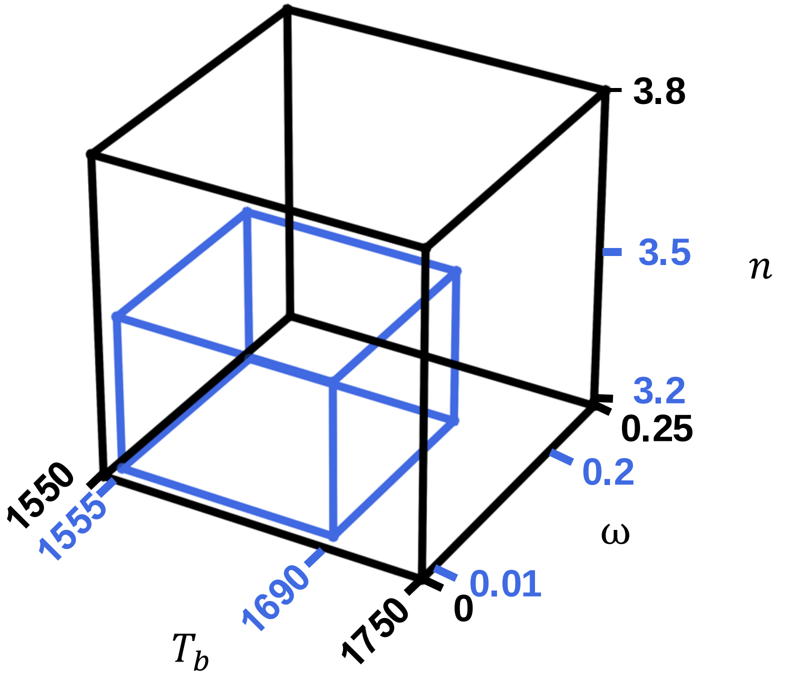
Leave One Out Cross-Validation (LOOCV) error

For all $\mathbf{q}_k \in \mathbf{Q}$, build ROM using $\widetilde{\mathbf{X}} = \mathbf{X} \setminus \mathbf{X}_k$ and approximate $\widetilde{\mathbf{X}}(\mathbf{q}_k)$.

$$CV(k) = \sup \left| \widetilde{\mathbf{X}}(\mathbf{q}_k) - \mathbf{X}_k \right|$$

- Errors > 100 K on edges of $\mathbf{Q}$
- Compute **sub-region** of $\mathbf{Q}$ where CV < 30 K
- Mean error in **sub-region** is 12 K



Reduced-order model is 10^5 times faster to evaluate

Offline ROM construction	
Run forward models	~ 5400 sec on 128 MPI ranks x 550 models = 105,600 core-hrs
Compute the SVD	800 sec on 1 MPI rank
Construct the RBF interpolant	0.96 sec on 1 MPI rank

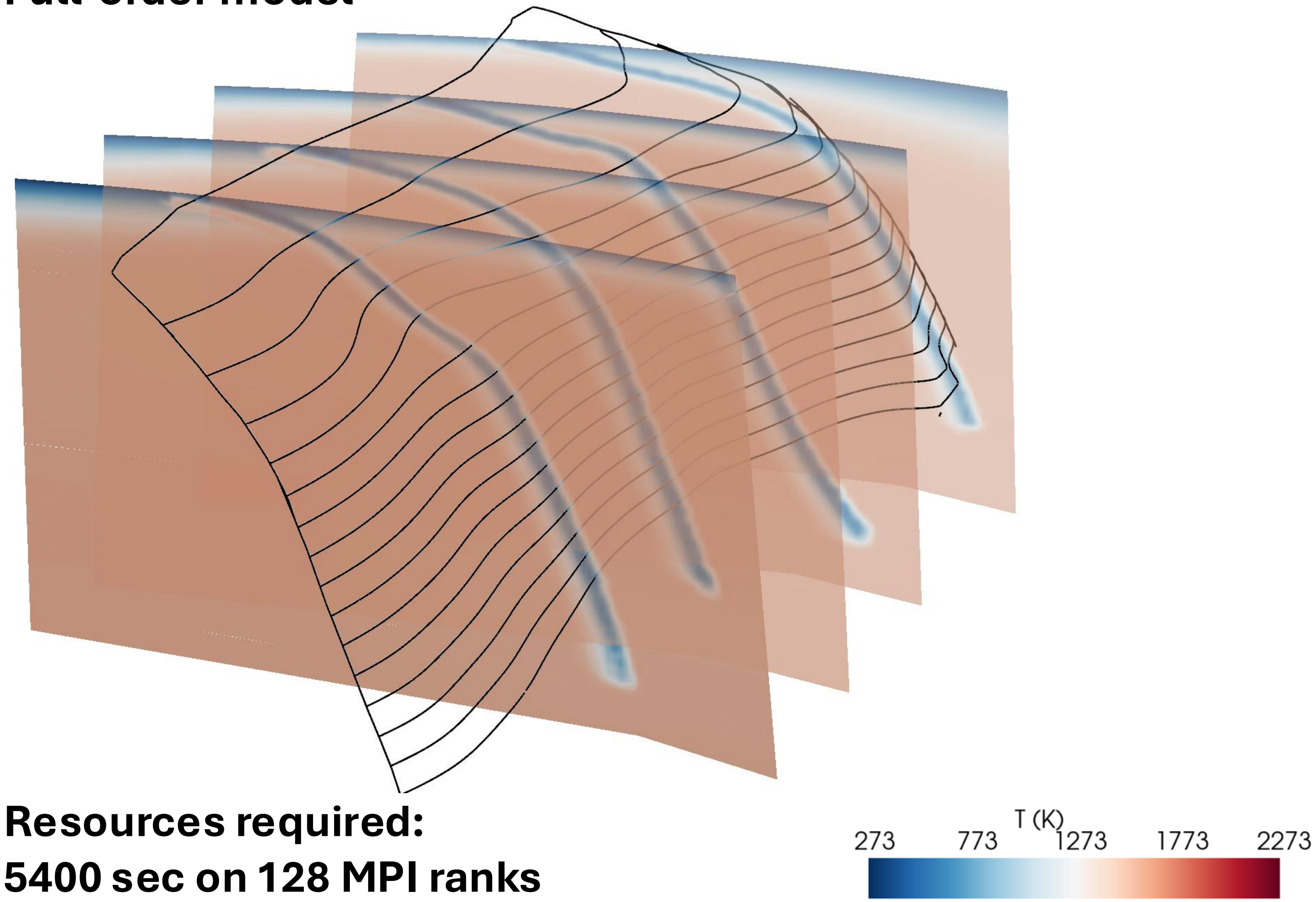
Online phase	
RBF evaluation time	0.001 sec on 1 MPI rank
Matrix multiplication, $\widehat{\mathbf{X}}(\widehat{\mathbf{q}}) = \mathbf{U}\,\widehat{\boldsymbol{\alpha}}$	4 sec on 1 MPI rank

→ **Speedup factor of 10^5** once ROM is constructed.

Reduced-order model is 10^5 times faster to evaluate

ROM evaluation is performed for full 3D domain, with slices of Cascadia shown here for clarity.

Full-order model



Resources required:
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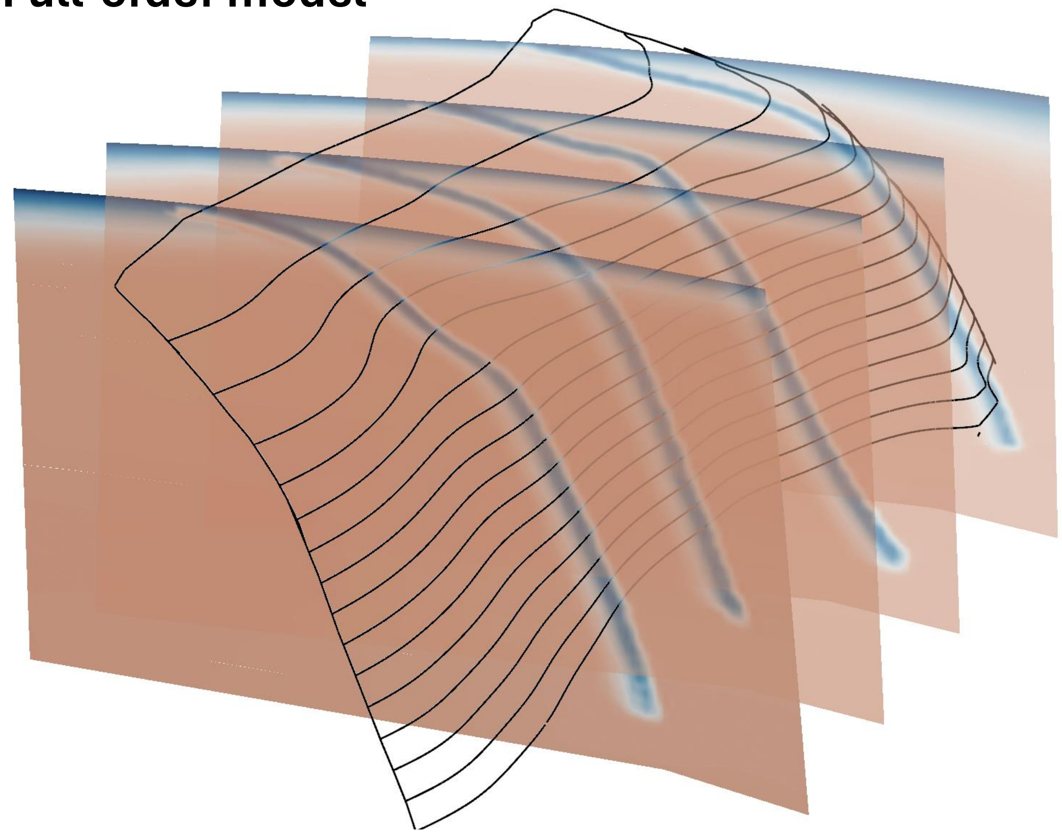
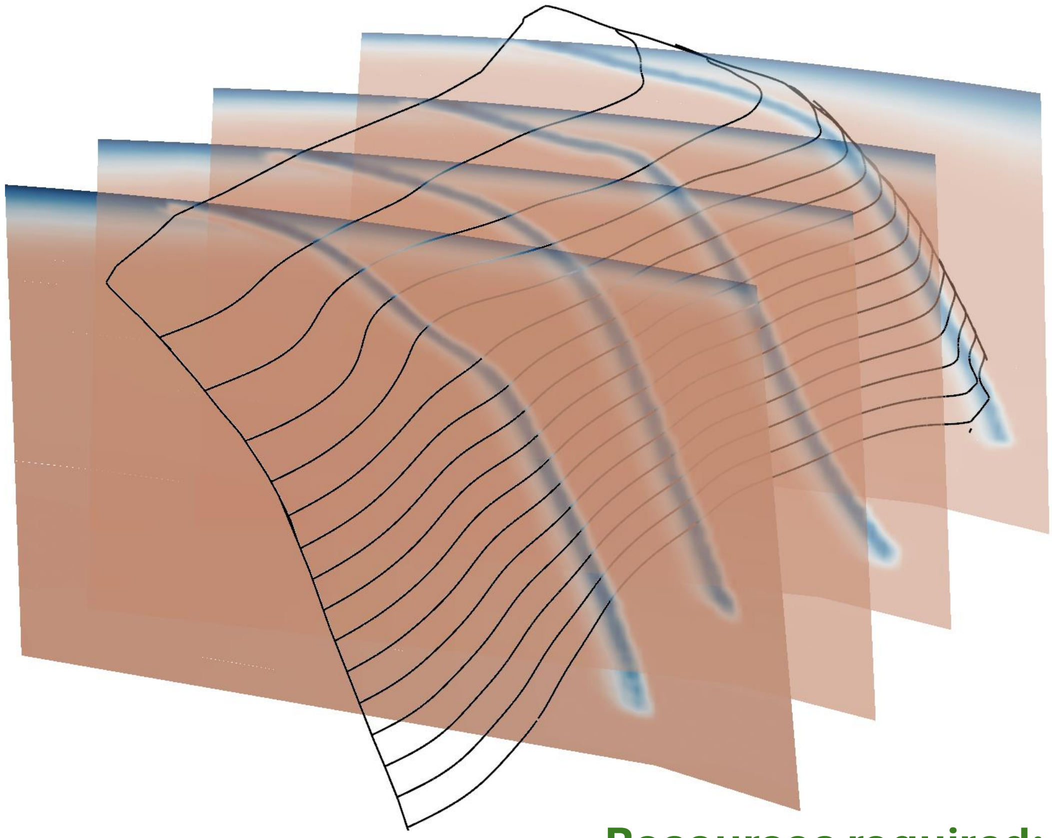


Reduced-order model



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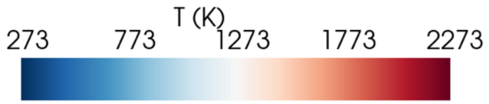
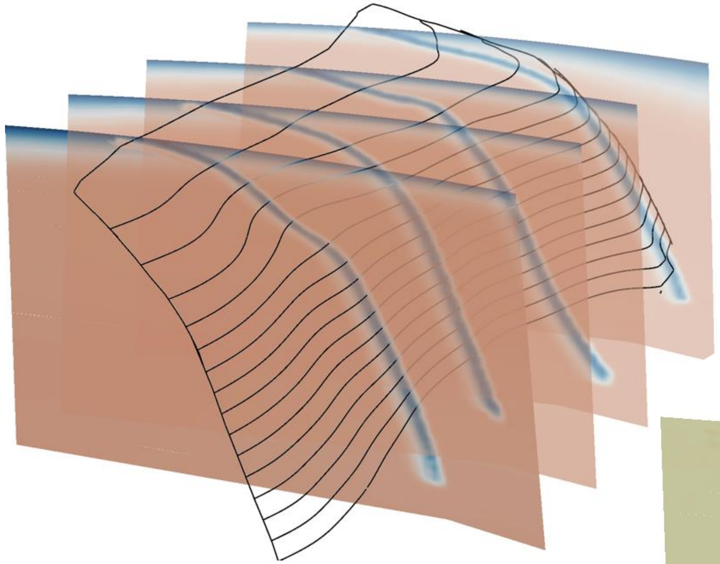


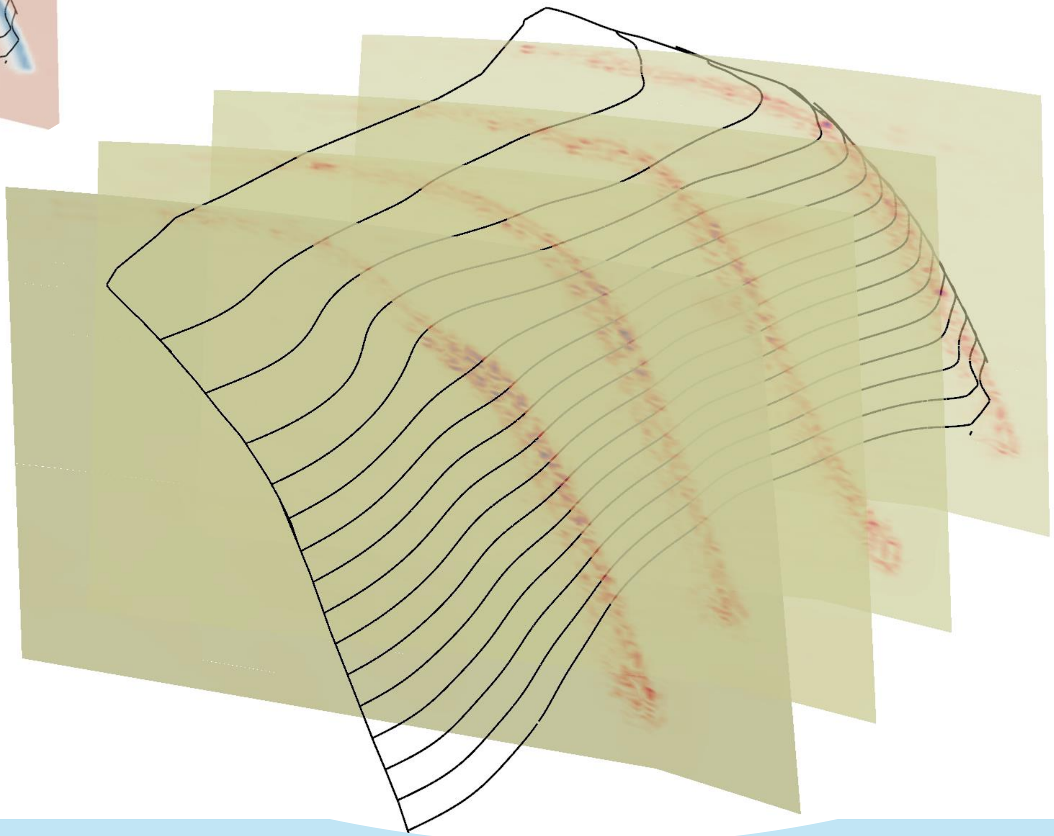
Resources required:
4 sec on 1 MPI rank

ROM errors are low in the mantle wedge, higher within the slab

Full-order model



ROM error, $T_{\mathrm{FOM}} - T_{\mathrm{ROM}}$ (K)



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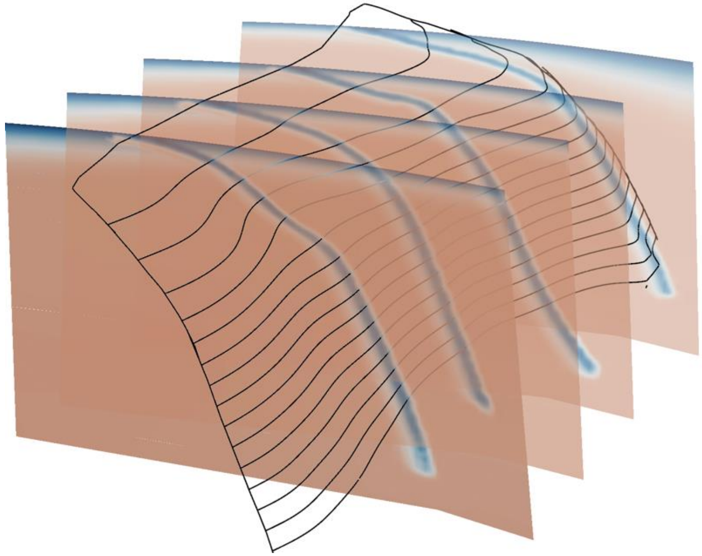

Summary

Key Takeaways

- Building a ROM to approximate global temperature is feasible.
- FOM-ROM error is < 30 K globally in sub-region of parameter space.
- For Cascadia, errors are low in the mantle wedge and higher within the slab.
- The ROM is 10^5x faster to evaluate than the full-order model.

Preprint for 2D study available
https://arxiv.org/abs/2410.02083

arXiv

Outlook

- ROM permits rigorous global sensitivity analysis.
- Plan to expand the ROM to include additional model input parameters such as age of the incoming lithosphere and sediment cover.
- Aim to estimate uncertainty in temperature and potential rupture extent given variability in:
  - Model inputs (T_b, ω, n),
  - Along-margin effects (lithosphere age, sediment cover, along-margin flow).
- Preliminary results indicate that the ROM can be used for viscosity as accurately and efficiently as for temperature.

We would like to thank NSF FRES (grant EAR-2121568) and our MTMOD collaborators including Thorsten Becker at UTIG.