Simulating Complex Flows in the Earth Mantle: Time stepping in the ASPECT code

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WHERE DISCOVERIES BEGIN

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

There are no “Conclusions” to this talk.

Take-away message (charitable version):

The world is messy:

- **Models are messy**
- **Development histories are messy**

Take-away message (not-so-charitable version):

The developers of this code are amateurs:

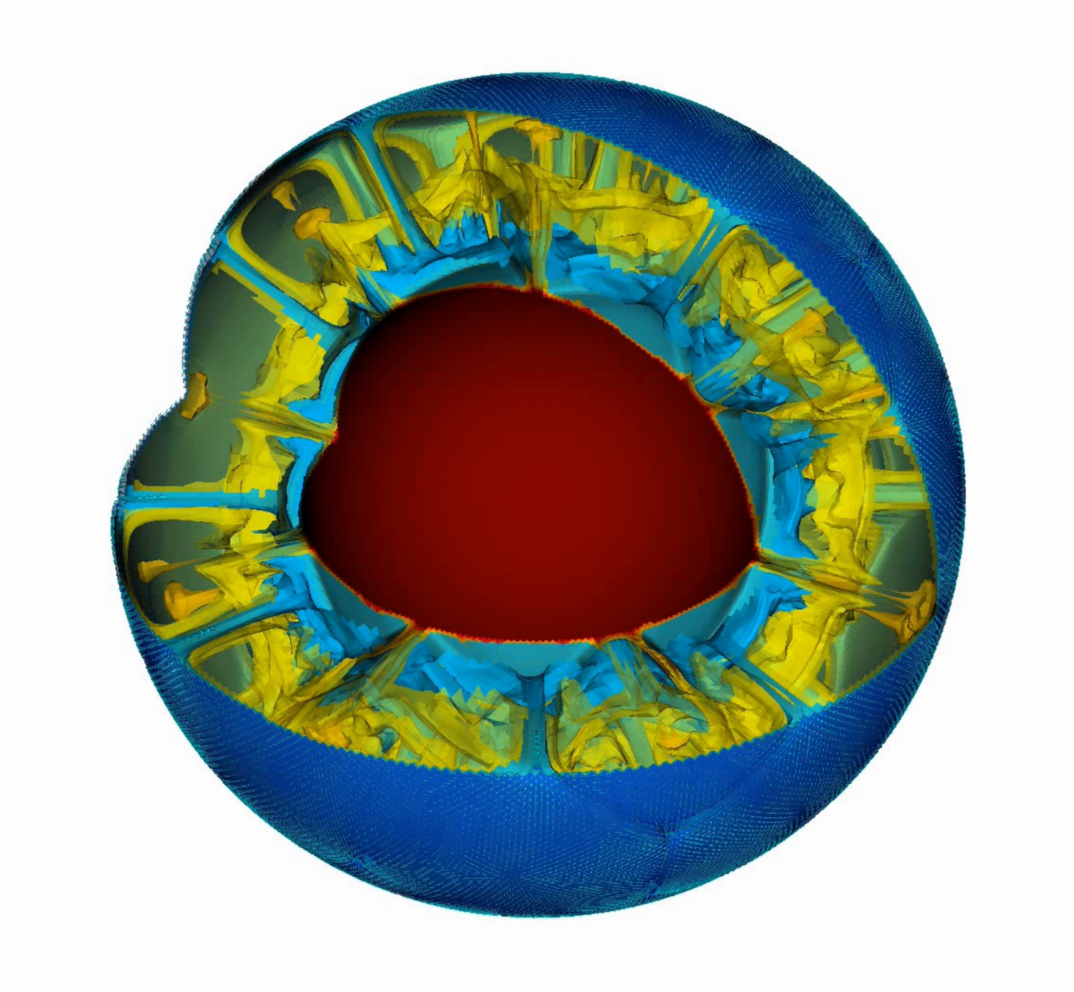
- **We were (and are) not experts in time stepping**
- **We failed to anticipate future directions when coming up with the original design**

In particular: There is no “holistic design”.

Introduction:

What and why?

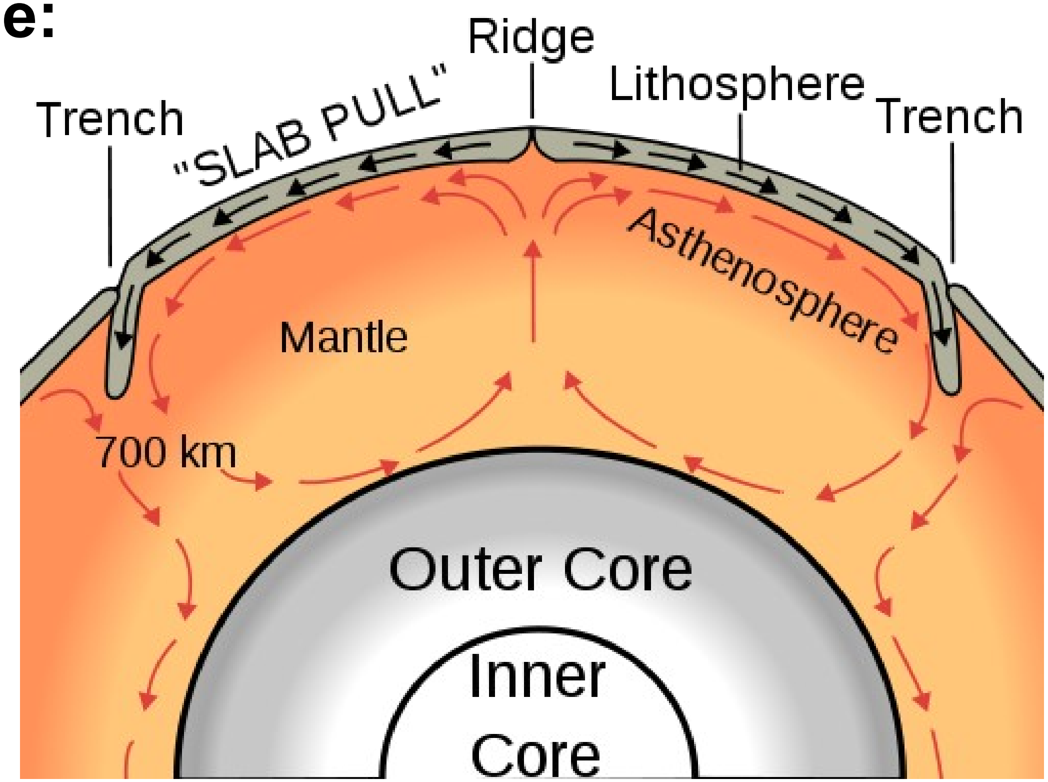
The what and the why



The what and the why

Brief recap on the Earth mantle:

- It makes up the largest component of Earth (~80%)
- It is solid
- It flows on long time scales
- Thermal gradients drive convection



- It is probably Earth's component we understand the least
- Yet, it has a large impact on basically everything else
- It's relevance lies in the interaction with the rest of Earth

The what and the why

“Big” questions one may ask about the mantle in relation to other systems:

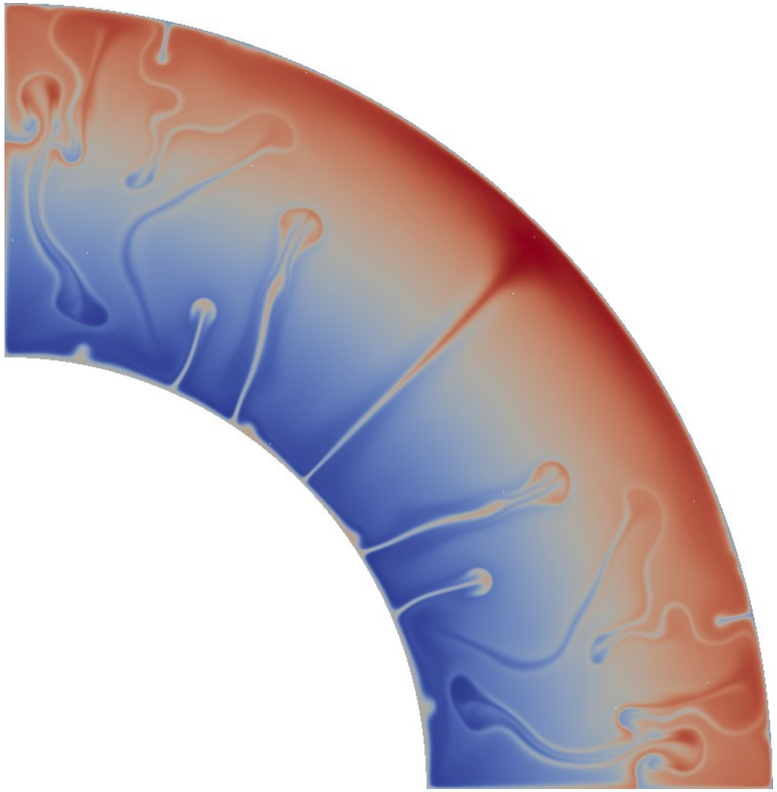
- *Mantle vs. Lithosphere (the “crust”):*
  How does mantle convection interact with plate tectonics?
  How does mantle convection affect natural resources?

- *Mantle vs. Atmosphere:* How does carbon cycle in the Earth?
  Mantle vs. Oceans: How does water cycle in the Earth?
  → Does mantle convection affect the habitability of planets?

- *Mantle vs. Core:* How is heat transported from core to surface?
  → impact on the magnetic field
  → thermal history of Earth
  → history of the inner core

Part I:

“Classical” mantle convection



The model

Thermal convection is described by the relatively “simple” Boussinesq approximation (or variations):

$$-\nabla\cdot[2\eta\epsilon(u)]+\nabla p=g\rho(T)$$

$$\nabla\cdot u=0$$

$$\frac{\partial T}{\partial t}+u\cdot\nabla T-\kappa\Delta T=\gamma+\alpha\left(\frac{\partial p}{\partial t}+u\cdot\nabla p\right)+\eta(\nabla u)^2$$

This is not dissimilar from a typical “model problem”.

Challenges: Problem size

For (global) convection in the earth mantle:

- Depth: ~35 – 2890 km
- Volume: $\sim 10^{12}$ km^3
- Resolution required: <10 km
- Uniform mesh: $\sim 10^9$ cells
- Using Taylor-Hood (Q_2/Q_1) elements: 33B unknowns
- At 100k-1M DoFs/processor: 30k-300k processors!

Consequence: We need adaptive mesh refinement.

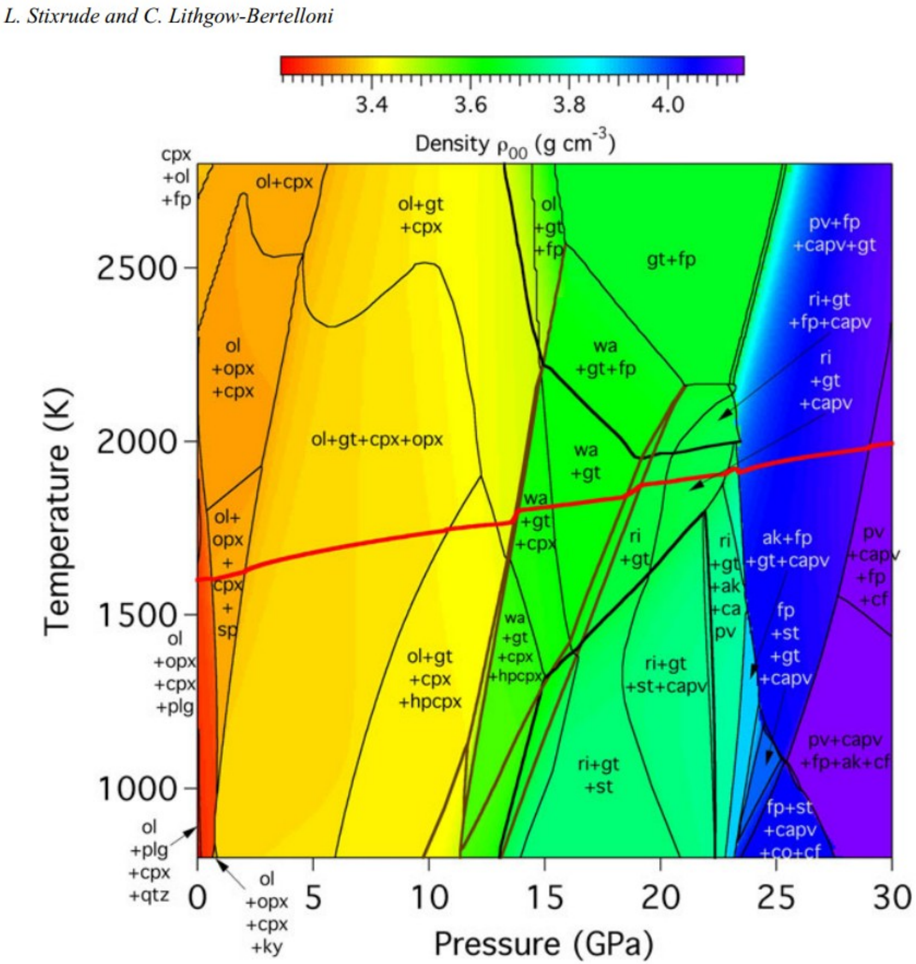
Challenges: Model complexity

However, in reality:

- All coefficients depend nonlinearly on
  - pressure
  - temperature
  - strain rate
  - chemical composition
- Dependency is not continuous

Moreover:

- Viscosity varies by at least 10^6
- Material is compressible
- Geometry depends on solution



Solutions

Among the mathematical techniques we use are:

- *"Higher" order time stepping schemes*
- Higher order finite elements
- Fully adaptive, dynamically changing 3d meshes
- Iterate out the nonlinearity via fixed-point and Newton methods
- Silvester/Wathen-style block preconditioners with F-GMRES
- Algebraic or geometric multigrid for the elliptic part
- Parallelization using MPI, threads, and tasks

To make the code usable by the community:

- Use object-oriented programming, build on external tools
- Make it modular, separate concerns
- Extensive documentation
- Extensive and frequent testing

Time discretization

Recall the model:

$$-\nabla\cdot[2\eta\epsilon(u)]+\nabla p=g\rho(T)$$

$$\nabla\cdot u=0$$

$$\frac{\partial T}{\partial t}+u\cdot\nabla T-\kappa\Delta T=\gamma+\alpha\left(\frac{\partial p}{\partial t}+u\cdot\nabla p\right)+\eta(\nabla u)^2$$

Time discretization

Overall algorithm:

While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field
- Advance time

Time discretization for the temperature

Time equation:

$$\frac{\partial T}{\partial t} + u \cdot \nabla T - \kappa \Delta T = \gamma + \alpha \left(\frac{\partial p}{\partial t} + u \cdot \nabla p \right) + \eta (\nabla u)^2$$

Considerations:

- Adaptive mesh refinement → no high-order multistep methods
- Variable time step size → no high-order multistep methods
- Segregated solver → velocity not available at intermediate times → what to do about RK methods?
- Spatial error dominant (?) → high order not necessary (?)

Our choice: BDF2

Time discretization for the temperature

BDF2 applied to

$$\frac{\partial T}{\partial t} + u \cdot \nabla T - \kappa \Delta T = \gamma + \alpha \left(\frac{\partial p}{\partial t} + u \cdot \nabla p \right) + \eta (\nabla u)^2$$

results in

$$\alpha_n T^n + u^n \cdot \nabla T^n - \kappa \Delta T^n = F(u^{n-1}, T^{n-1}, u^{n-2}, T^{n-2})$$

Considerations:

- We need an efficient linear solver for the discretized system
- The matrix is non-symmetric
- Treat advection as explicit instead:

$$\alpha_n T^n - \kappa \Delta T^n = -u^n \cdot \nabla T^* + F(u^{n-1}, T^{n-1}, u^{n-2}, T^{n-2})$$

Time discretization for the temperature

Semi-implicit BDF2:

$$\alpha_n T^n - \kappa \Delta T^n = -u^n \cdot \nabla T^* + F\left(u^{n-1}, T^{n-1}, u^{n-2}, T^{n-2}\right)$$

Consequences:

- The matrix is now symmetric
- Efficient linear solvers are easy to construct
- **But:** We now have a time step restriction

$$k_n \;\leq\; C_{\mathrm{BDF2}} \min_{K \in T} \frac{h_K}{\|u\|_{L_\infty(K)}}$$

Time discretization for the temperature

CFL condition – the struggle is real:

$$k_n \leq C_{\mathrm{BDF2}} \min_{K \in T} \frac{h_K}{\|u\|_{L_\infty(K)}}$$

Questions:

- What is C_{BDF2}?
- What is h_K on unstructured 3d meshes with curved edges?
- How does all of this relate to the eigenvalues of the matrix?

After much experimentation:

- Choose h_K as the diameter of K
- Choose C_{BDF2}=0.085 → quite small actually

Time discretization for the temperature

After much agony, change of mind – go back to fully implicit:

$$\alpha_n T^n + u^n \cdot \nabla T^n - \kappa \Delta T^n = F\left(u^{n-1}, T^{n-1}, u^{n-2}, T^{n-2}\right)$$

Considerations:

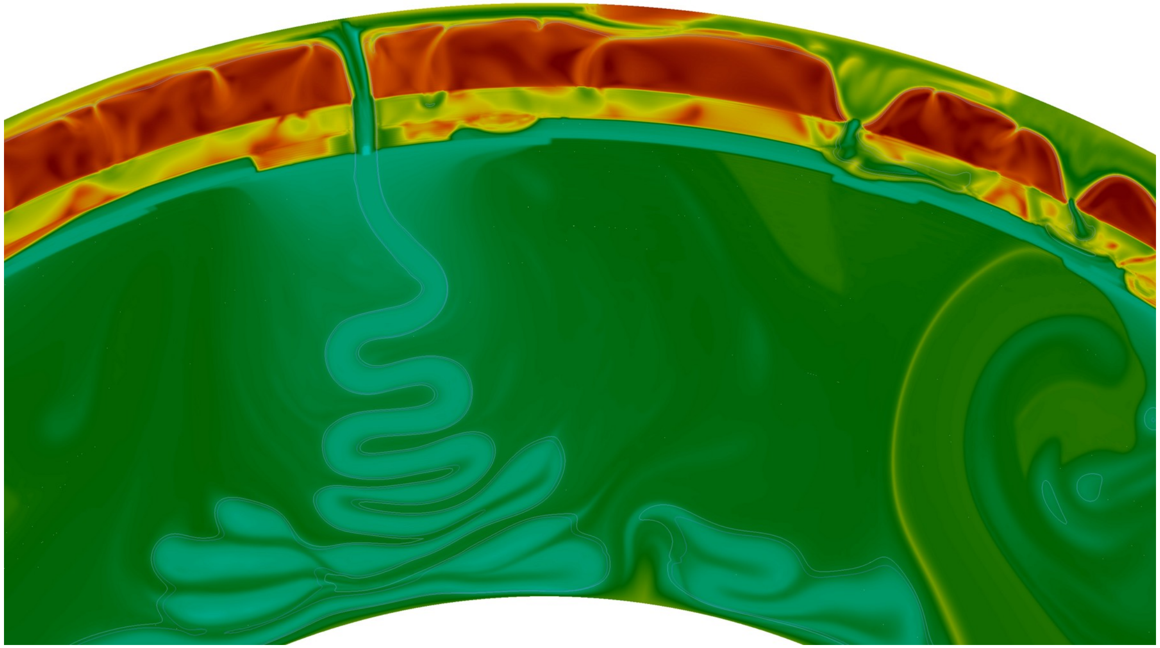
- Need to work harder to solve linear system
- But no longer time-step restricted; choose

$$k_n = 1 \cdot \min_{K \in T} \frac{h_K}{\|u\|_{L_\infty(K)}}$$

Because the Stokes solve is so expensive, the larger time step easily balances the more expensive temperature solve.

Part II:

What then? – Compositional fields



Compositional fields

Juliane Dannberg comes along (2012):

We also want to track chemical compositions:

$$-\nabla\cdot[2\eta\epsilon(u)]+\nabla p=g\rho(T)$$

$$\nabla\cdot u=0$$

$$\frac{\partial T}{\partial t}+u\cdot\nabla T-\kappa\Delta T=\gamma+\alpha\left(\frac{\partial p}{\partial t}+u\cdot\nabla p\right)+\eta(\nabla u)^2$$

$$\boxed{\begin{gathered}\frac{\partial c_1}{\partial t}+u\cdot\nabla c_1-\kappa\Delta c_1=q_1(u,p,T,\vec{c})\\ \ldots\\ \frac{\partial c_N}{\partial t}+u\cdot\nabla c_N-\kappa\Delta c_N=q_N(u,p,T,\vec{c})\end{gathered}}$$

Chemical compositions

Considerations:

- Originally meant to track *compositions* → zero right hand sides
- Then *mineral compositions* → chemical reactions
- Then also other quantities (melting, accumulated strains, level sets, …) → many many such fields

- Would like to solve in a coupled fashion, but too memory expensive
- Solving advection equations suddenly becomes expensive

- Solve in segregated fashion, treat rhs explicitly

Time discretization

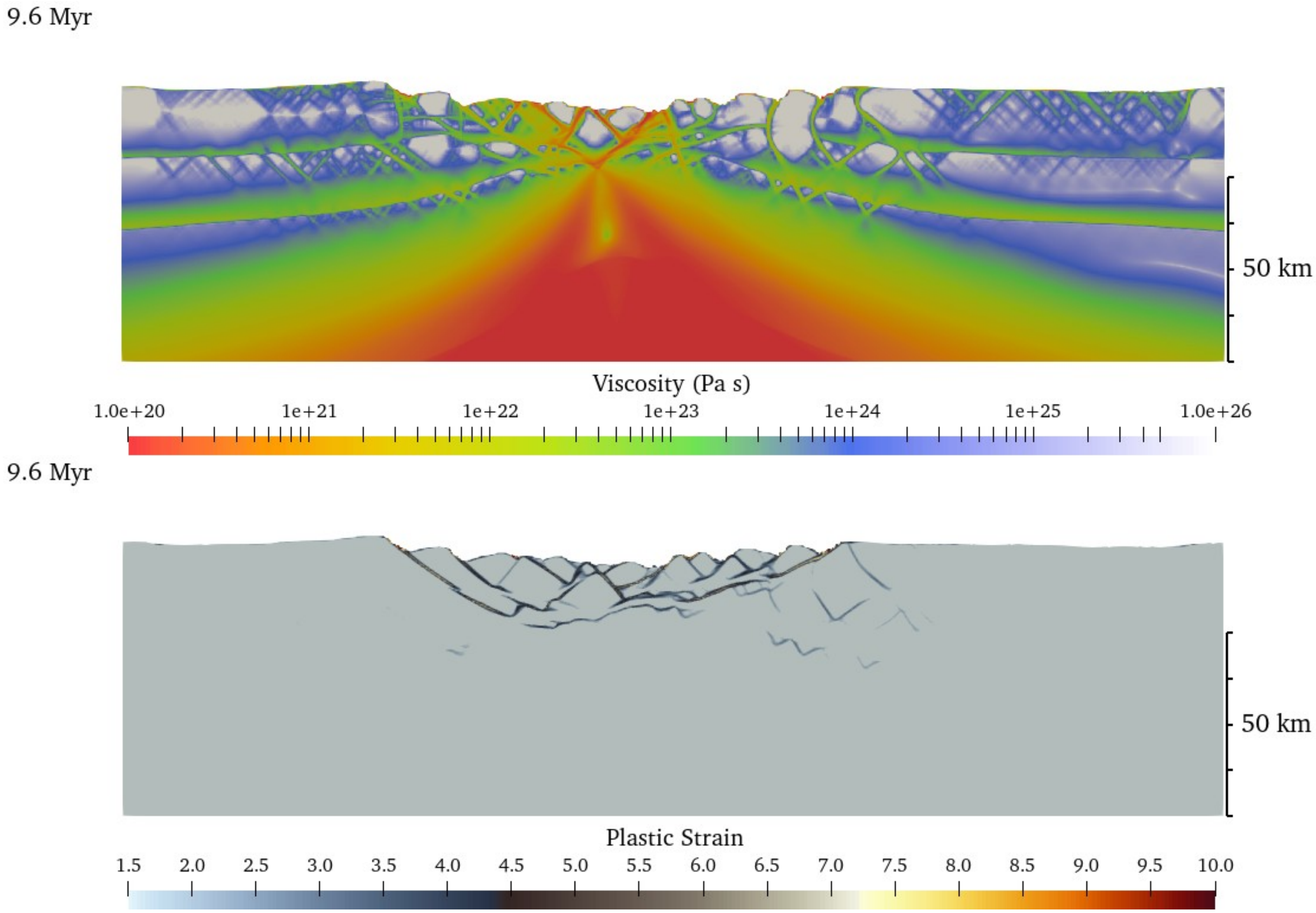
Overall algorithm:

While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1 with implicit BDF2, explicit rhs
- …
- Solve for compositional field N with implicit BDF2, explicit rhs
- Advance time

Part III:

What then? – Stiff source terms



Stiff source terms

John Naliboff, Juliane Dannberg, et al. come along (2017):

"compositional field" is elastic stress, which decays quickly in time:

$$-\nabla \cdot [2\eta\epsilon(u)] + \nabla p = g\rho(T)$$

$$\nabla \cdot u = 0$$

$$\frac{\partial T}{\partial t} + u \cdot \nabla T - \kappa \Delta T = \gamma + \alpha\left(\frac{\partial p}{\partial t} + u \cdot \nabla p\right) + \eta(\nabla u)^2$$

$$\frac{\partial c_1}{\partial t} + u \cdot \nabla c_1 - \kappa \Delta c_1 = q_1(u, p, T, \vec{c})$$

$$\ldots$$

$$\frac{\partial c_N}{\partial t} + u \cdot \nabla c_N - \kappa \Delta c_N = q_N(u, p, T, \vec{c})$$

Stiff source terms

Considerations:

- Elastic stress relaxes on a time scale faster than the flow → "multirate" system
- Impossible to resolve this time scale in a coupled scheme
- Treat rhs via operator splitting:
  – currently uses Lie splitting
  – currently integrates pointwise ODE with a fixed micro timestep

Time discretization

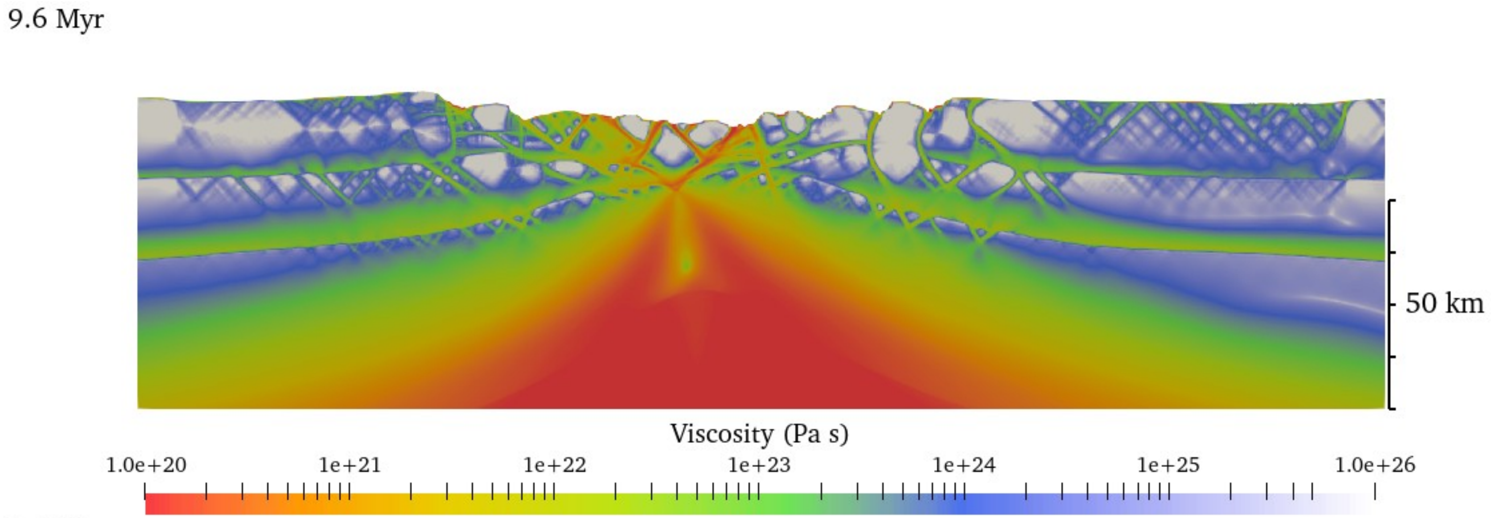
Overall algorithm:

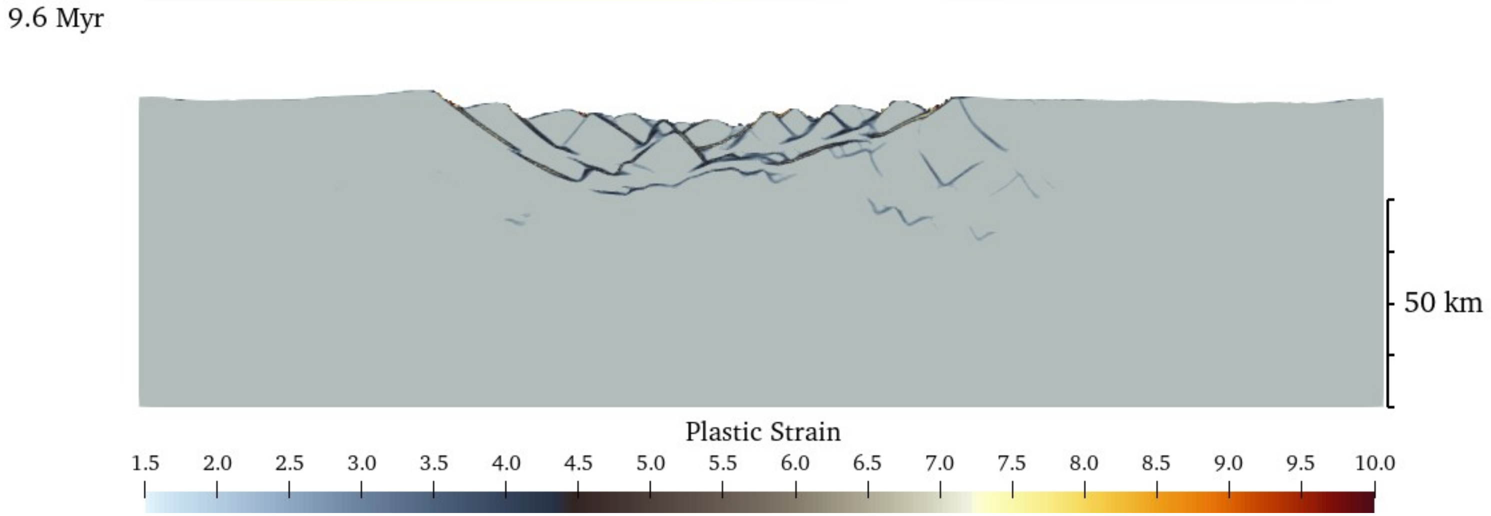
While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1, implicit BDF2, operator splitting
- …
- Solve for compositional field 1, implicit BDF2, operator splitting
- Advance time

Part IV:

What then? – Free surfaces





Free surfaces

Then Ian Rose and Timo Heister come along (2014):

- We also want to deform the surface of the domain
- Evaluate residual stresses at the surface, move nodes at boundary and in domain
- Requires one Laplace solve

Then Anne Glerum comes along (2020):

- Diffuse the surface to mimic erosion

Free surfaces

Equations now:

$$-\nabla\cdot[2\eta\epsilon(u)]+\nabla p=g\rho(T)$$

$$\nabla\cdot u=0$$

$$\frac{\partial T}{\partial t}+u\cdot\nabla T-\kappa\Delta T=\gamma+\alpha\left(\frac{\partial p}{\partial t}+u\cdot\nabla p\right)+\eta(\nabla u)^2$$

$$\frac{\partial c_1}{\partial t}+u\cdot\nabla c_1-\kappa\Delta c_1=q_1(u,p,T,\vec{c})$$

$$\ldots$$

$$\frac{\partial c_N}{\partial t}+u\cdot\nabla c_N-\kappa\Delta c_N=q_N(u,p,T,\vec{c})$$

$$\boxed{\frac{\partial h}{\partial t}-A\Delta h=r(u,p)}$$

Time discretization

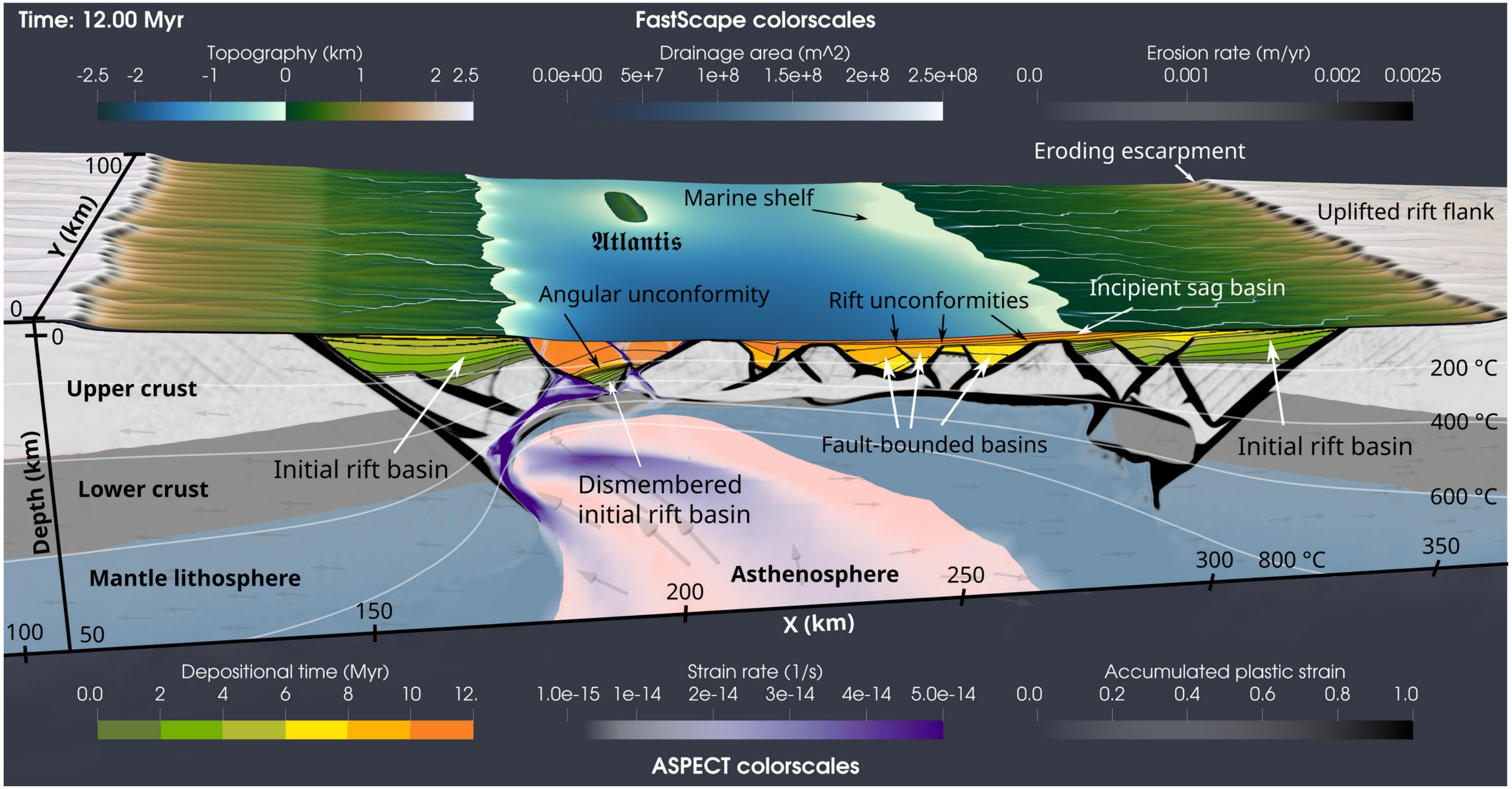
Overall algorithm:

While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1, implicit BDF2, operator splitting
- …
- Solve for compositional field 1, implicit BDF2, operator splitting
- Solve for surface deformation
- Advance time

Part V:

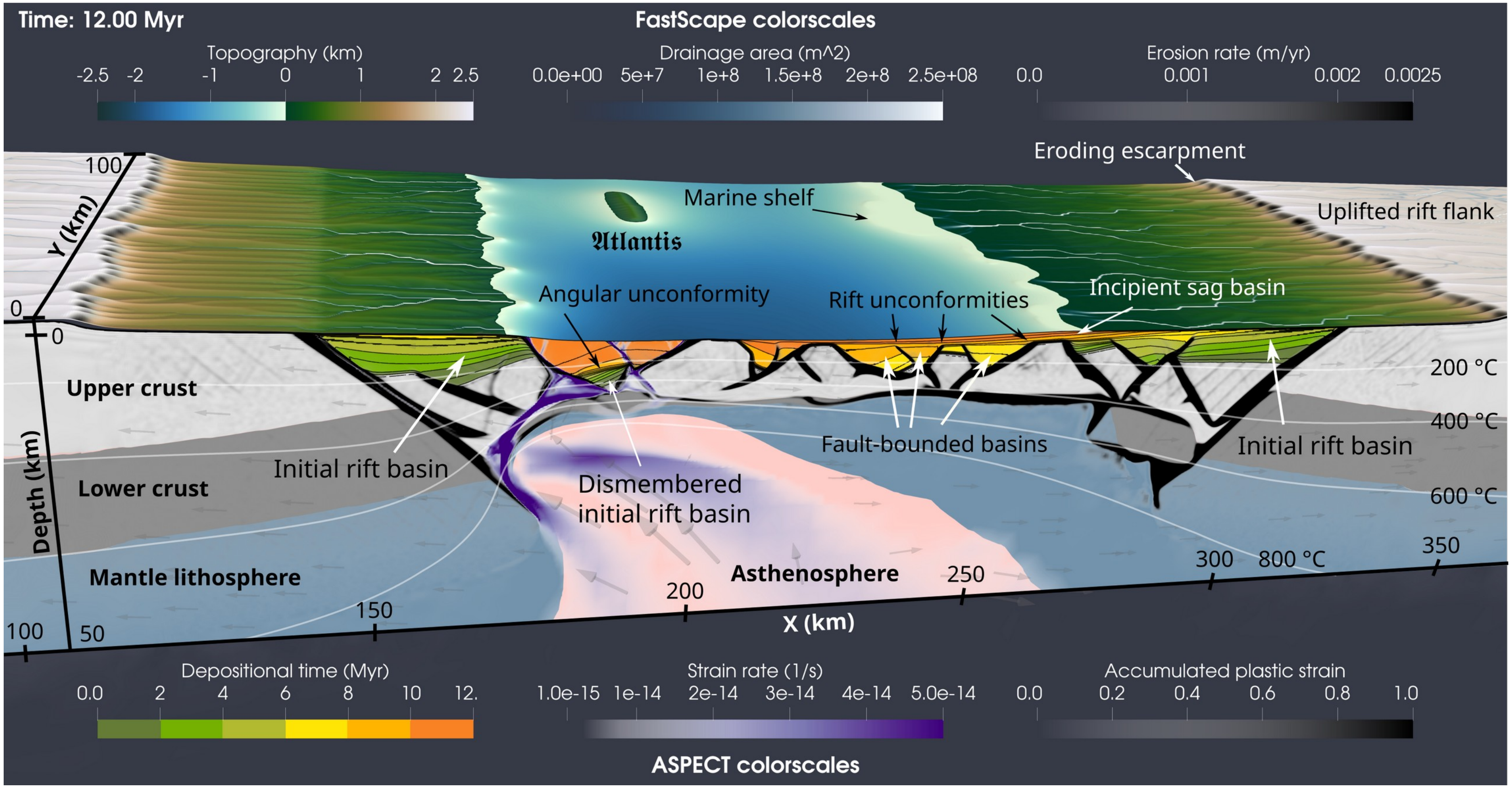
What then? – Surface evolution



Realistic surfaces

Derek Neuharth et al. come along (2021):

“Real” surface models are too complicated to re-implement in ASPECT. Couple with an external code: FastScape



Time discretization

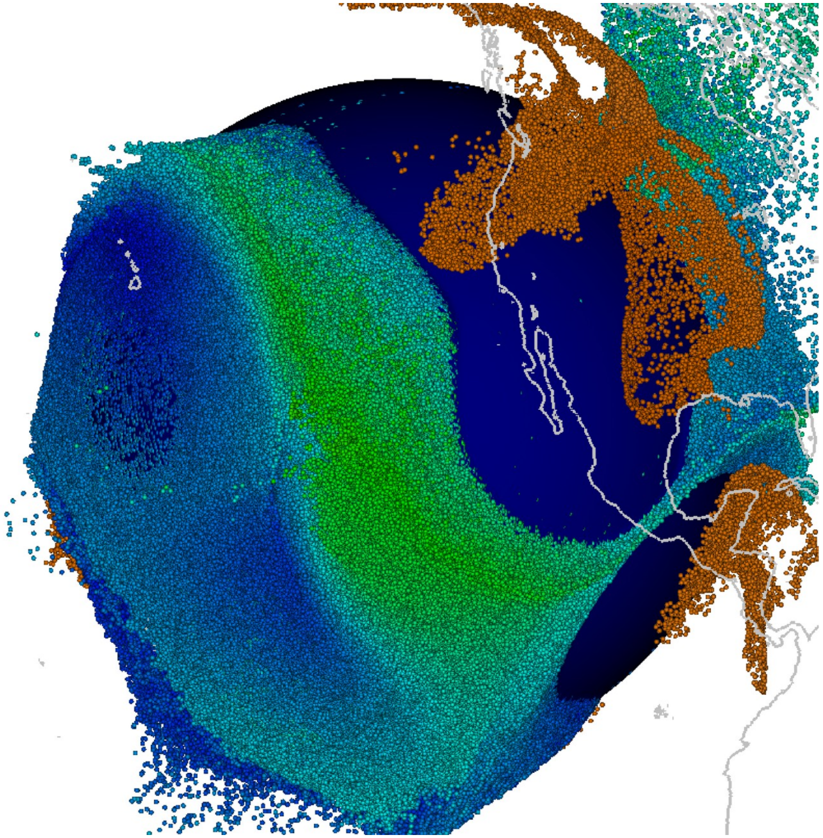
Overall algorithm:

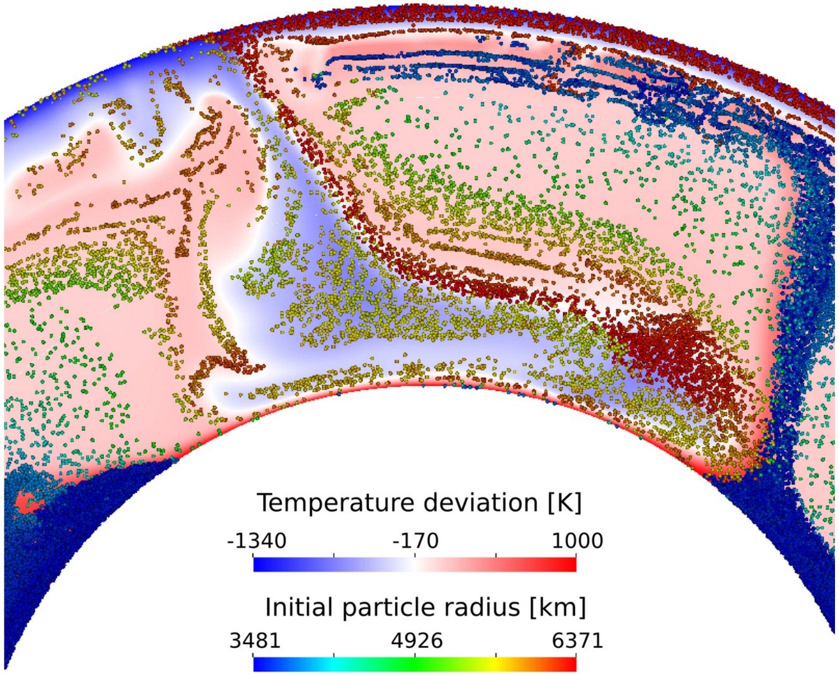
While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1, implicit BDF2, operator splitting
- …
- Solve for compositional field 1, implicit BDF2, operator splitting
- Solve for surface deformation, couple with FastScape
- Advance time

Part VI:

What then? – Particles

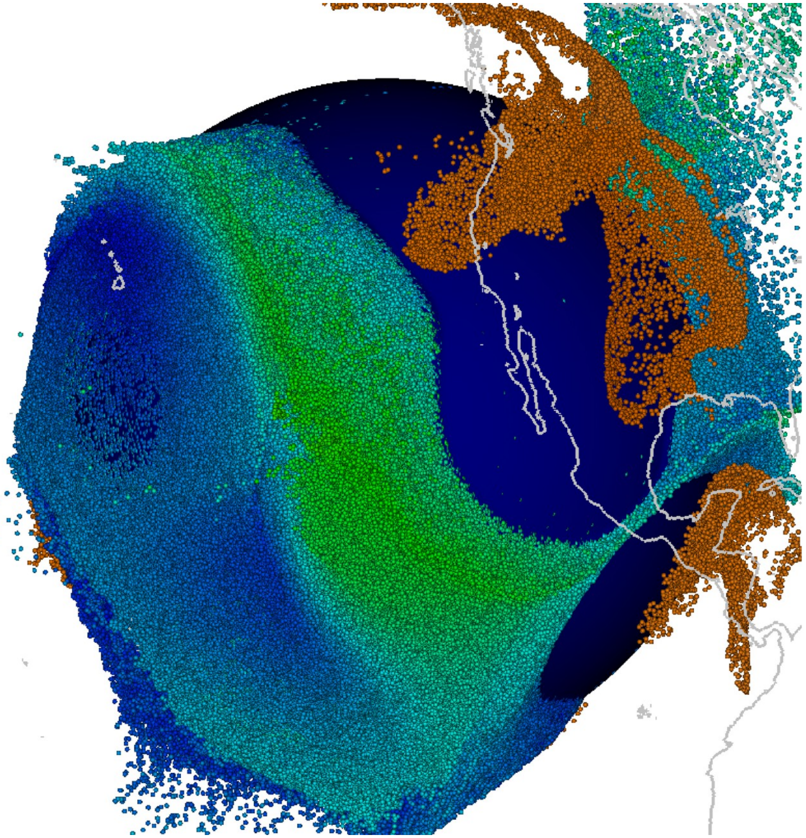


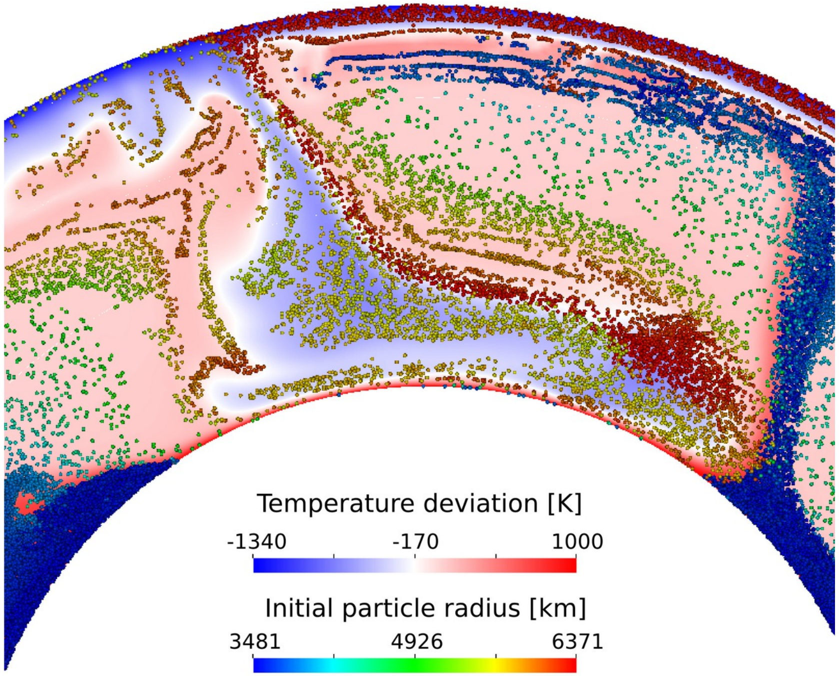


Compositional fields

Rene Gassmoeller comes along (2013?):

Fields are expensive. We want to track particles move along with the flow.





Free surfaces

Equations now:

$$-\nabla\cdot[2\eta\epsilon(u)]+\nabla p=g\rho(T)$$

$$\nabla\cdot u=0$$

$$\frac{\partial T}{\partial t}+u\cdot\nabla T-\kappa\Delta T=\gamma+\alpha\left(\frac{\partial p}{\partial t}+u\cdot\nabla p\right)+\eta(\nabla u)^2$$

$$\frac{\partial c_1}{\partial t}+u\cdot\nabla c_1-\kappa\Delta c_1=q_1(u,p,T,\vec{c})$$

$$\dots$$

$$\frac{\partial c_N}{\partial t}+u\cdot\nabla c_N-\kappa\Delta c_N=q_N(u,p,T,\vec{c})$$

$$\frac{\partial h}{\partial t}-A\Delta h=r(u,p)$$

$$\boxed{\frac{dx_i(t)}{dt}=u(x_i(t)) \qquad \frac{dp_{i,j}(t)}{dt}=s(u,p,T,\vec{c},\vec{p}_i)}$$

Compositional fields

Considerations:

- Velocity affects particle locations
- Sometimes particle properties affect flow equations

- Computationally quite different from field-based methods
- Efficiency requires CFL<=1 → Particles transported at most one cell per time step
- Evaluation of rhs is *very* expensive

- Do one explicit Euler/RK4 step per (macro) step

Time discretization

Overall algorithm:

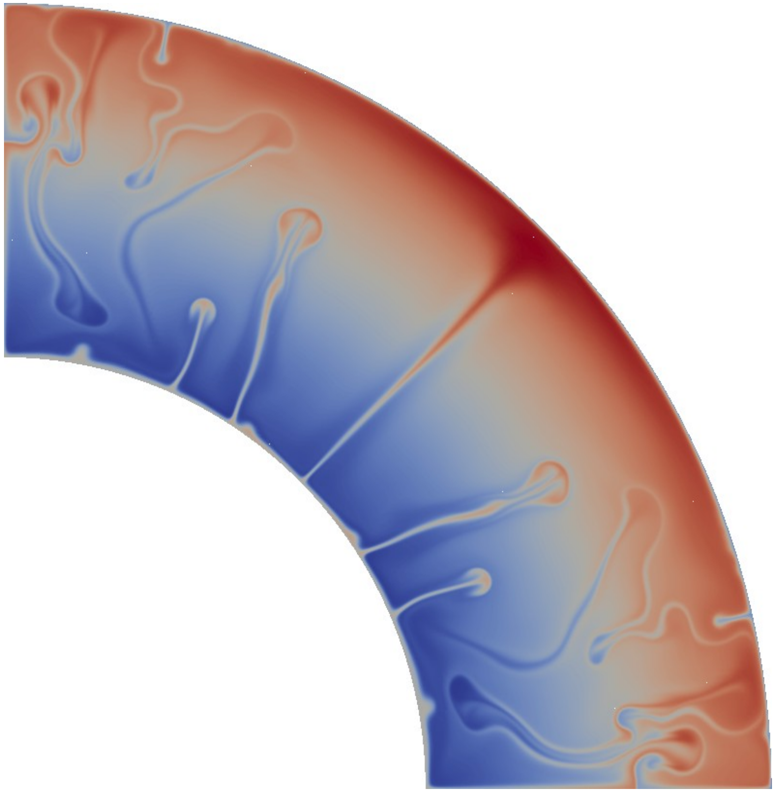
While ($T<T_{end}$):

- Solve Stokes equation
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1, implicit BDF2, operator splitting
- …
- Solve for compositional field 1, implicit BDF2, operator splitting
- Solve for surface deformation, couple with FastScape
- Advance cell positions and properties
- Advance time

Conclusions

ASPECT has turned out to be a very good tool to do interesting science!

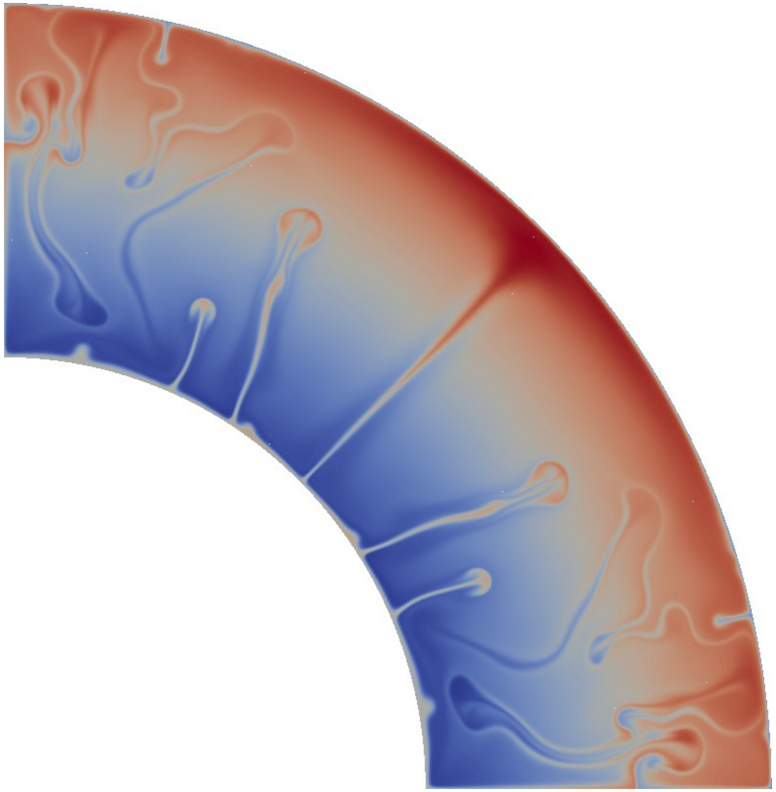
- We can produce lots of colorful pictures → something must be right!
- ***But is this the right approach?***



Questions I don't know the answer to

Question 1: What would be the costs of a better approach?

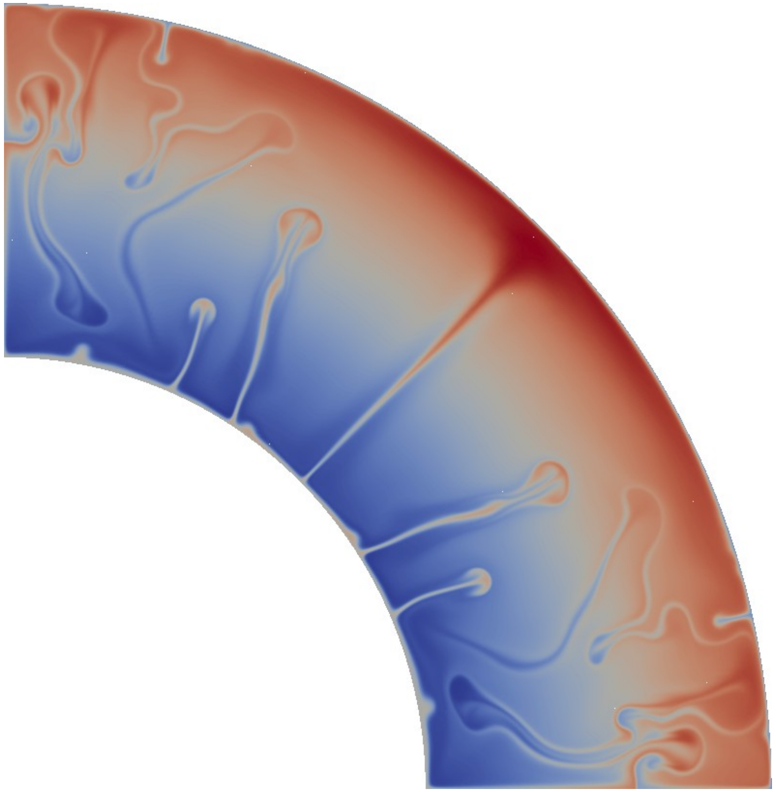
- Coupled solvers will require more memory, likely more computations
- How would one even approach integrating multiple modalities (solving in the bulk, on the surface, particles, external codes)?



Questions I don't know the answer to

Question 2: What would be the benefits of a better approach?

- How big is the time discretization error?
- What is the dominant contribution to the overall error?
- What is the *error* anyway?



Conclusions

Aspect – Advanced Solver for Problems in Earth's ConvecTion:

http://aspect.geodynamics.org/

References:
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