Thoughts about time stepping in real-world multiphysics PDE solvers

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Joint work with Juliane Dannberg, Menno Fraters, Rene Gassmoeller, Anne Glerum, Timo Heister, Bob Myhill, John Naliboff, and many many other contributors

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WHERE DISCOVERIES BEGIN

CIG COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Theory v Practice

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WHERE DISCOVERIES BEGIN

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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 was no “holistic design” at the beginning.

Take-away message (realistic version):

Real-world simulators often do not fit into typical categories.

Practicalities of code development limit both original choice of and later conversion to different methods.

Overview:

- The model, and how we solve it in the Advanced Solver for Planetary Evolution, Convection and Tectonics (ASPECT)

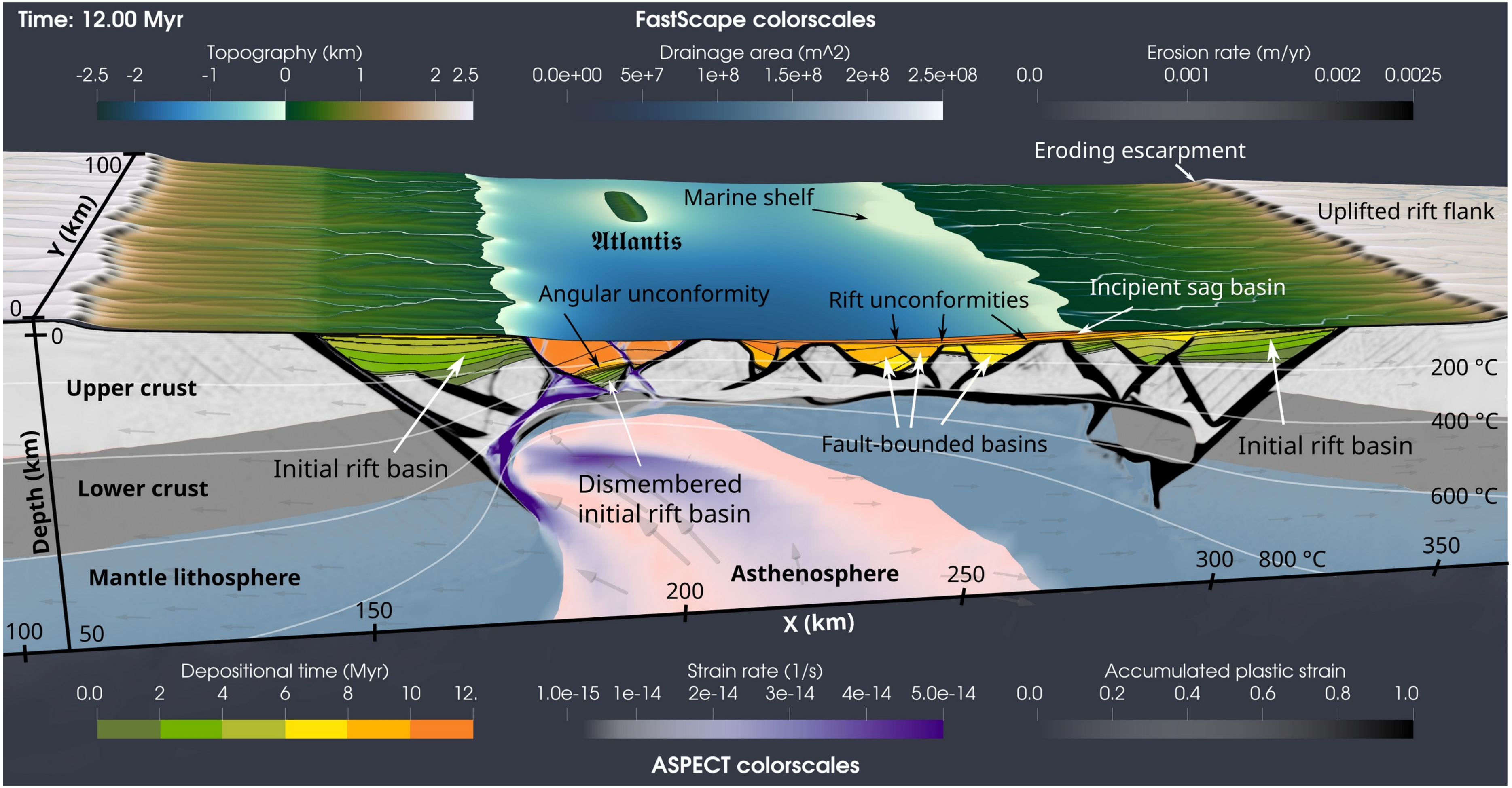
- What I would love to do

- Why I can’t do it

- What *does* work today

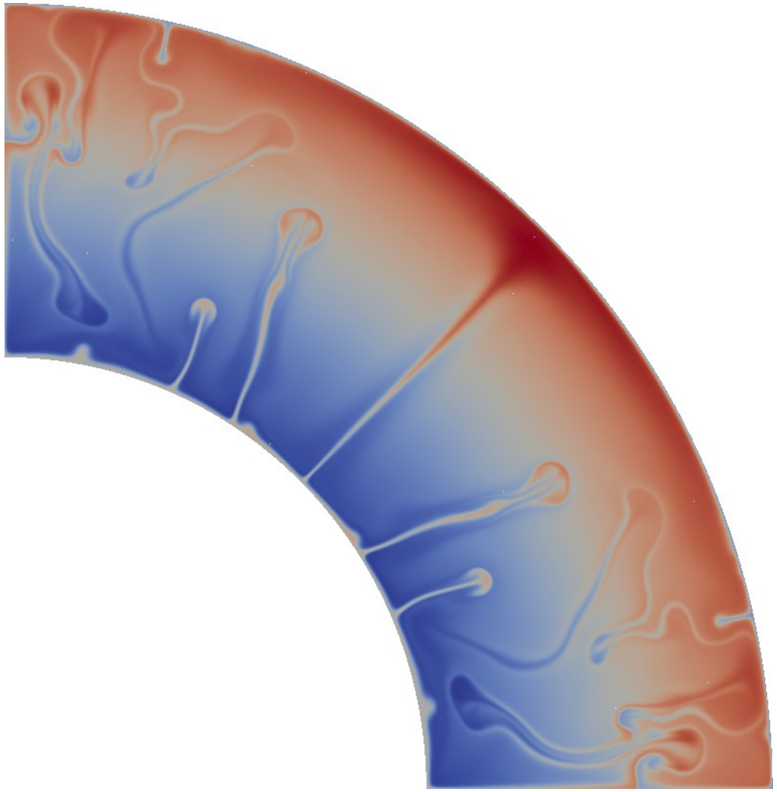
The model and how we solve it

The what and the why



Component 1:

“Classical” mantle convection



The model

Motion in the deep Earth is driven by density differences due temperature differences ("convection").

On long time scales, rocks behave like viscous Stokes flow:

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

$$\nabla \cdot u = 0$$

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

Stokes + advection-diffusion: not dissimilar from a typical "model problem". (But note: It's a DAE.)

Challenges: Problem size

For (global) convection in the earth mantle:

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

Better: Can reduce these numbers 10x to 100x through adaptive mesh refinement.

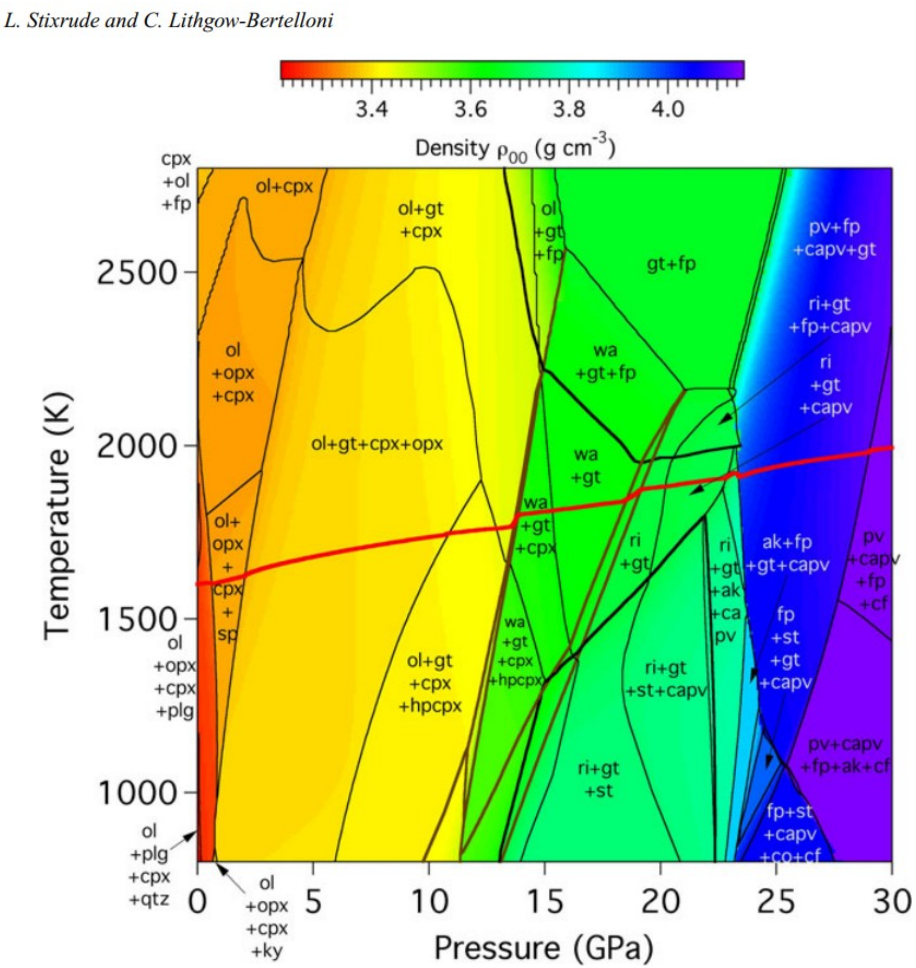
Challenges: Model complexity

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:

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

$$\nabla\cdot u=0$$

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

This is a nonlinear Differential-Algebraic Equation (DAE).

In practice:

- Solve Stokes with extrapolated *T* for *u*,*p*
- Solve advection/diffusion with *u*,*p* for temperature *T*

Time discretization

Overall algorithm:

While ($t<t_{end}$):

- Solve Stokes equation
- From velocity, compute time step via CFL condition
- 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

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

Considerations:

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

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

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:

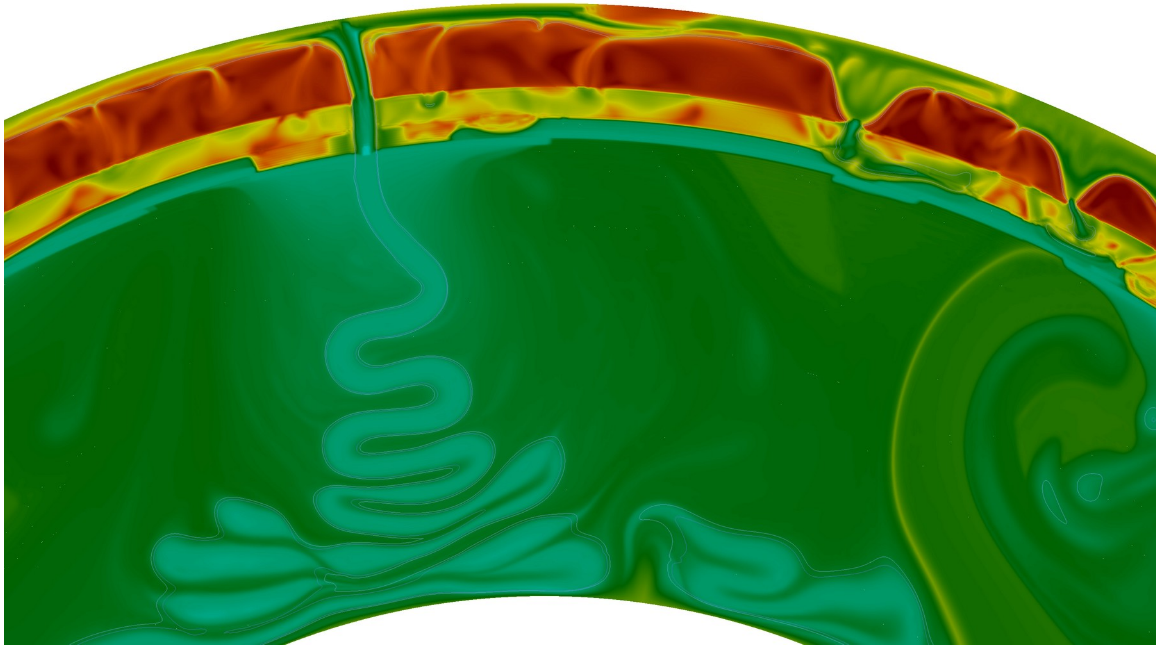
- Need to work harder to solve linear system
- But no longer time-step restricted; choose

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

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

Component 2:

Compositional fields



Compositional fields

Juliane Dannberg (2012):

We also want to track chemical compositions:

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

$$\nabla\cdot u=0$$

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

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

$$\ldots$$

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

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

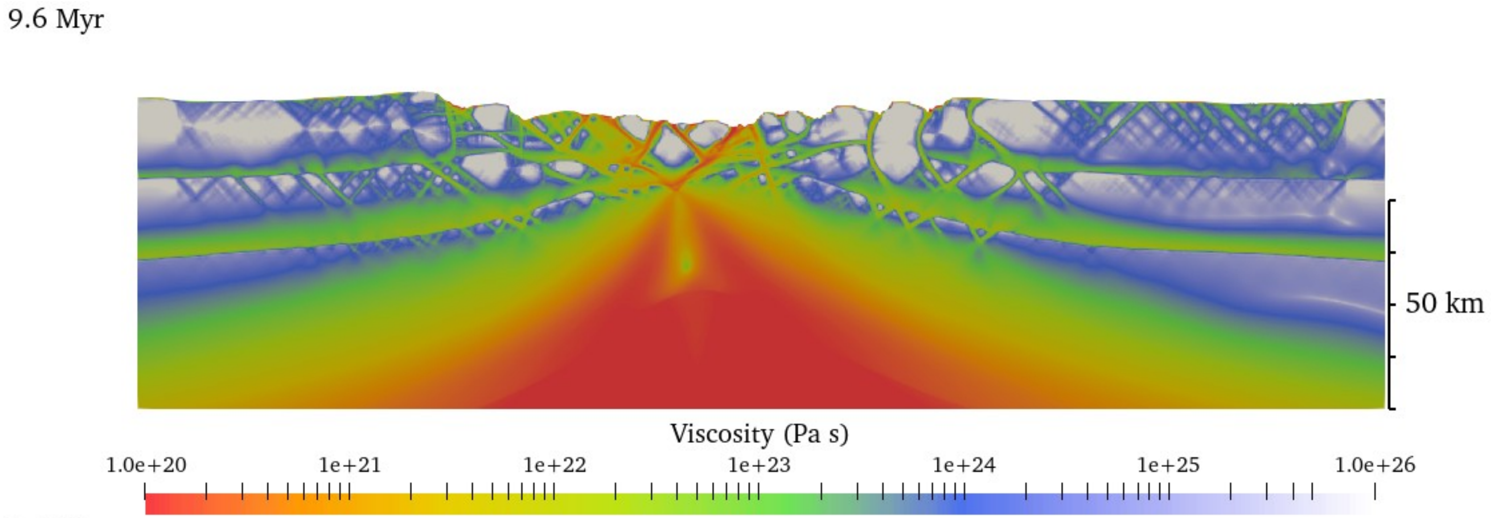
Overall algorithm:

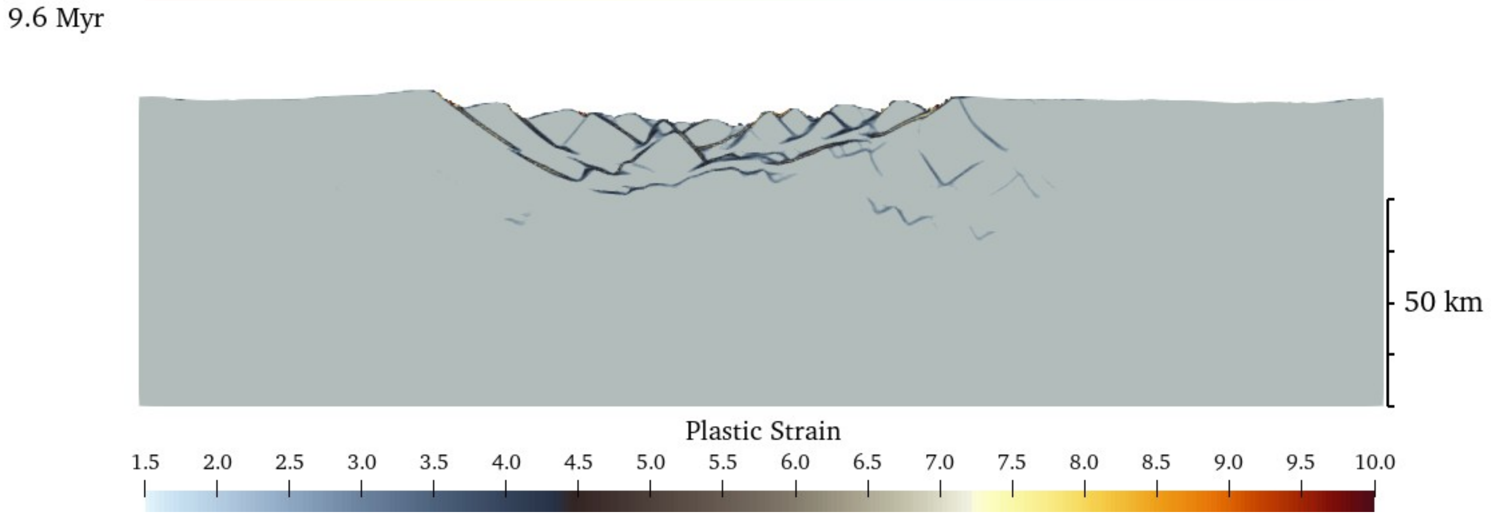
While ($t<t_{end}$):

- 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

Component 3:

Stiff source terms





Stiff source terms

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

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

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

$$\nabla\cdot u=0$$

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

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

$$\ldots$$

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

Stiff source terms

Considerations:

- Elastic stress relaxes on a time scale faster than the flow
  $\rightarrow$ "multirate" system
- Impossible to resolve this time scale in a coupled scheme
- Treat rhs via operator splitting:
  – currently uses Lie splitting
  – originally used pointwise ODE with fixed micro timestep
  – now uses SUNDIALS ARKODE

Time discretization

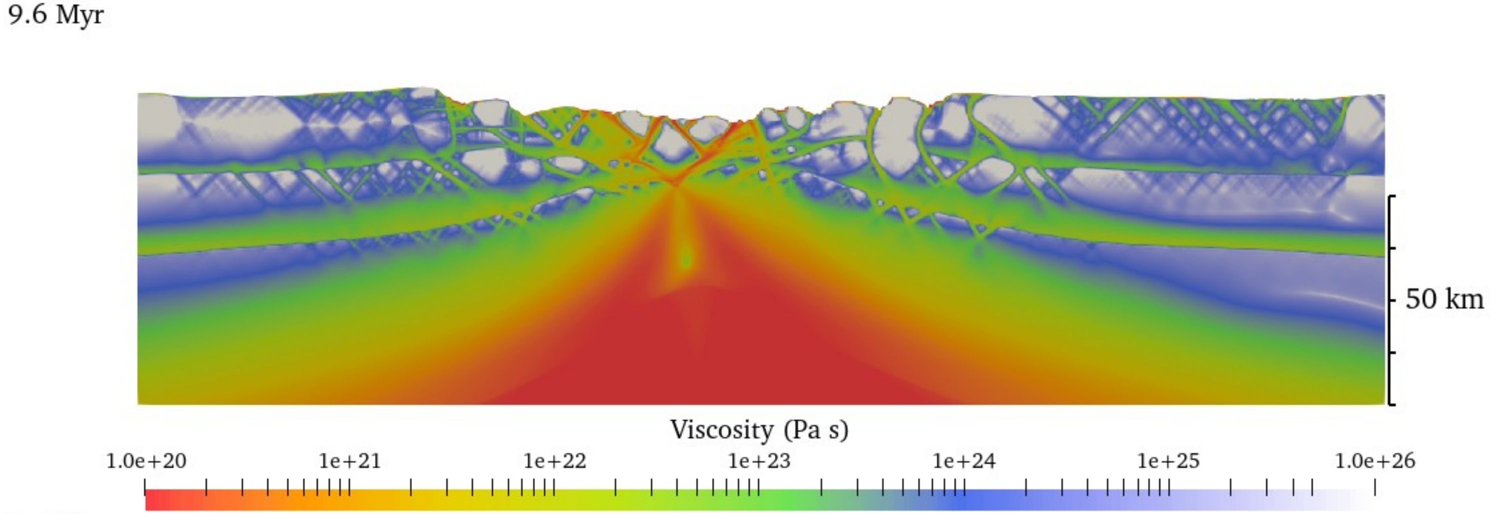
Overall algorithm:

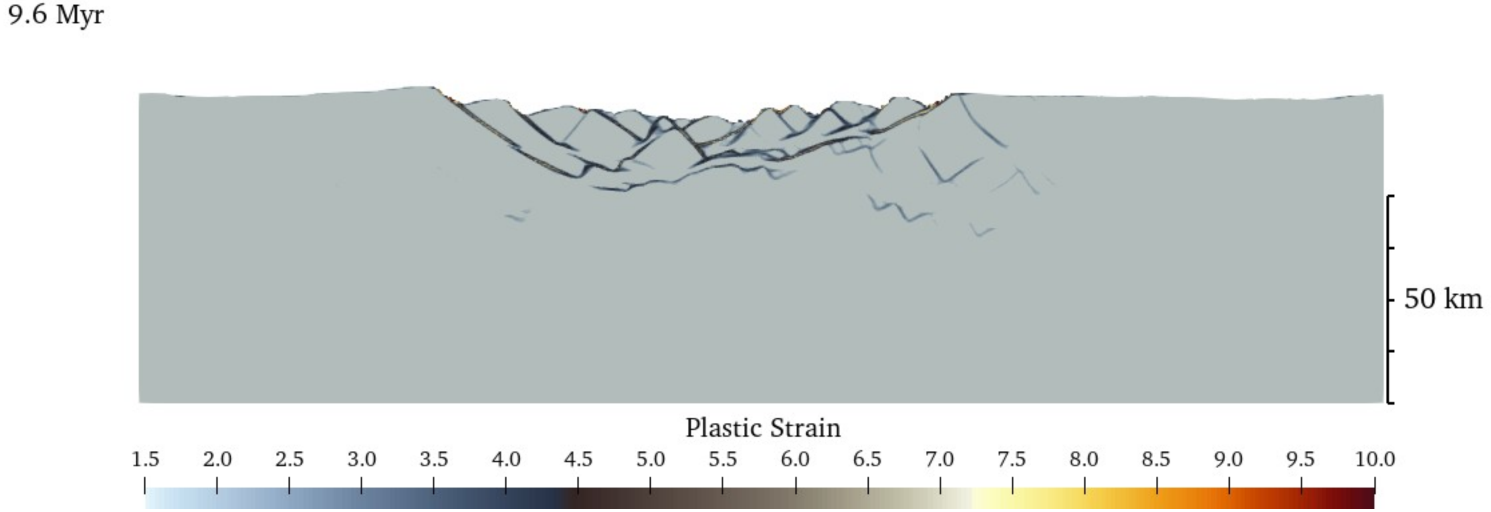
While ($t<t_{end}$):

- 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

Component 4:

Free surfaces





Free surfaces

Ian Rose and Timo Heister (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

Anne Glerum (2020):

- Diffuse the surface to mimic erosion

Free surfaces

Equations now:

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

$$\nabla\cdot u=0$$

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

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

$$\dots$$

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

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

Time discretization

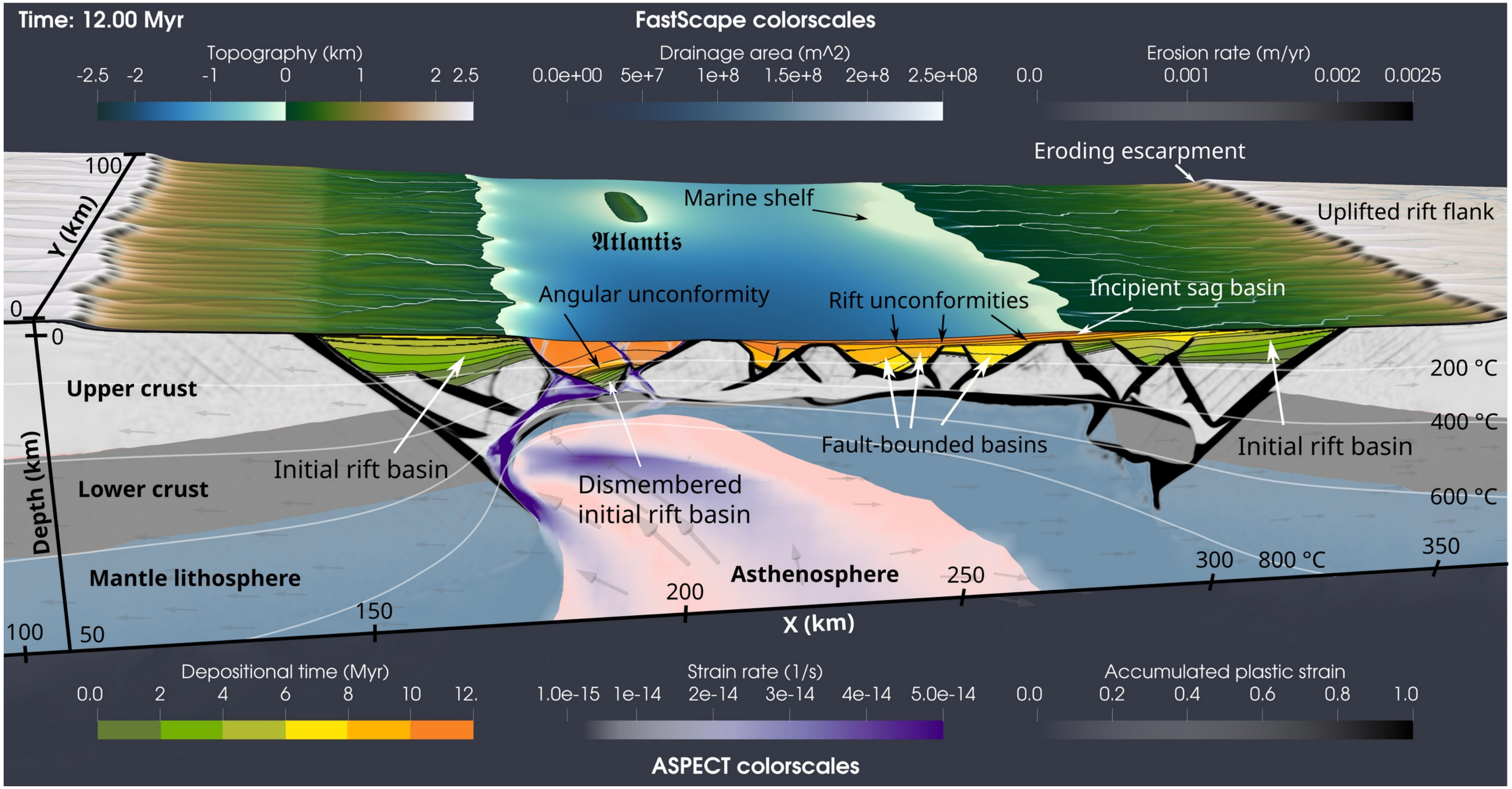
Overall algorithm:

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

Component 5:

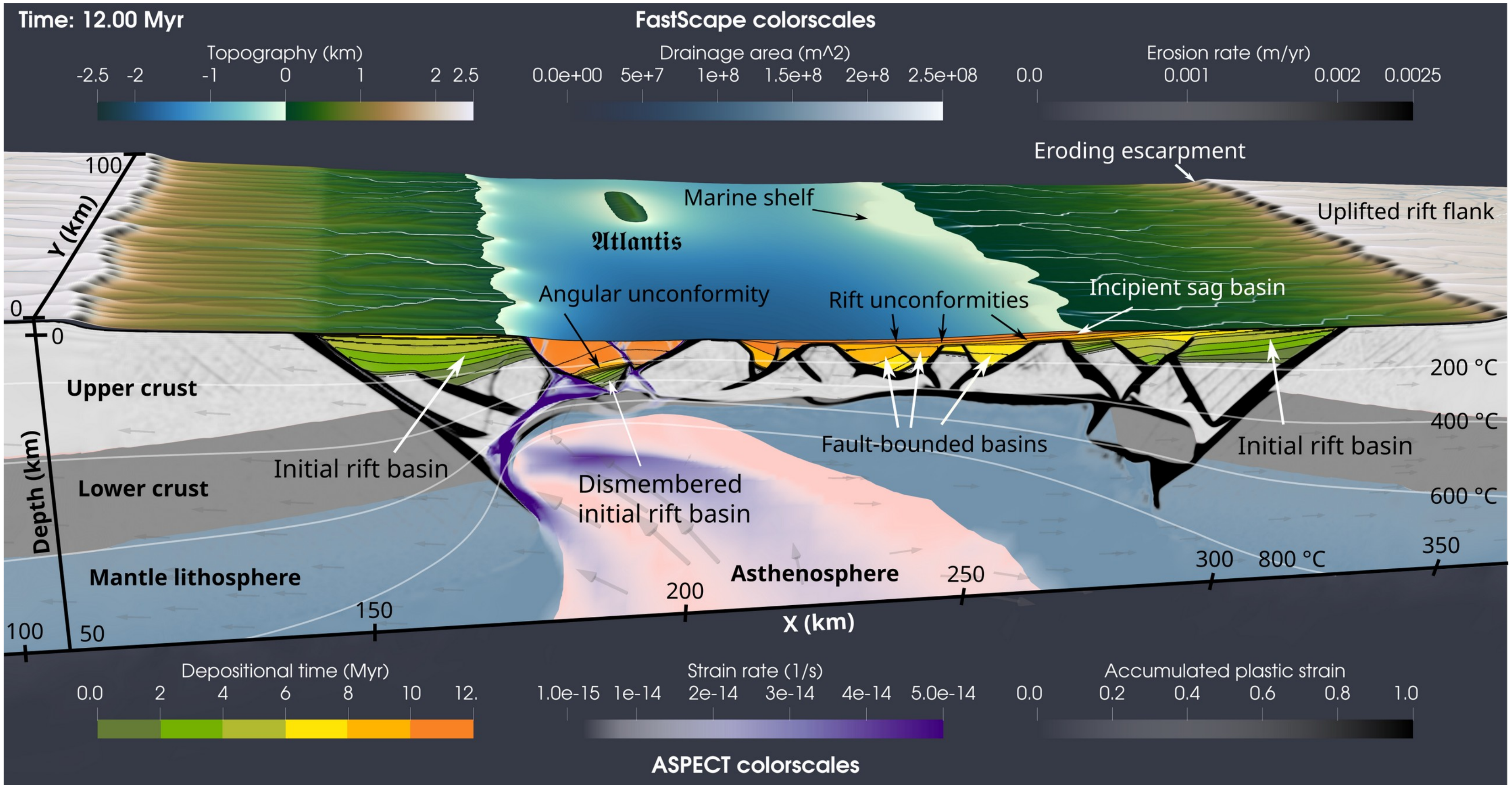
Surface evolution



Realistic surfaces

Derek Neuharth et al. (2021):

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



Time discretization

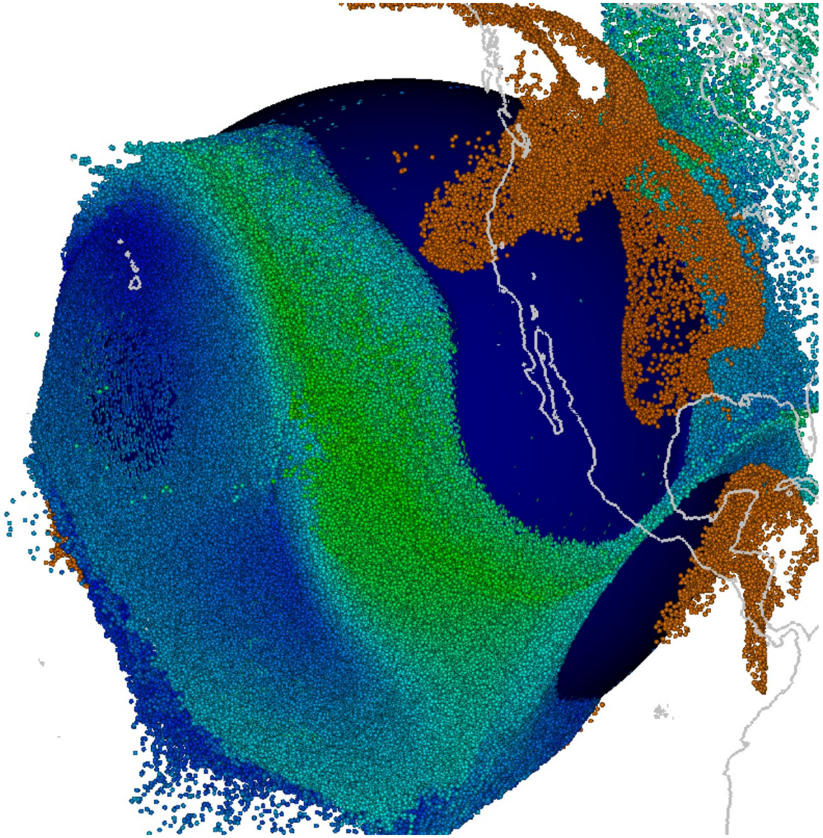
Overall algorithm:

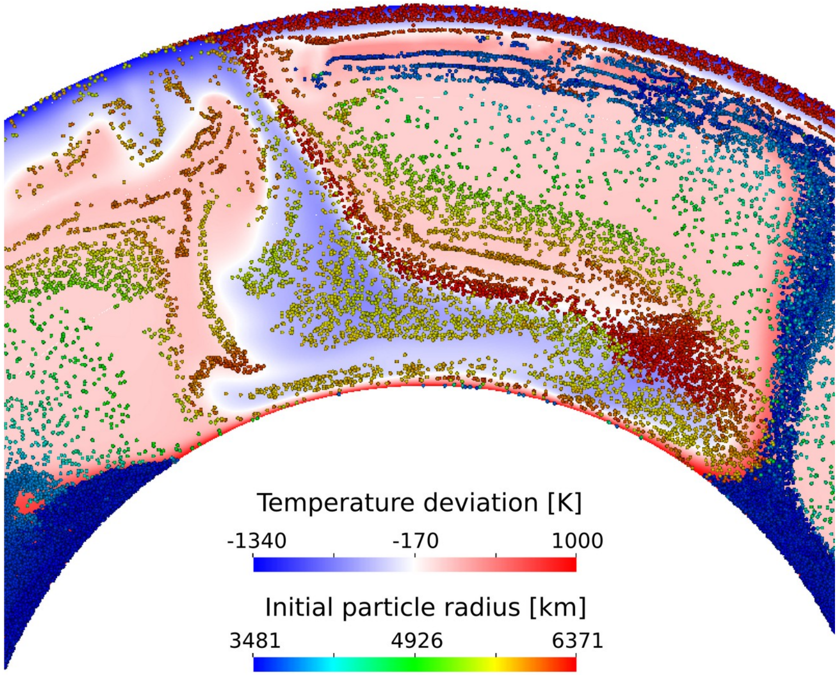
While ($t<t_{end}$):

- 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, coupled with external tool
- Advance time

Component 6:

Particles

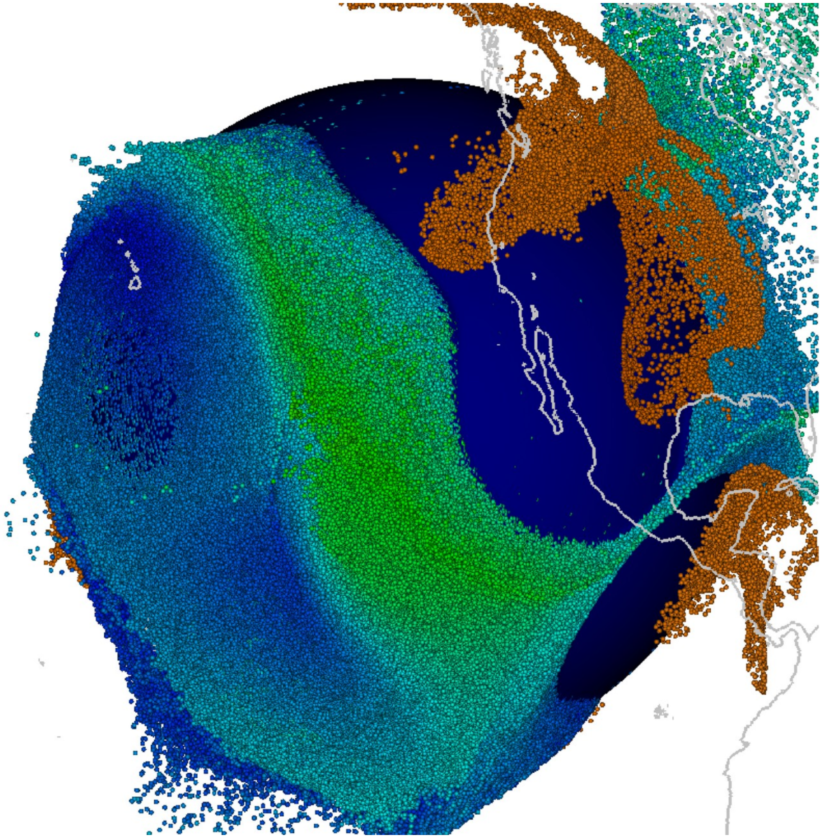


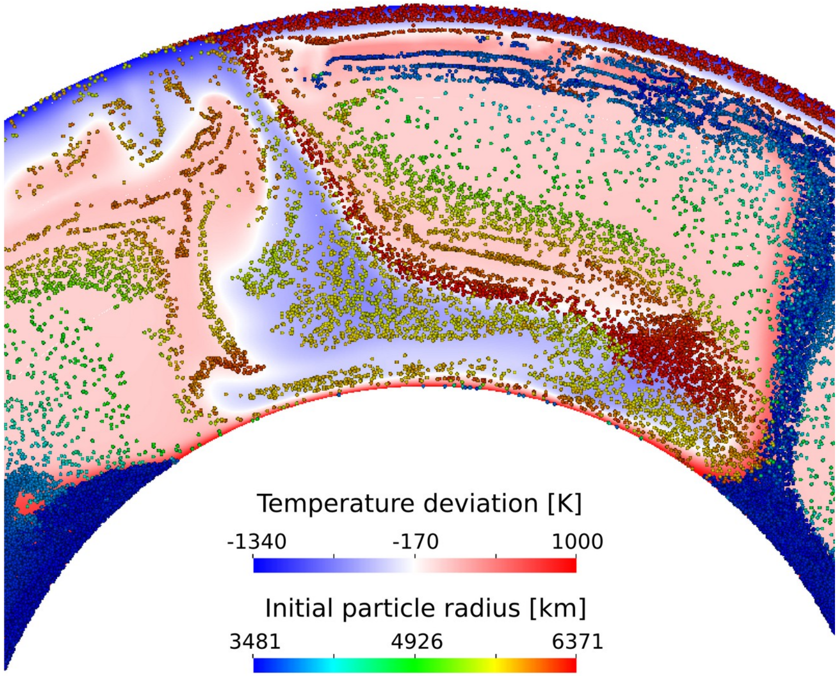


Particles

Rene Gassmoeller (~2013):

Fields are expensive. We want to track particles (and properties) as they move along with the flow.





Particles

Equations now:

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

$$\nabla\cdot u=0$$

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

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

$$\dots$$

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

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

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

Particles

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/RK2/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, coupled with external tool
- Advance particle positions and properties
- Advance time

Time discretization

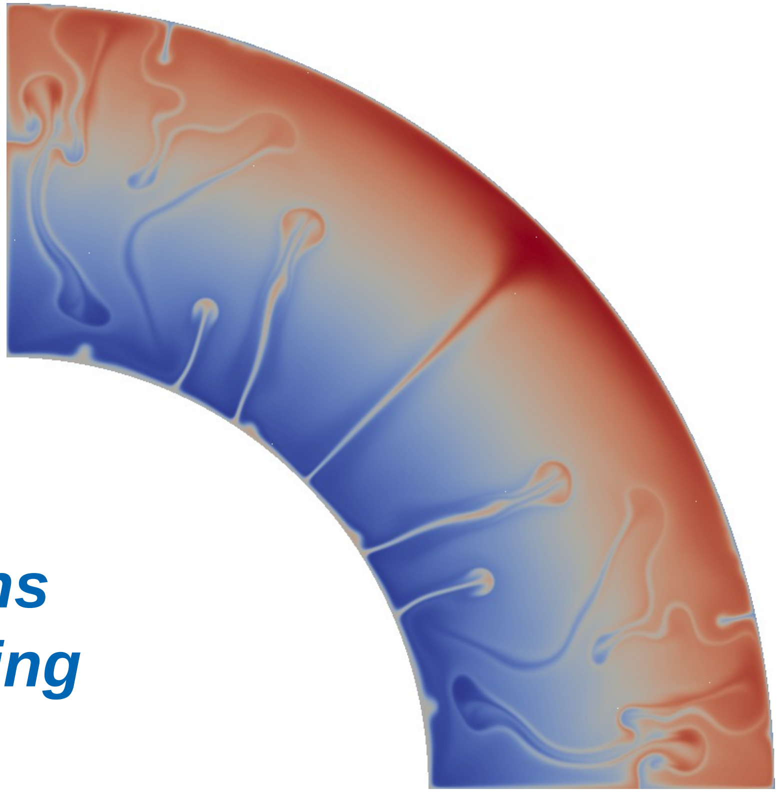
Overall algorithm:

While ($t<t_{end}$):

- Solve Stokes equation **60%**
- From velocity, compute time step
- Solve for temperature field with implicit BDF2
- Solve for compositional field 1, implicit BDF2, operator splitting
- … **15%**
- Solve for compositional field 1, implicit BDF2, operator splitting
- Solve for surface deformation **10%**
- Advance particle positions and properties **15%**
- Advance time

Conclusions of this part

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 it is not an easy set of equations***
- ***We use a first-order operator splitting***
- ***How could we do this better?***

What I would love to do

My wishlist

Right now:

- First order operator splitting: Solve one physics after the other

What I wished:

- The system is a DAE. Solve it as such.
- Or at least use a (second-order) Strang splitting.

- At least do a study that assesses how much of an error we introduce – perhaps time discretization is not a major source of error?

My wishlist

Right now:

- Temperature + compositional fields used fixed-order BDF2
- BDF-2 (like all multistep methods) requires awkward start-up procedure

What I wished:

- Build on a library that abstracts the details (hard-coded coefficients, special-casing first time step)
- Adjusts method order automatically
- Allows playing with different methods

My wishlist

Right now:

- Particle integrator can use forward Euler ... RK4
- Time step is fixed fraction of global time step

What I wished:

- Build on a library that abstracts the details (hard-coded coefficients, special-casing first time step)
- Is able to adjust method order, time step length

- Should probably use SUNDIALS' ARKODE

My wishlist

Right now:

- Global time step is based on CFL condition, not error
- We have methods of iterating out the nonlinearity in each time step, but their use is not automatic

What I wished:

- Default to nonlinear iteration
- Control all this with an error criterion
- Let some library handle the details, rather than do it ourselves

Why I can’t do what I’d love to do

Obstacles

Human issues:

Complexity:

- Core of ASPECT has ~40,000 lines of code
- Core has contributions from ~25 people over 15 years

Modularity is an important consideration!

Obstacles

Historical issues:

- Core of ASPECT was written in ~2010
- SUNDIALS first released early 2000s, but not widely known in the PDE community
- PETSc TS paper is from ~2018

Building on others’ code is important – put your ideas into widely used packages!

Obstacles

Technical factors:

- Solving *coupled* system requires *much* more peak memory
- Coupling different codes in one time stepping scheme is *hard*!
- Discretized PDEs are *not* just large systems of ODEs:
  - Boundary conditions
  - Constraints (e.g., hanging nodes)
  - Meshes change from time step to time step
- High order operator splitting/multirate integrators not widely available (until recently?)

Again, put new ideas into widely used packages that know how to deal with these practicalities!

Obstacles

Needs assessment:

- It isn't actually clear that more accurate time stepping methods are necessary
- The only clear need is for larger time steps
  (Caveat: Accuracy, particles requires CFL ~ 1)

Things that do work already today

What does work

Packaging works:

- SUNDIALS, PETSc TS are good solutions
- We use the SUNDIALS KINSOL and PETSc SNES as nonlinear solvers elsewhere
- ASPECT uses SUNDIALS' ARKODE for stiff compositional right hand sides

What does work

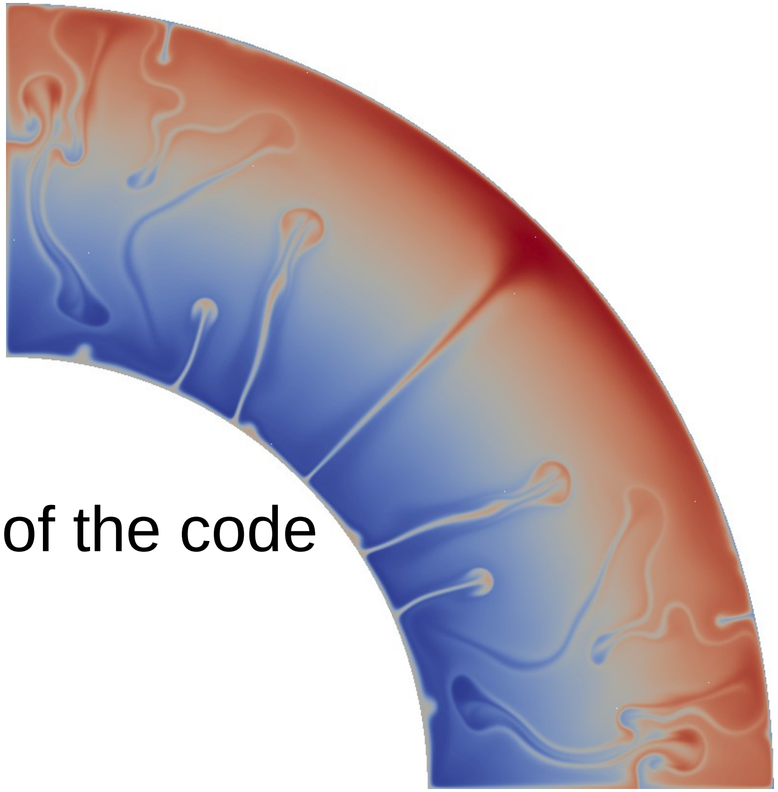
PDEs vs ODEs:

Packaged solvers (e.g. PETSc TS) understand that discretized PDEs are not just large ODE systems:

- Know how to deal with constrained DoFs
- Know how to deal with changing meshes
- Are used in large-scale multiphysics codes

Summary

Dealing with real world problems is hard:



- Problems are coupled, aren't always easy to characterize
- Software is written by humans:
  - Who are not experts in everything
  - With limited knowledge of the rest of the code
  - Over a long time
- The *need* for higher order methods is not always clear
- Packaging makes everyone's life easier!

Conclusions

Aspect – the Advanced Solver for Planetary Evolution, Convection, and Tectonics:

http://aspect.geodynamics.org/

References:

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