ETH
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Overview of modelling challenges in Lithospheric Dynamics

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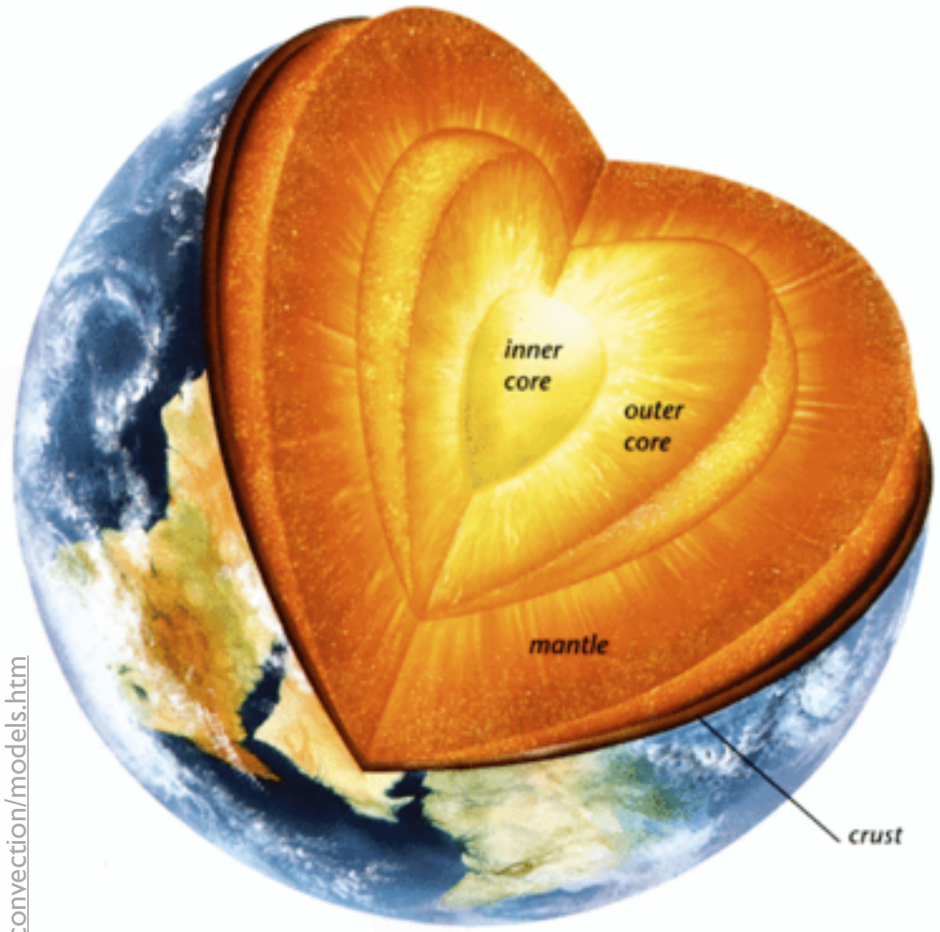
Philippe Yamato

Outline

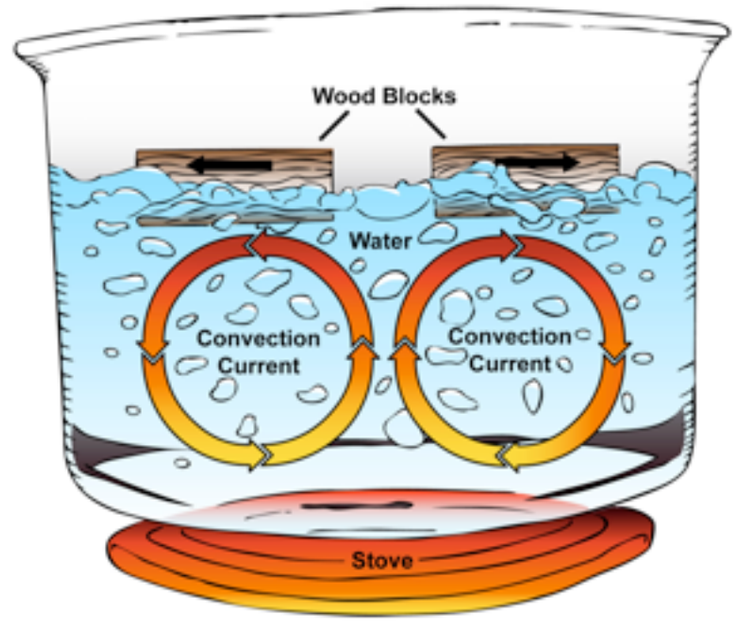
- Geodynamic background and motivations
- Physics motivated modelling requirements
- Practical requirements
- State of the art methods for lithospheric dynamics

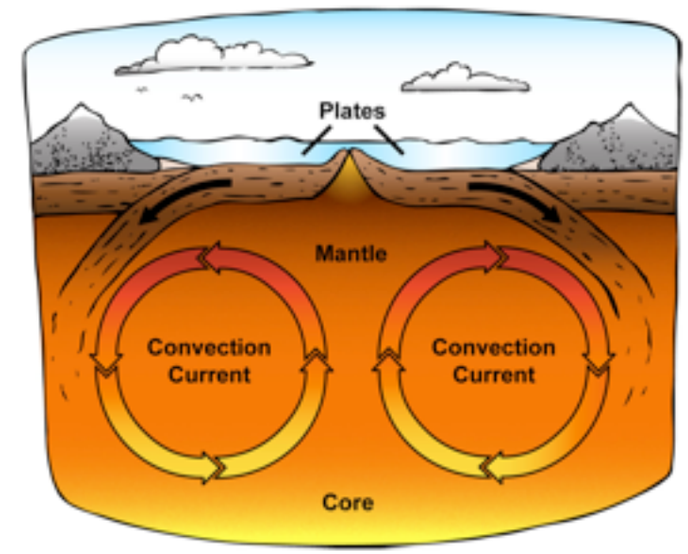
Convective Engine of the Earth

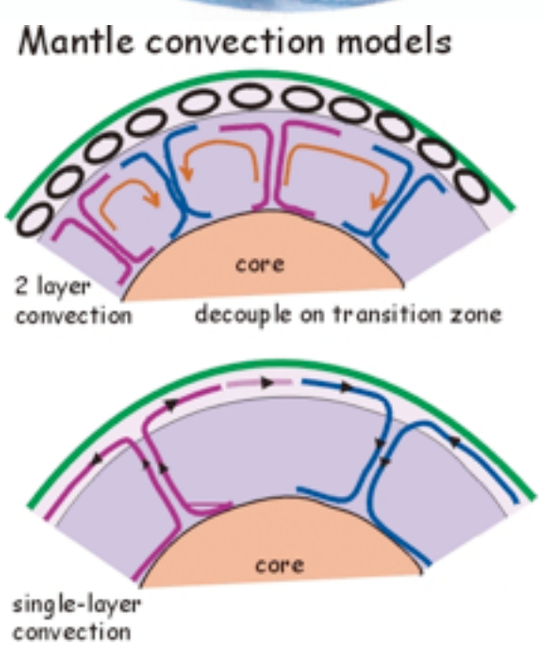


http://asapscience.tumblr.com/post/50419005208/the-earths-center-is-out-of-sync-we-all-know

http://dreamtigers.wordpress.com/2011/05/11/plate-tectonic-metaphor-illustrations-cmu/



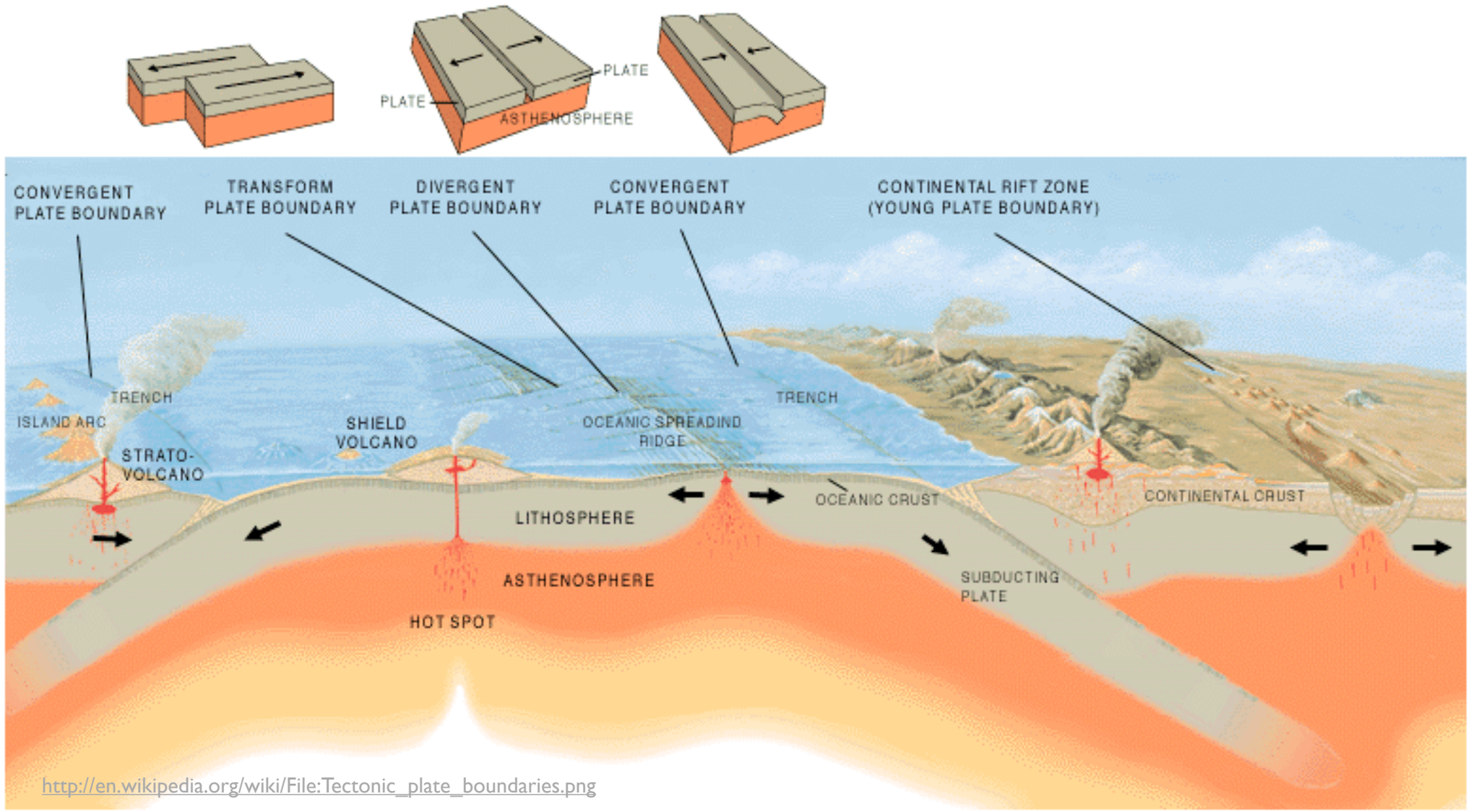




http://www.see.leeds.ac.uk/structure/dynamicearth/convection/models.htm

- Long time scale process. Very viscous, creeping flow regime
- Highly temperature dependent viscosity - large contrast in material properties (1e10)
- Stokes like Rayleigh-Bénard convection with strongly variable viscosity

Regional Geodynamic Processes

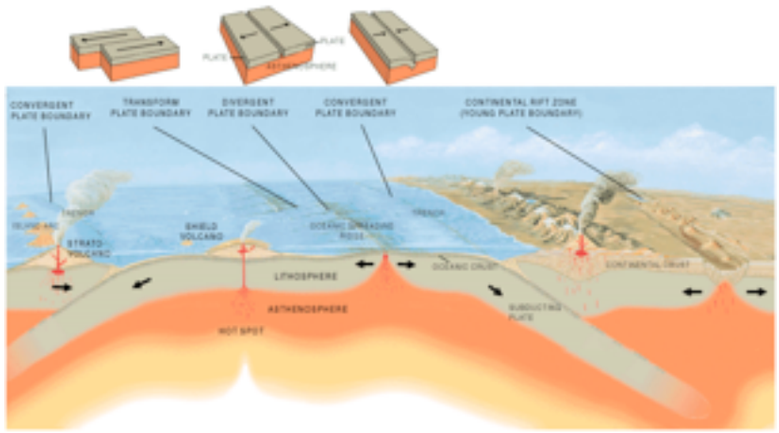


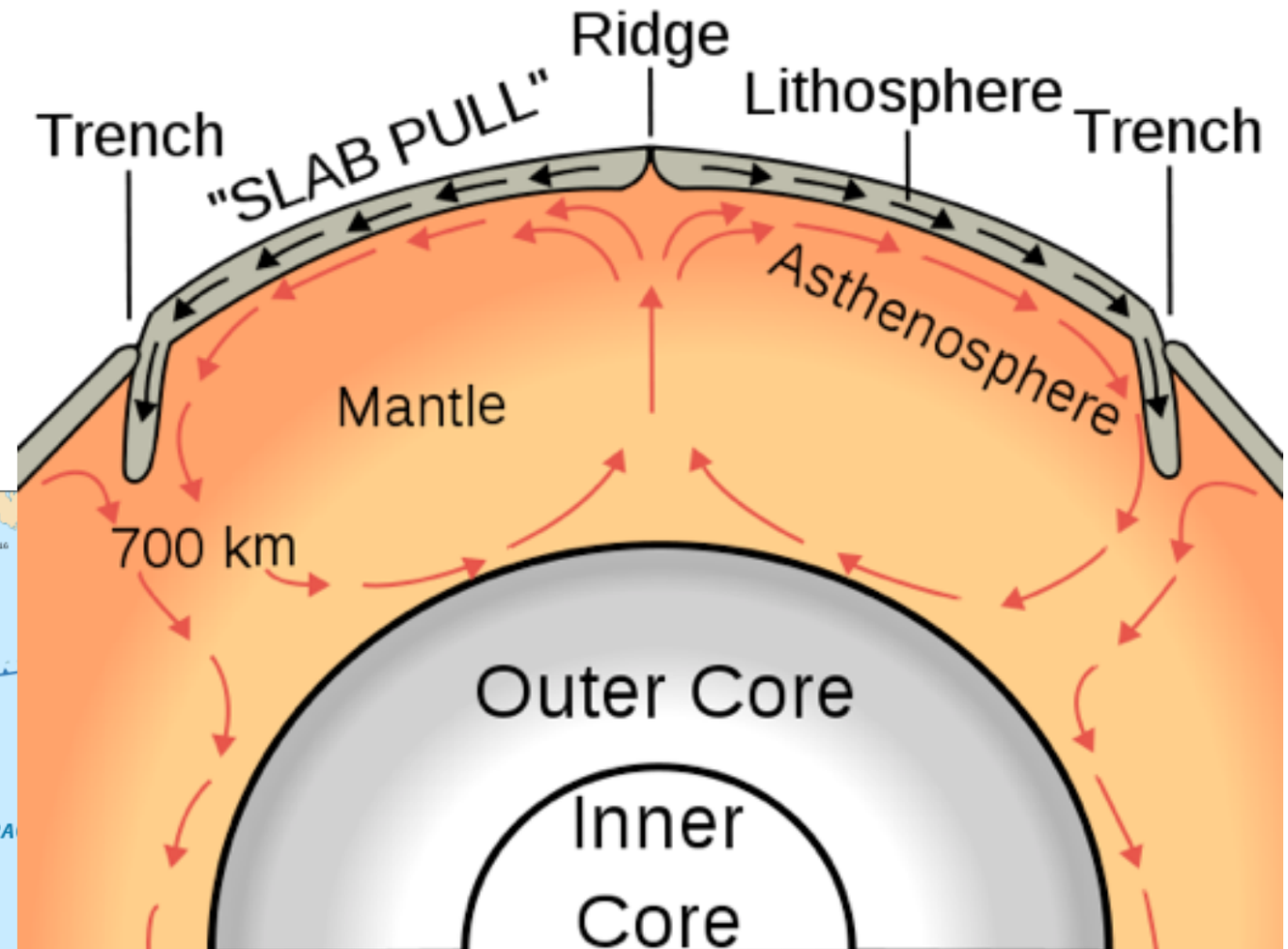
http://en.wikipedia.org/wiki/File:Tectonic_plate_boundaries.png

- Topography variations
- Large variation in length scales
- Presence of faults (material failure)
- Melting

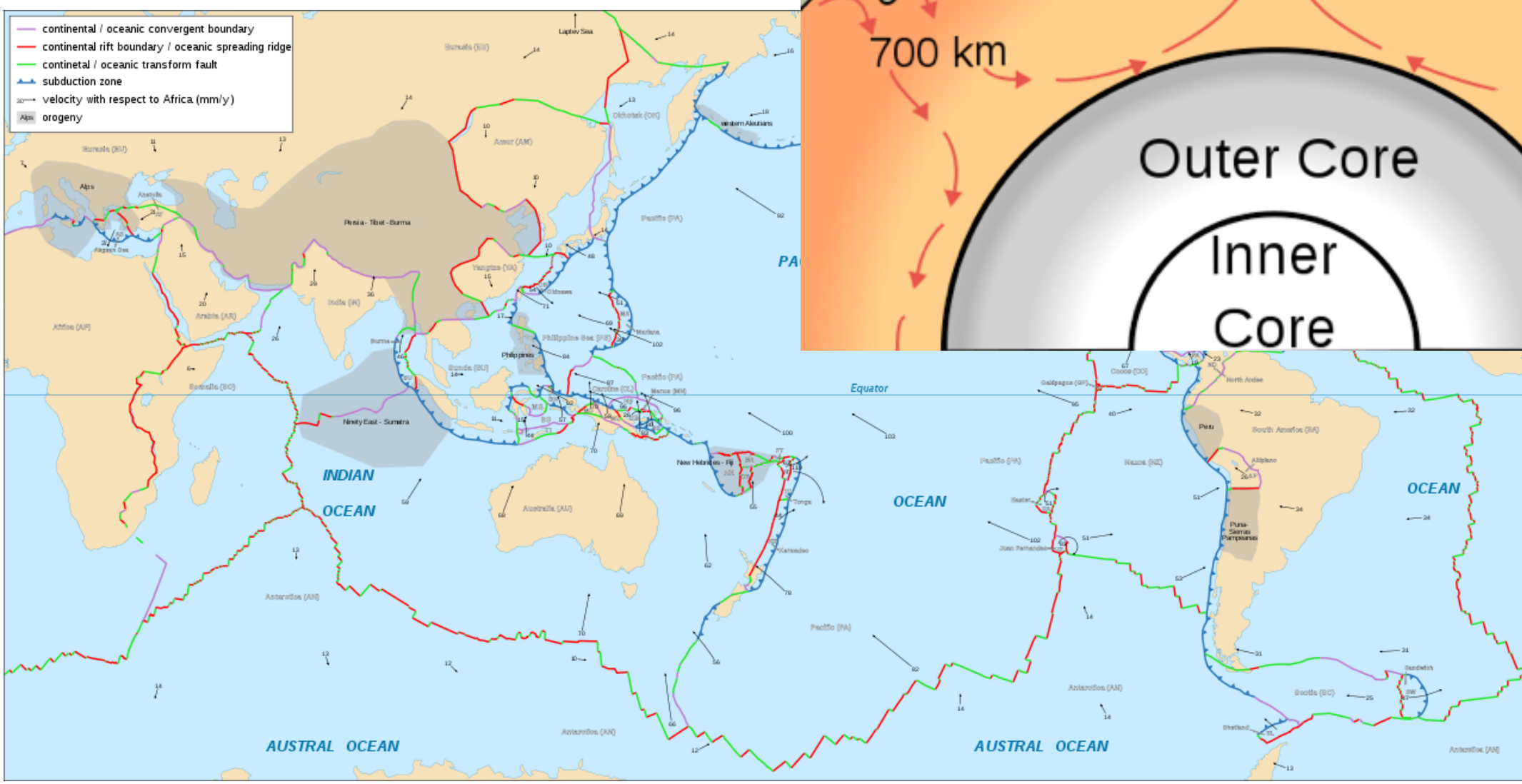
- Complex constitutive behaviour
- Large deformation
- Deformation past the onset of material failure

Coupled Regional / Global Processes





http://en.wikipedia.org/wiki/File:Oceanic_spreading.svg



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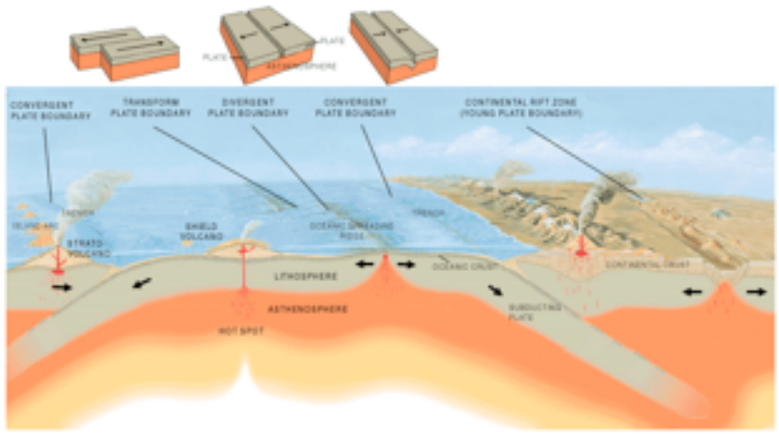

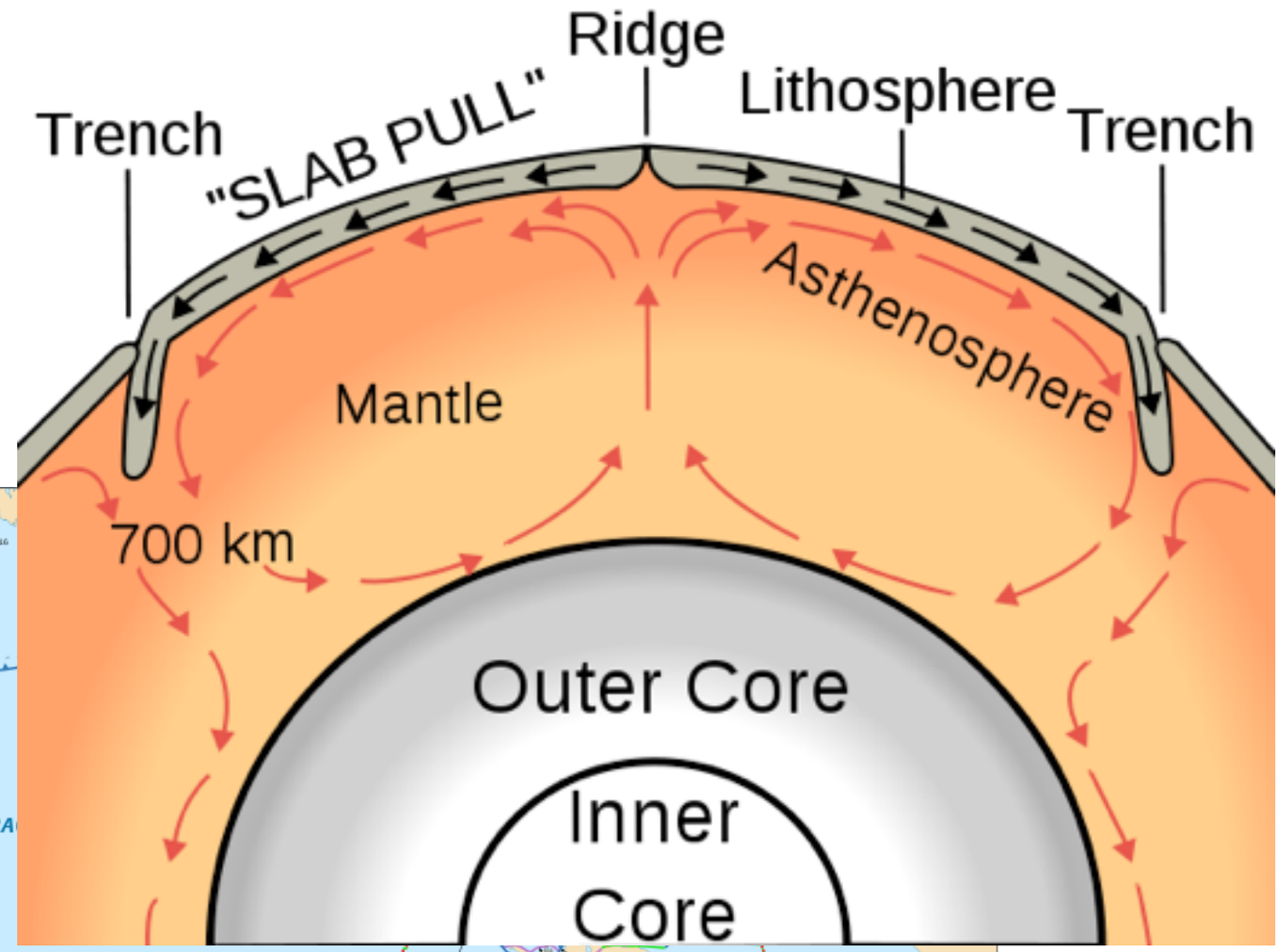

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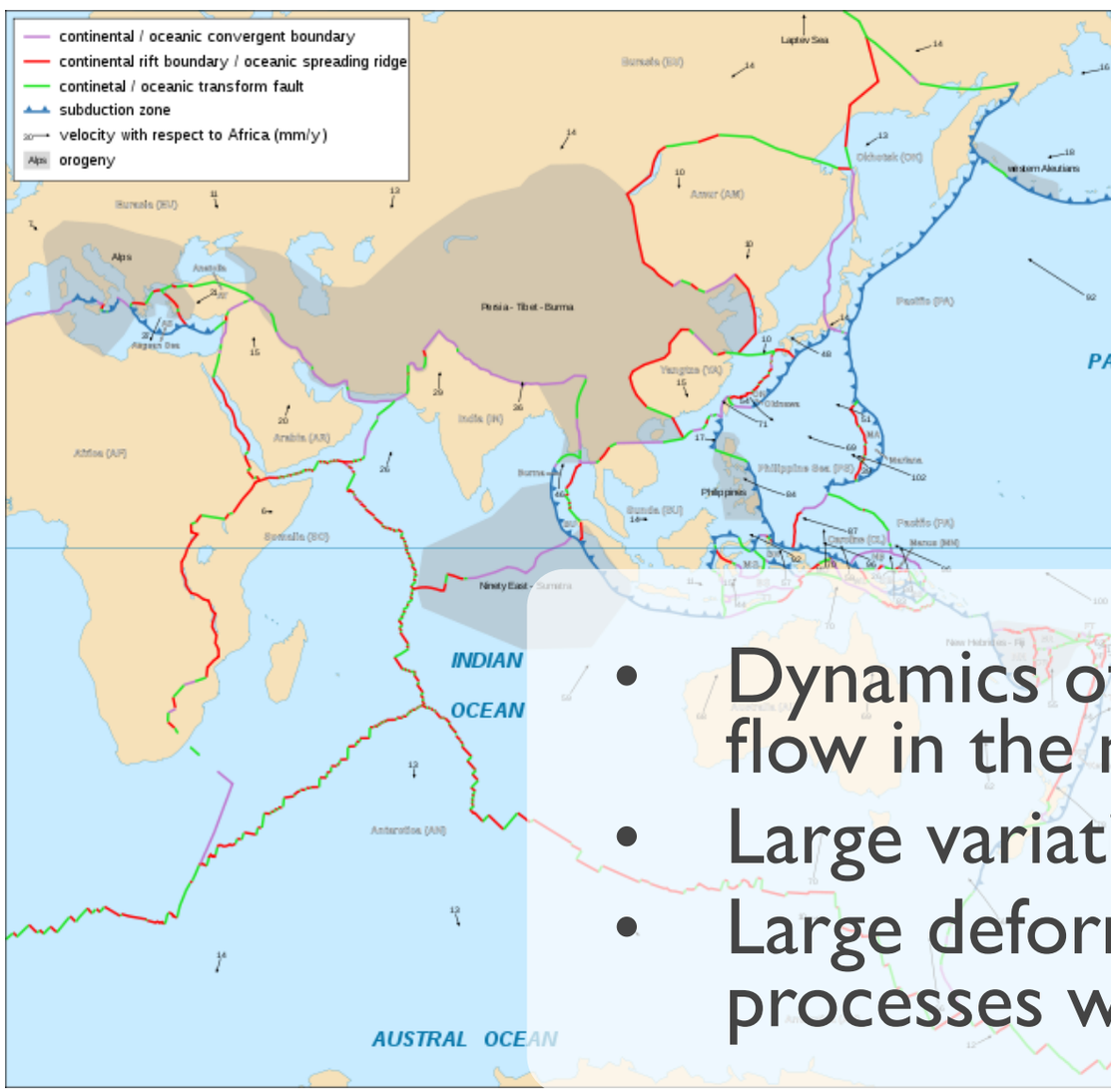
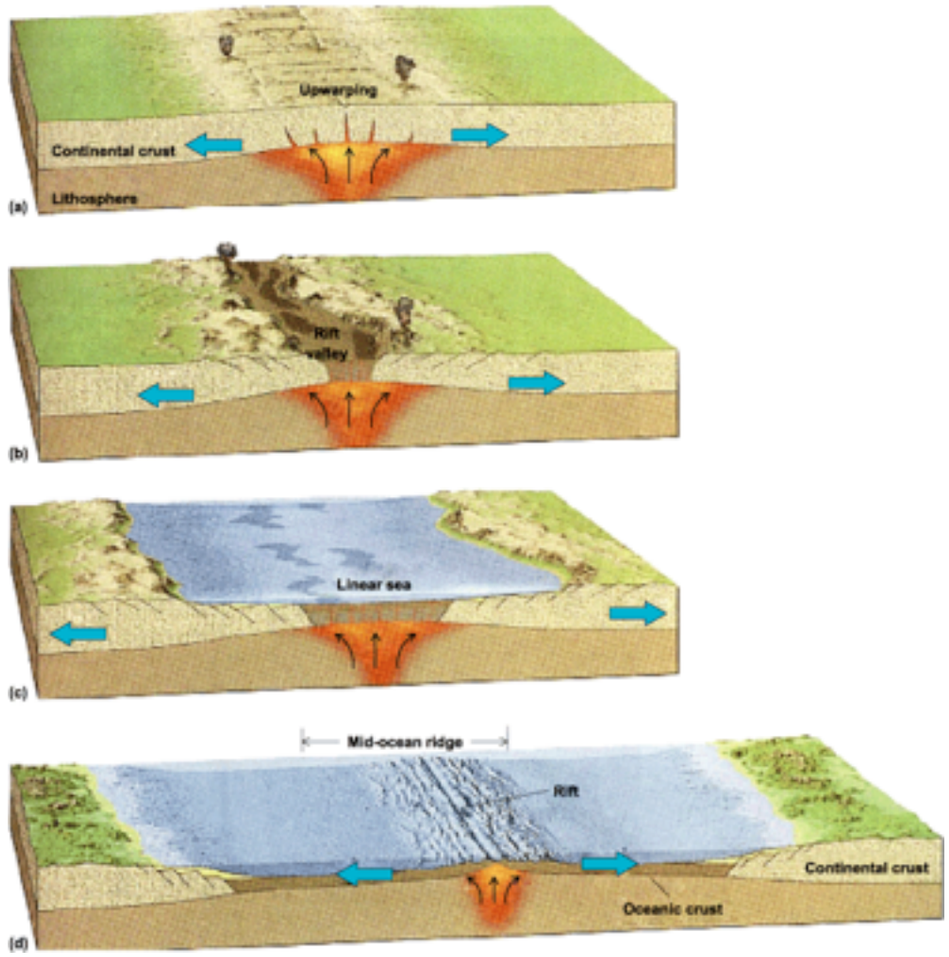


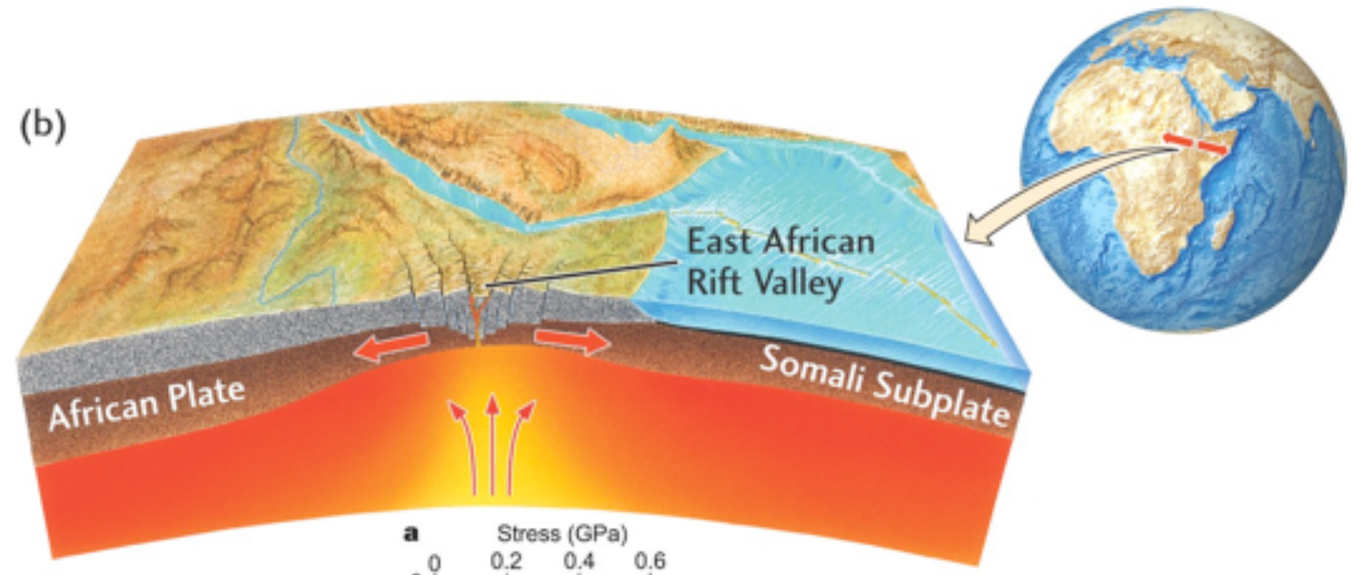
- Dynamics of small length scales influence large scale flow in the mantle
- Large variation in length scales
- Large deformation, coupled thermo-mechanical processes with material failure

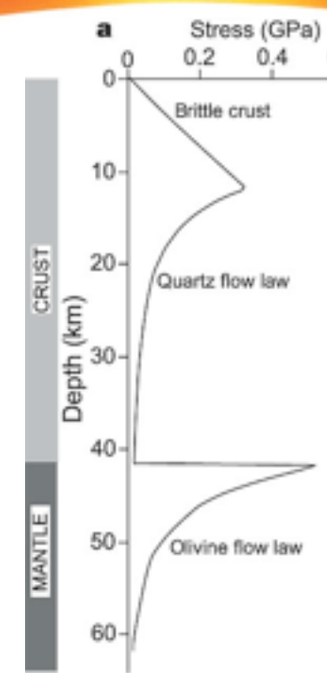
Geodynamic Motivations

Continental rifting

20 million years of evolution







- Follow the **4D** evolution of rocks over millions year time spans ⟶ large deformation
- Complex constitutive laws
- Large contrast in material properties
- Deformation past the onset of material failure

Physics Overview

- Incompressible, non-linear Stokes problem:

$$\left[2\eta D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i \quad \text{in } \Omega$$

$$u_{k,k} = 0$$

$$u_i = \bar{u}_i \quad \text{on } \Gamma_D$$

$$\sigma_{ij} n_j = \bar{t}_i \quad \text{on } \Gamma_N$$

Feedbacks

- Non-linear constitutive behaviour
- Evolution of coefficients and history variables
- Non-linear boundary conditions
- Conservation of energy
- Other physics...

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- Non-linear constitutive behaviour

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Physics Overview

- Non-linear constitutive behaviour

Arrhenius [u,p,T dependence]

$$\eta = A(\sqrt{I_2'})^{\alpha} \exp\left(\frac{E + Vp}{nRT}\right) \qquad I_2' = \tfrac{1}{2} D_{ij} D_{ij}$$

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Visco-elasticity

$$\frac{1}{2\eta}\tau_{ij} + \frac{1}{2\mu}\frac{\hat{D}\tau_{ij}}{\hat{D}t} = \dot{\epsilon}_{ij}$$

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- Evolution of coefficients

$$\frac{D\boldsymbol{x}}{Dt} = \boldsymbol{u}$$

$$\frac{D\eta}{Dt} = 0, \qquad \frac{Df_i}{Dt} = 0$$

$$\left[2\eta D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i$$

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Physics Overview

- Non-linear boundary conditions

Surface processes

$$\frac{D\boldsymbol{x}}{Dt} = \boldsymbol{u}$$

$$\frac{Dh}{Dt} = \nabla \cdot (\kappa(h)\nabla h) + s$$

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Frictional sliding

$$[(\boldsymbol{n}\cdot\nabla)(\boldsymbol{t}\cdot\boldsymbol{u})] - 2C\,[(\boldsymbol{t}\cdot\nabla)(\boldsymbol{t}\cdot\boldsymbol{u})] = \frac{C}{\eta_{\text{eff}}}p$$

$$c = \begin{cases} \frac{u^b}{|u^b|}\tan\delta, & u^b \neq 0, \\ 0, & u^b = 0. \end{cases}$$

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- Conservation of energy

$$\frac{DT}{Dt} = \left[\kappa\, T_{,k}\right]_{,k} + Q$$

$$f_i = \rho_0 \left[1 - \alpha(T - T_0)\right] g_i$$

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- Other physics
  - melting / fluids (two phase flow) ⟶ more coupling and non-linearities
  - ...

Modelling Requirements

Our choice of space-time discretisation must allow for

- the representation of large material deformation (large strain)
- the prescription of complex non-linear constitutive behaviour
- the representation and tracking of distinct rock types (and any history variables)

- the evolution of material both pre- and post- failure
- a diverse range of boundary conditions (potentially non-linear)
- multi-physics coupling
- three-dimensional
- stable space-time discretisations
- accurate and convergent space-time discretisations

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- the representation of large material deformation (large strain)
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- the representation and tracking of distinct rock types (and any history variables)

  ⟶ *gives rise to large jumps in material properties*
- the evolution of material both pre- and post- failure
- a diverse range of boundary conditions (potentially non-linear)
- multi-physics coupling
- three-dimensional
- stable space-time discretisations
- accurate and convergent space-time discretisations

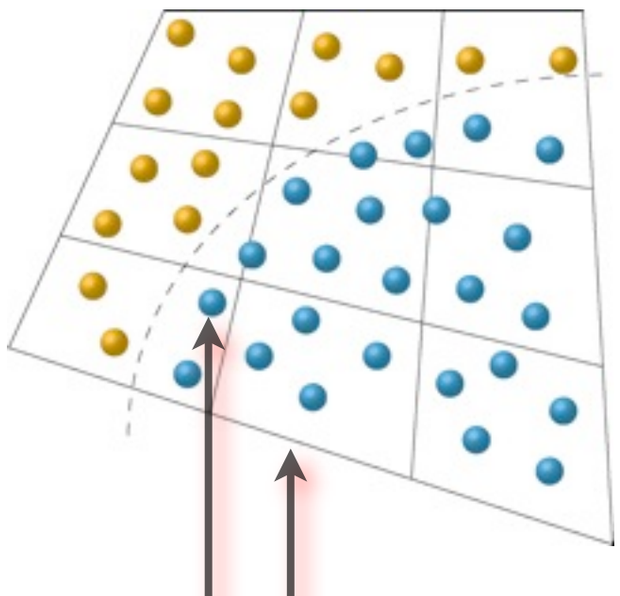
Practical Requirements

- Robustness over a wide range of multi-physics applications
- Flexible w.r.t. boundary condition and rheological prescription
- "Fast" turn around time between simulations
  - optimal solvers, or
  - discretisations/solvers which are scalable on massively parallel hardware
  - (or ideally both of the above)
- Amenable to three-dimensional simulations

Addressing Modelling Requirements

State of the Art

- "Material Point Method" like spatial discretisation



Particle In Cell (PIC) *Harlow & Welch, Phys. Fluids, (1965)*

Material Point Method (MPM) *Sulsky & Brackbill, JCP, (1991)*

a) Discretise the continuum problem on a mesh

b) Discretise constitutive behaviour and history variables on Lagrangian points (markers)

c) Coupling between markers and continuum discretisation

Material Point Method Family

- Extremely popular technique in computational geodynamics

Finite element variants

PARAVOZ / FLAMAR [Podladchikov, Burov, 1993]

SOPALE [Fullsack, 1995]

Underworld / GALE [Moresi, 2003]

DOUAR [Braun, 2008]

LaMEM [Kaus, 2008]

SLIM3D [Popov, 2008]

FANTOM [Thieulot, 2011]

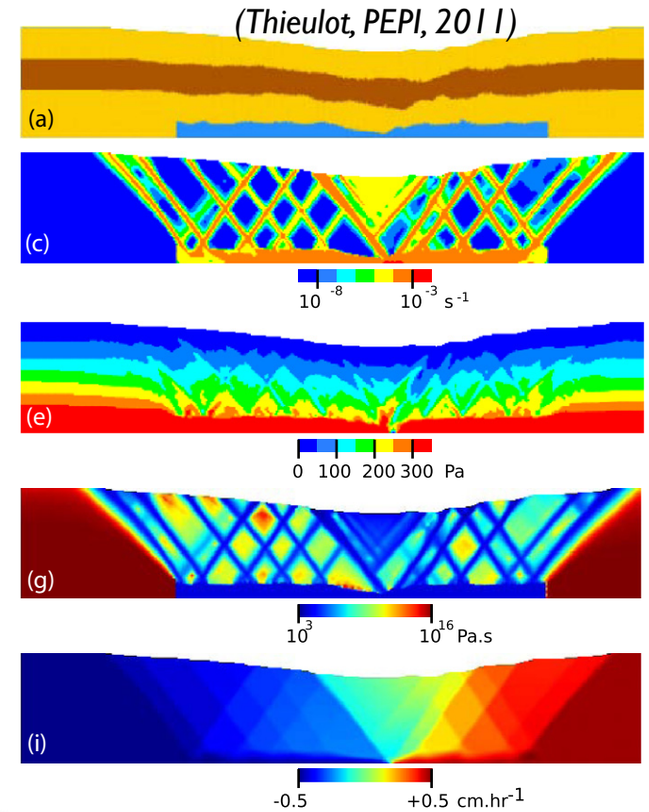
ELEFANT [Thieulot, 2013]

pTatin3d [May, 2014]

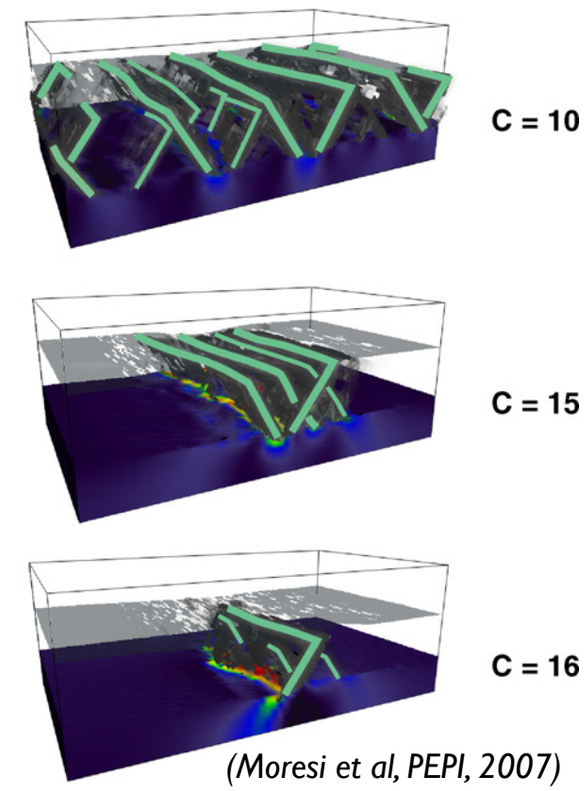
MILAMIN2 [Dabrowski, TBA]

Finite difference variants

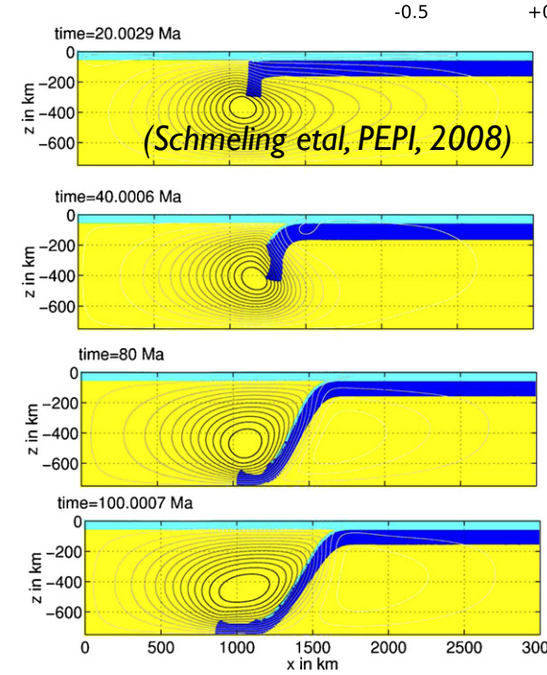
I2VIS / I3VIS [Gerya, 2003]



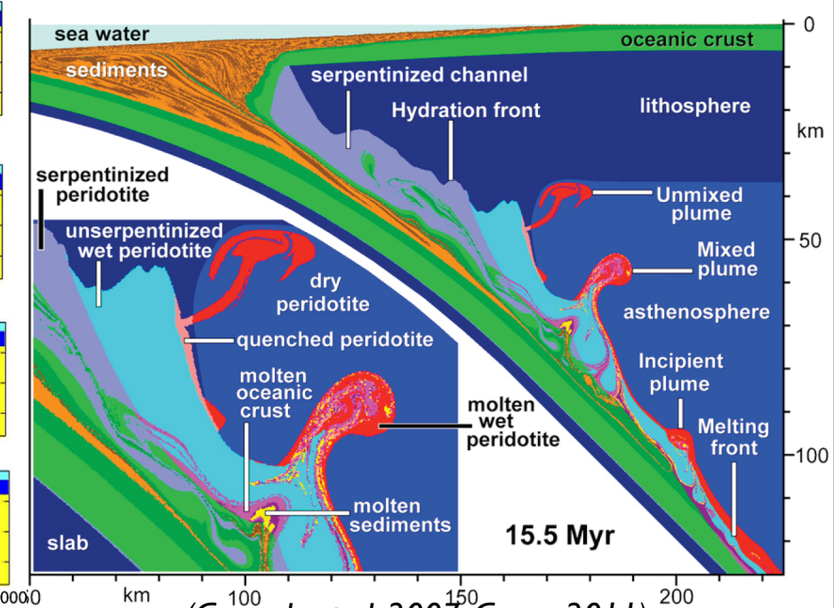
(Thieulot, PEPI, 2011)



(Moresi et al, PEPI, 2007)



(Schmeling etal, PEPI, 2008)



(Gorczyk, et al, 2007; Gerya, 2011)

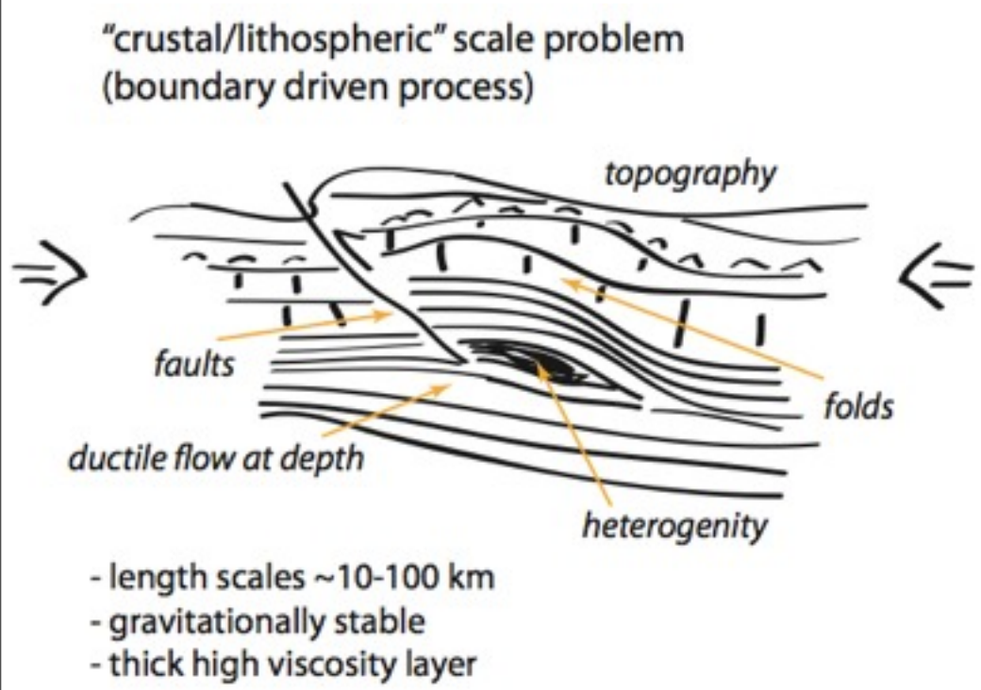
FE-Material Point Method Family

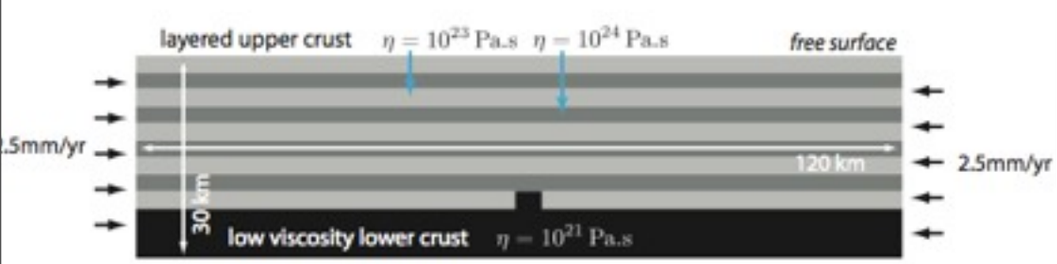
- the representation of large material deformation (large strain) ☑
- the prescription of complex non-linear constitutive behaviour ☑
- the representation and tracking of distinct rock types ☑
- the evolution of material both pre- and post- failure ☑
- a diverse range of boundary conditions (potentially non-linear) ☑
- multi-physics coupling ☑
- three-dimensional ☑
- *stable space-time discretisations [WITH A COST]* ?
- *accurate and convergent space-time discretisations [SEE NEXT SLIDE]* ?

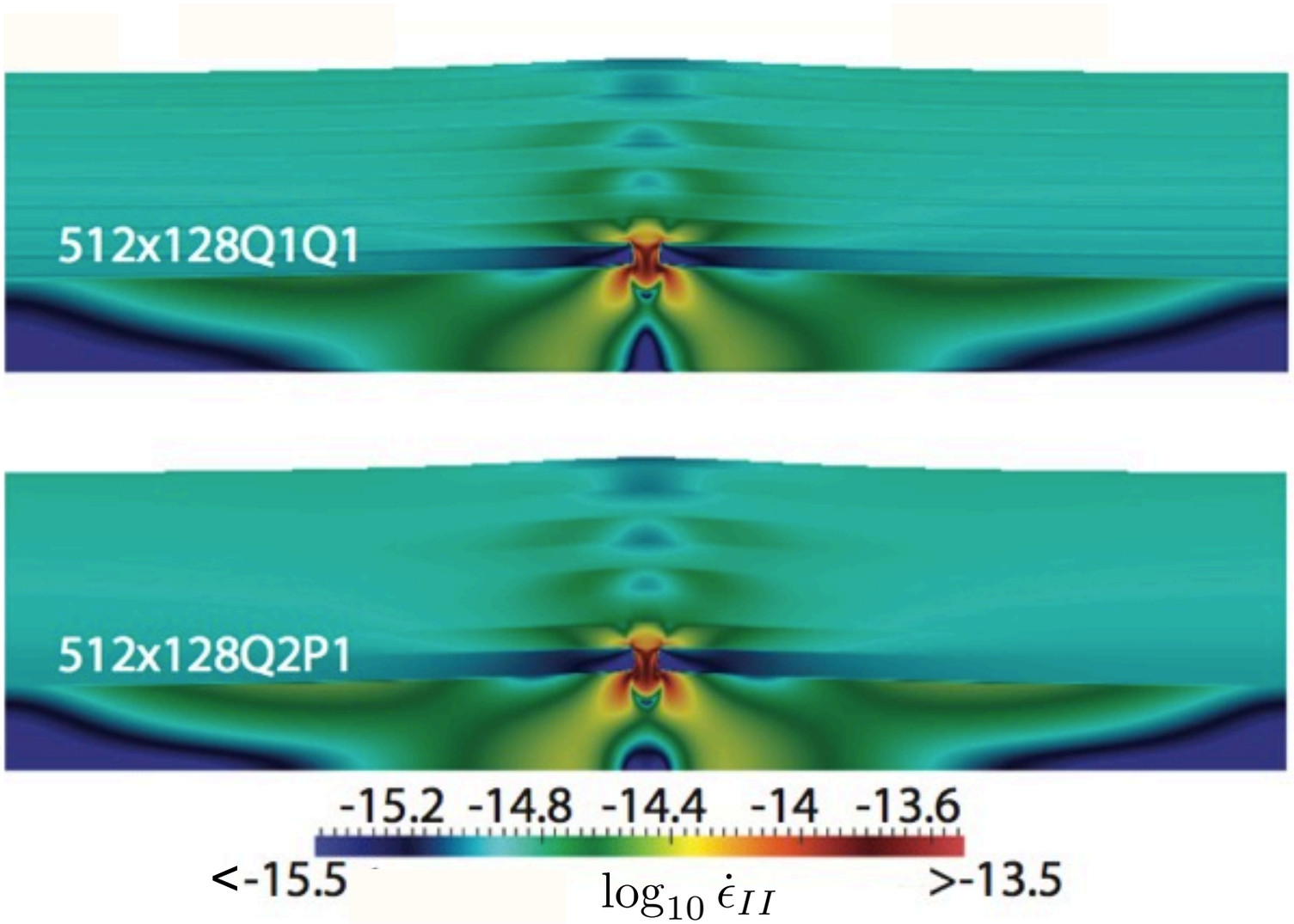
FE-Material Point Method Family

Stability concerns

- Choice of Stokes element type is important
- Stability and robustness may come at a different cost



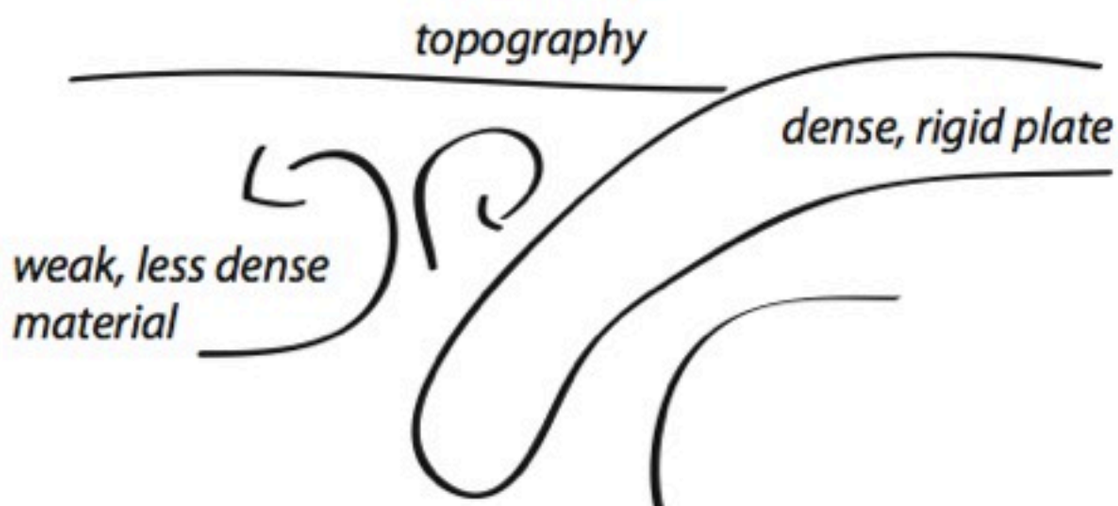




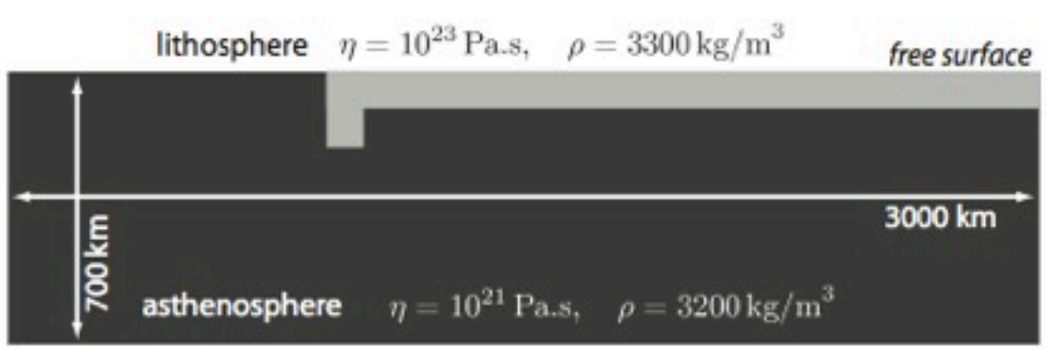
FE-Material Point Method Family

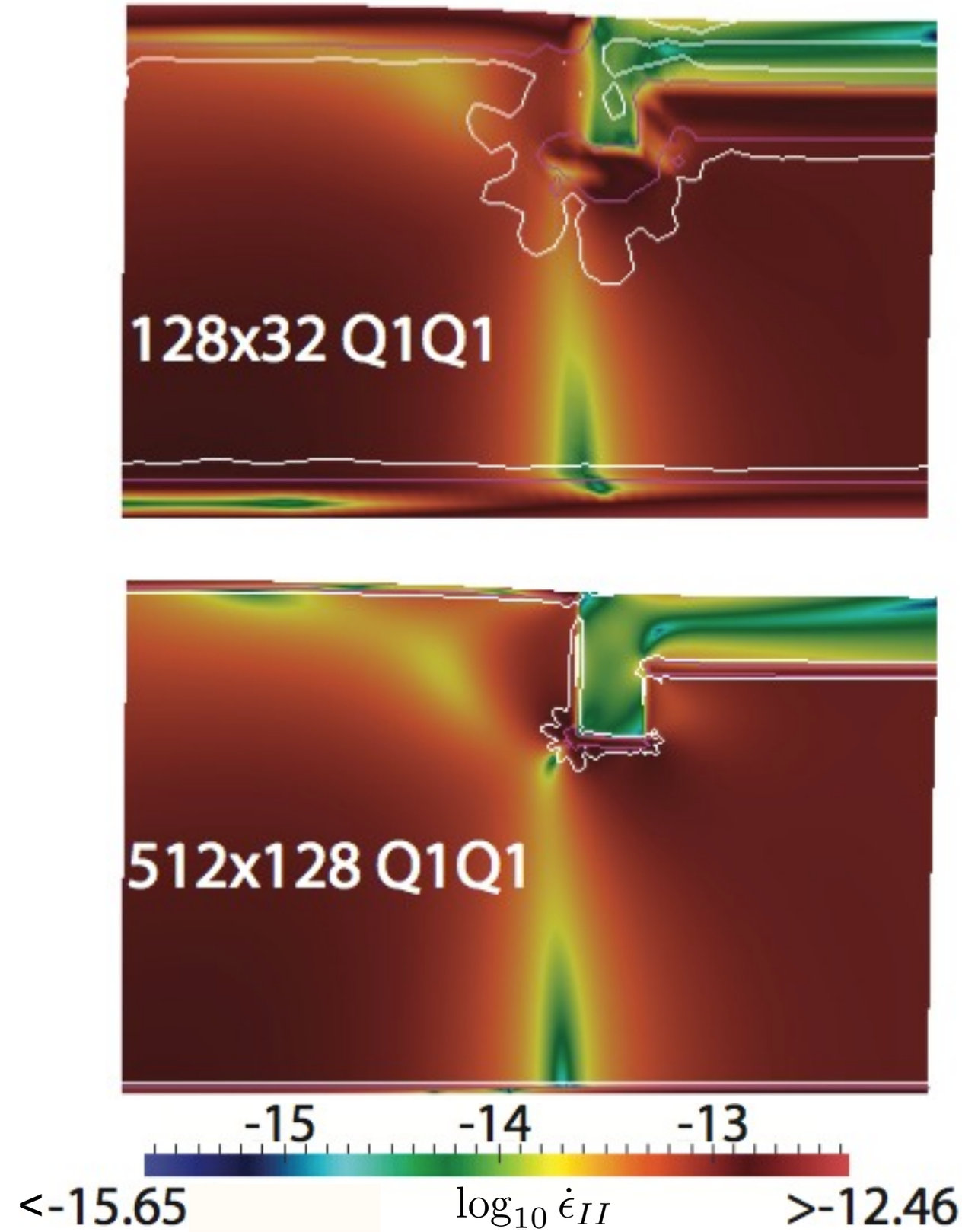
Stability concerns

"upper mantle" scale problem
(bouyancy driven process)



- length scale ~100-1000 km
- inverted density gradient
- thick low viscosity layer





FE-Material Point Method Family

Stability concerns

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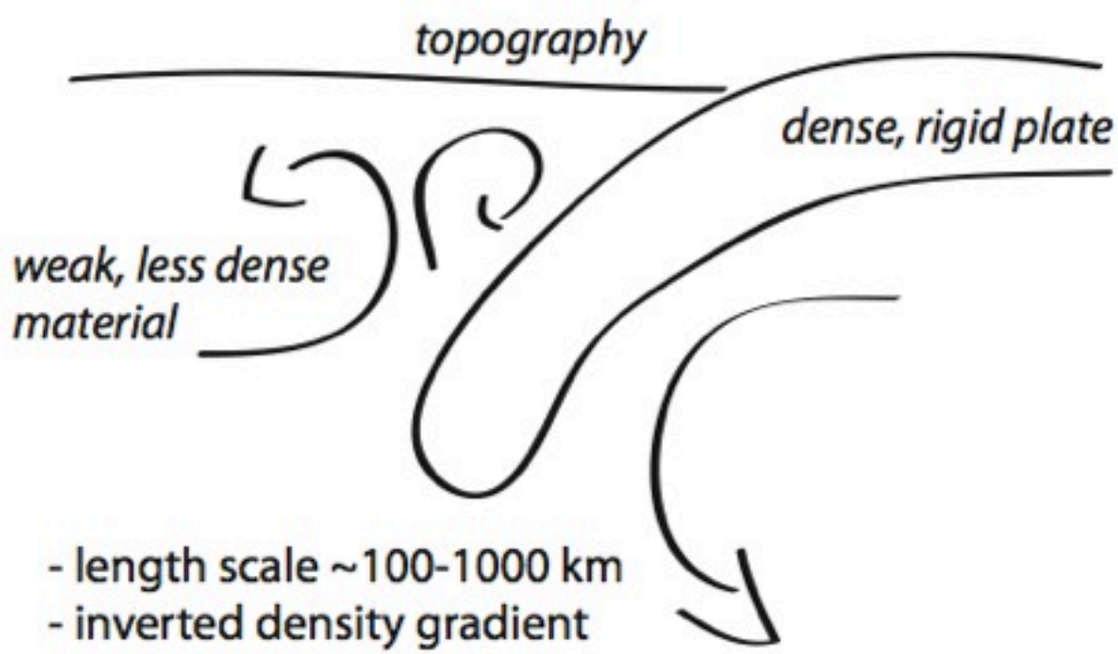

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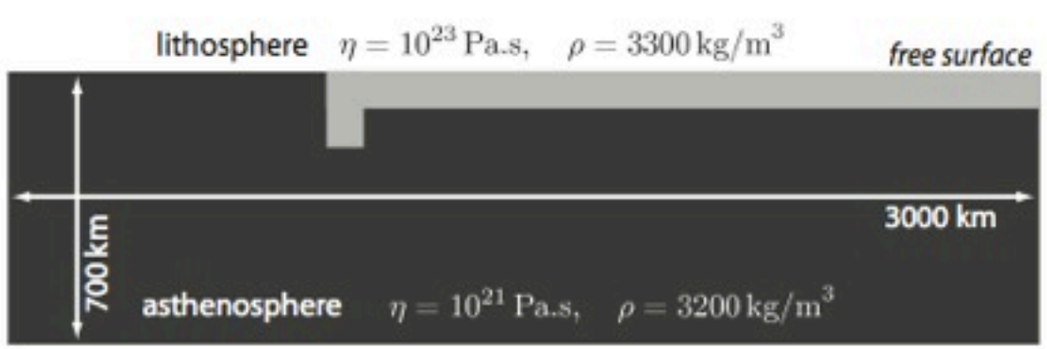
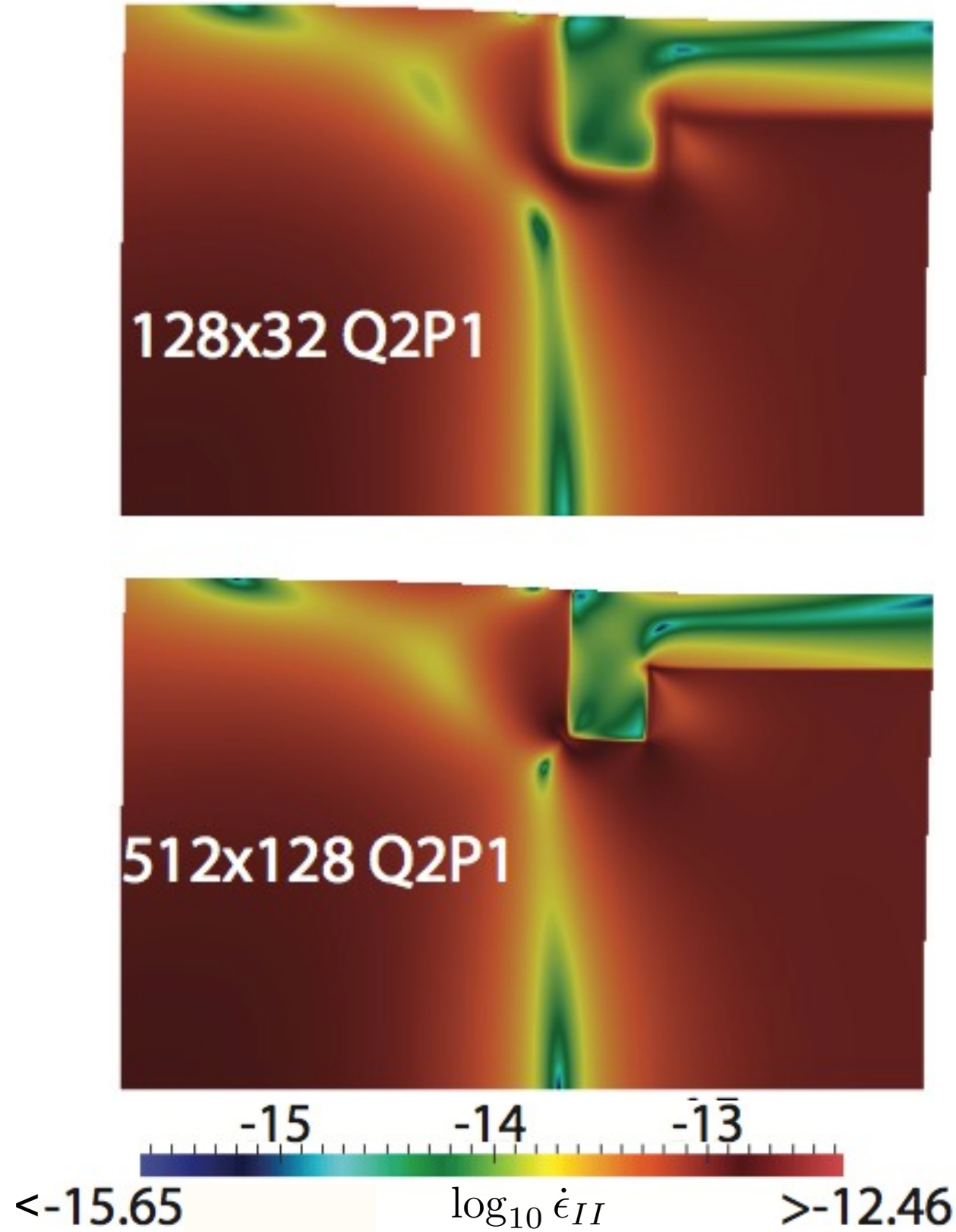
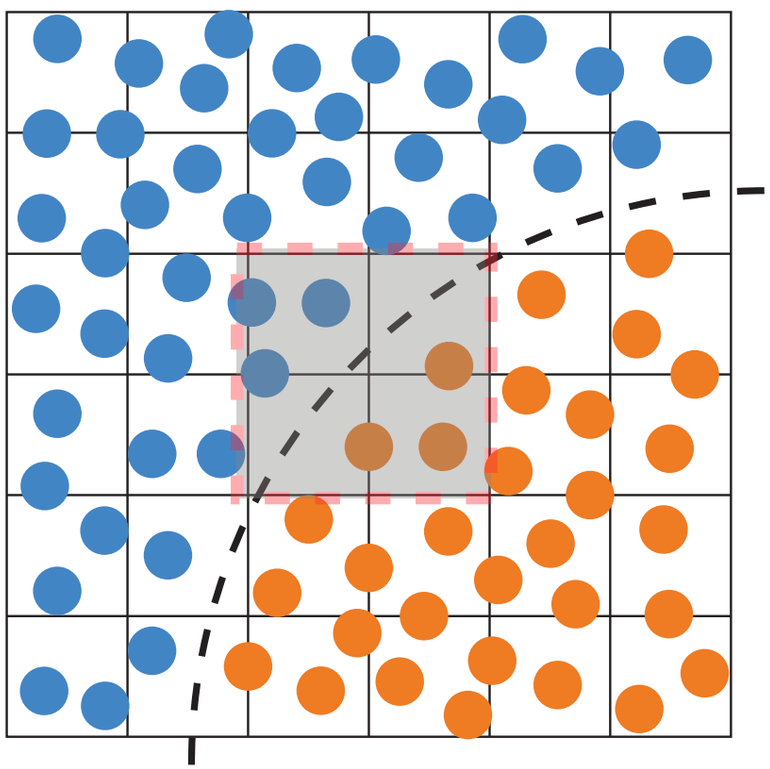




FE-Material Point Method Family

Accuracy concerns



- MPM formulation naturally leads to elements which contain inter-element jumps in material properties (viscosity)
- Physically, the discontinuous viscosity produces a jump in the strain-rate and pressure
- Consequences, sub-optimal order of accuracy of the velocity and pressure approximations

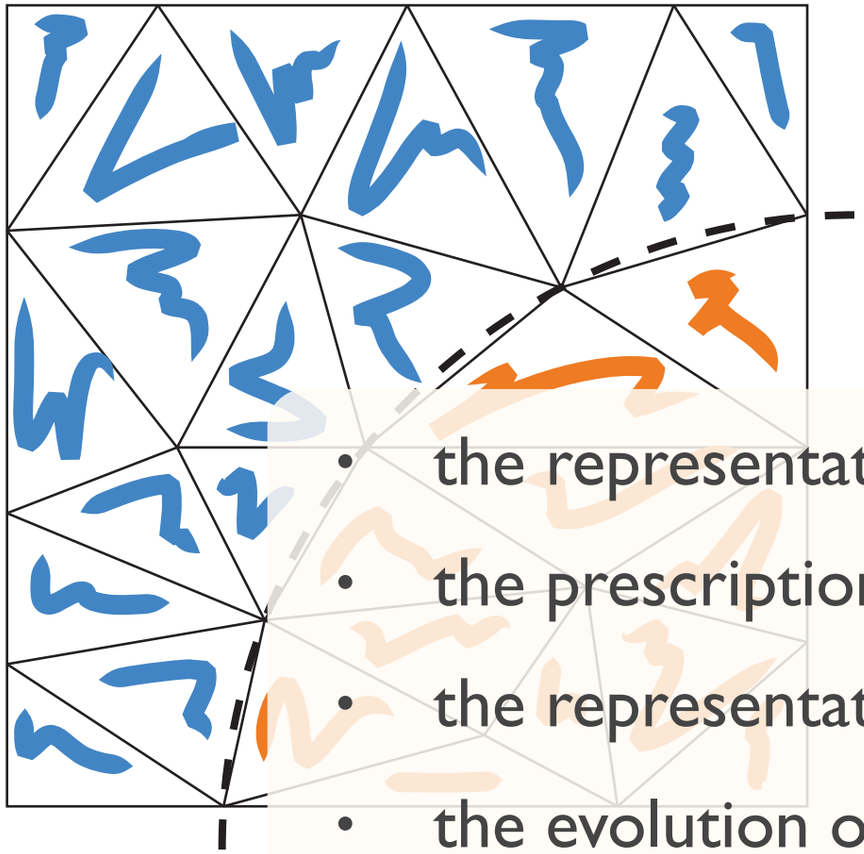
$$\|e_u\|_{L_2} = O(h)$$

$$\|e_p\|_{L_2} = O(h^{0.5}) \rightarrow O(h)$$

(Thielmann etal, PAAG, 2013)
(May etal, JCP, 2014)

Order of accuracy is *independent* of the polynomial order used for the u, p basis functions

Body Fitted FEM [MILAMIN]



$$\|e_u\|_{L_2} = O(h^{q+1})$$

$$\|e_p\|_{L_2} = O(h^q)$$

- the representation of large material deformation (large strain) ✗
- the prescription of complex non-linear constitutive behaviour ✓
- the representation and tracking of distinct rock types ✓
- the evolution of material both pre- and post- failure ✓
- a diverse range of boundary conditions (potentially non-linear) ✓
- multi-physics coupling ✓
- three-dimensional ✗
- *stable space-time discretisations* ✓
- *convergent space-time discretisations* ✓

SGFD-Material Point Method Family

- the representation of large material deformation (large strain) ☑
- the prescription of complex non-linear constitutive behaviour ☑
- the representation and tracking of distinct rock types ☑
- the evolution of material both pre- and post- failure ☑
- a diverse range of boundary conditions (potentially non-linear) ☒
- multi-physics coupling ?
- three-dimensional ☑
- *stable space-time discretisations* ?
- *convergent space-time discretisations* ?

SGFD-Material Point Method Family

- *Diverse range of boundary conditions (potentially non-linear)* ✗
  - ➡ Necessary boundary condition for lithospheric modelling is a free surface. The error associated with the "sticky air" approximation cannot be determined a priori.
  - ➡ Furthermore, convergence cannot be achieved if the "air" viscosity is not reduced. In the limit $\eta_{\mathrm{air}} \rightarrow 0$, discretisation breaks down
- *Multi-physics coupling* ?
  - ➡ Possible, but often requires stencil development and analysis
- *Stable space-time discretisations* ?
  - ➡ Staggered grid finite difference (SGFD) scheme is stable
- *Convergent space-time discretisations* ?
  - ➡ Same result as the FEM. SGFD is optimally second order and discontinuous viscosity reduces scheme to first order

Alternative approaches

- Interface tracking methods
  - Replacing material points with an interface tracking scheme (e.g. level set) does prevent the accuracy degradation associated with inter-element jumps
- Interface capturing schemes

  Ghost Fluid Method

  Immersed Interface Method

  eXtended Finite Element Method (XFEM)

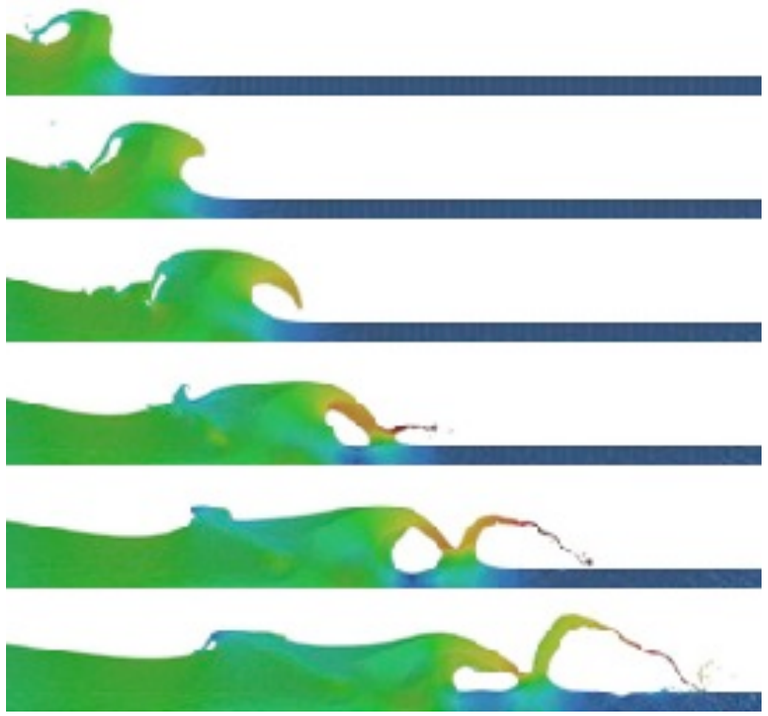
  Moment of Fluid (MOF)

  Such methods encounter difficulties when used in a multi-material context
  i) due to exponentially increase in cost with the number of materials
  ii) due to an inability to define discrete operators when >1 or 2 material interfaces intersect a cell

Alternative approaches

- Interface tracking methods
  - Replacing material points with an interface tracking scheme (e.g. level set) does prevent the accuracy degradation associated with inter-element jumps
- Pure particle methods

  Smoothed Particle Hydrodynamics (SPH)
  Element Free Galerkin (EFG)
  Natural Element Method (NEM)
  Lattice Boltzmann Method (LBM)
  Finite Pointset Method



- All have massive problems formulating a stable variable viscosity Stokes discretisations (no time splitting) when arbitrary point sets are considered

- Treatment of boundary conditions is non-trival

Addressing Practical Requirements

Practical Requirements

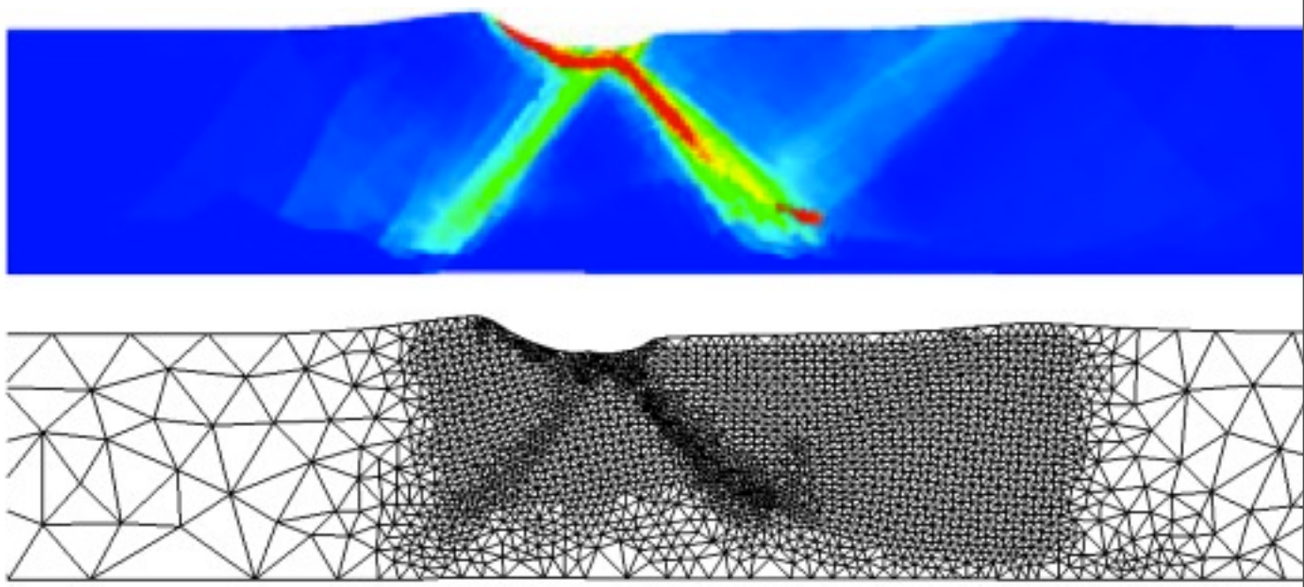
- Robustness over a wide range of multi-physics applications
- Flexible w.r.t. boundary condition and rheological prescription
- *"Fast" turn around time between simulations*
  - *optimal solvers, or*
  - *discretisations/solvers which are scalable on massively parallel hardware*
  - *(or ideally both of the above)*
- Amenable to three-dimensional simulations

Going Fast-I

FLAC / PARAVOZ / FLAMAR / LAPEX-2D / SNAC / DynEarthSol

- Alter the continuum formulation (compressible elasticity)

$$\rho^* \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{g}$$



- Fully explicit time integration --> huge number of cheap updates (no solve)
- Artificial density introduced to damp p- waves
- Massively parallel
- No way to ensure non-linearities are satisfied --> accuracy?
- Still require stable elements to avoid locking when yielding
- Frequent remeshing required --> problematic in 3D
  (also limits parallelism when using tetrahedrals)

Going Fast-II

- > 90% of CPU time is spent in solving the discrete non-linear (linear) Stokes system
- Obvious candidate to improve the time to solution

$$\left[2\eta D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i$$
$$u_{k,k} = 0$$

discretise

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f_u \\ 0 \end{bmatrix}$$

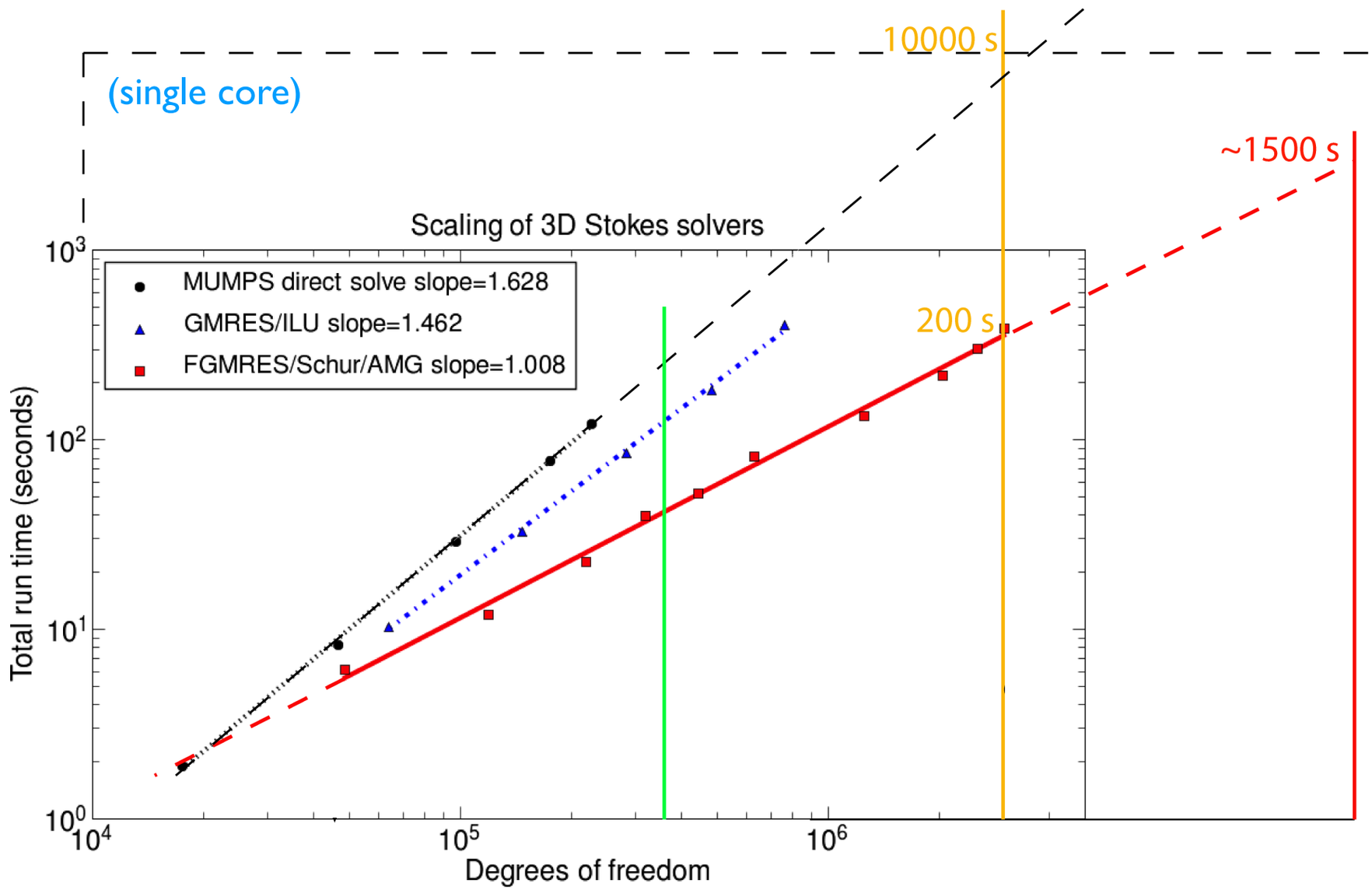
Going Fast-II

- > 90% of CPU time is spent in solving the discrete non-linear (linear) Stokes system

$$\left[2\eta D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} = f_i$$
$$u_{k,k} = 0$$

discretise

$$\begin{bmatrix} B \\ 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f_u \\ 0 \end{bmatrix}$$



3000 km x 2000 km x 200 km - 3 velocity components

with mesh resolution of 11 km --> 110 million unknowns

with mesh resolution of 20 km --> 1.8 million unknowns

with mesh resolution of 34 km --> 0.34 million unknowns

Choice of Solver (Preconditioner)

- Annoying trade-off's between

  robustness w.r.t. viscosity contrast (and boundary conditions, AR, ...)

  speed (algorithmic scalability)

  parallel implementation (OpenMP, MPI)

  parallel scalability

Sparse direct

Robust
Black box
Large scale MPI implementations exist
Sub-optimal alg. scaling ("slow") still limit computations:
(i) memory limitations
(ii) CPU time limitations (practicality)

Multi-grid

Sensitive to problem, requires tuning
White/grey box
Massively parallel implementations exist
Potential optimal alg. scaling ("fast")

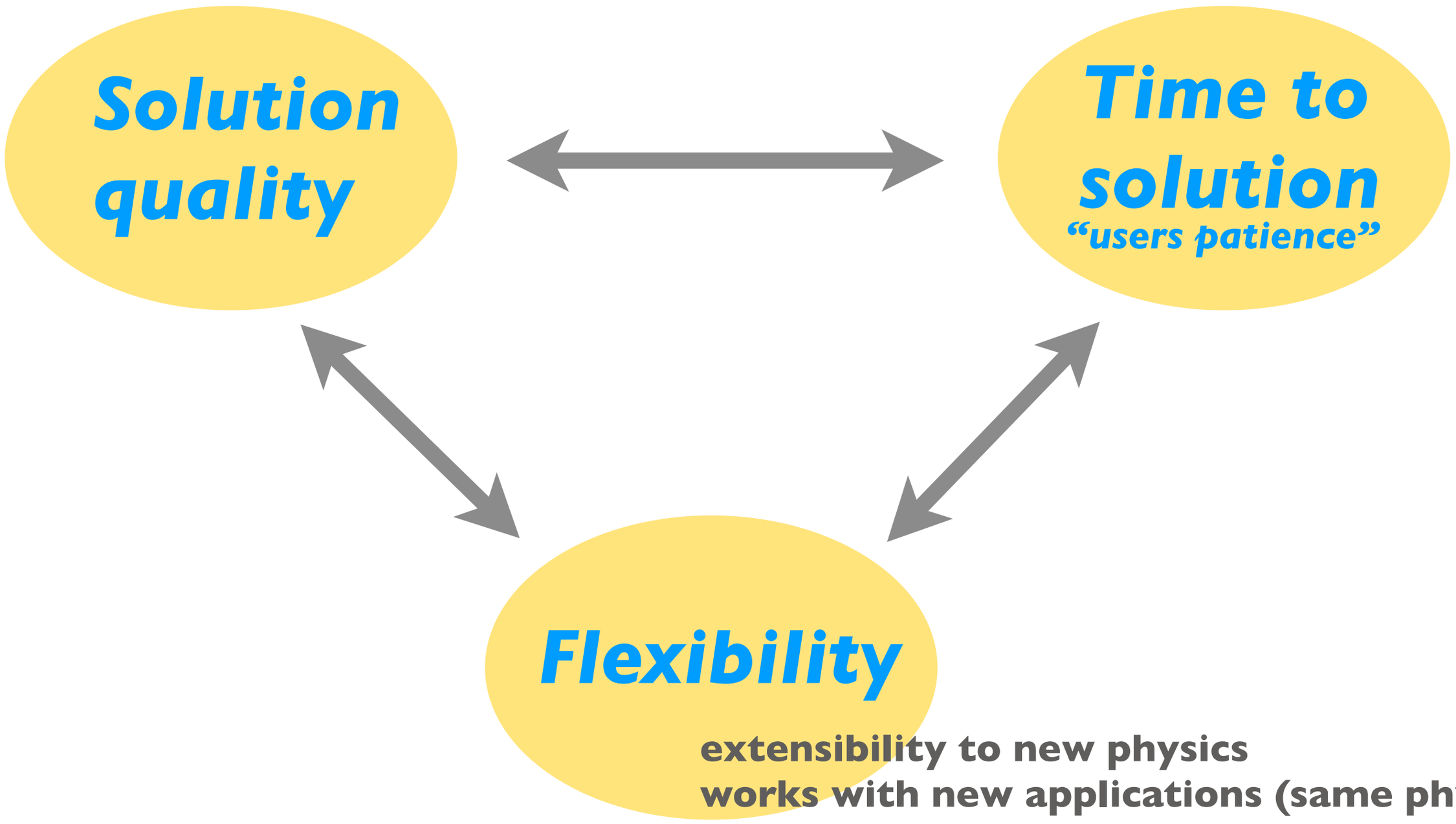
- Rich mathematical and experimental development for FE discretisations
- Less well developed for SGFD

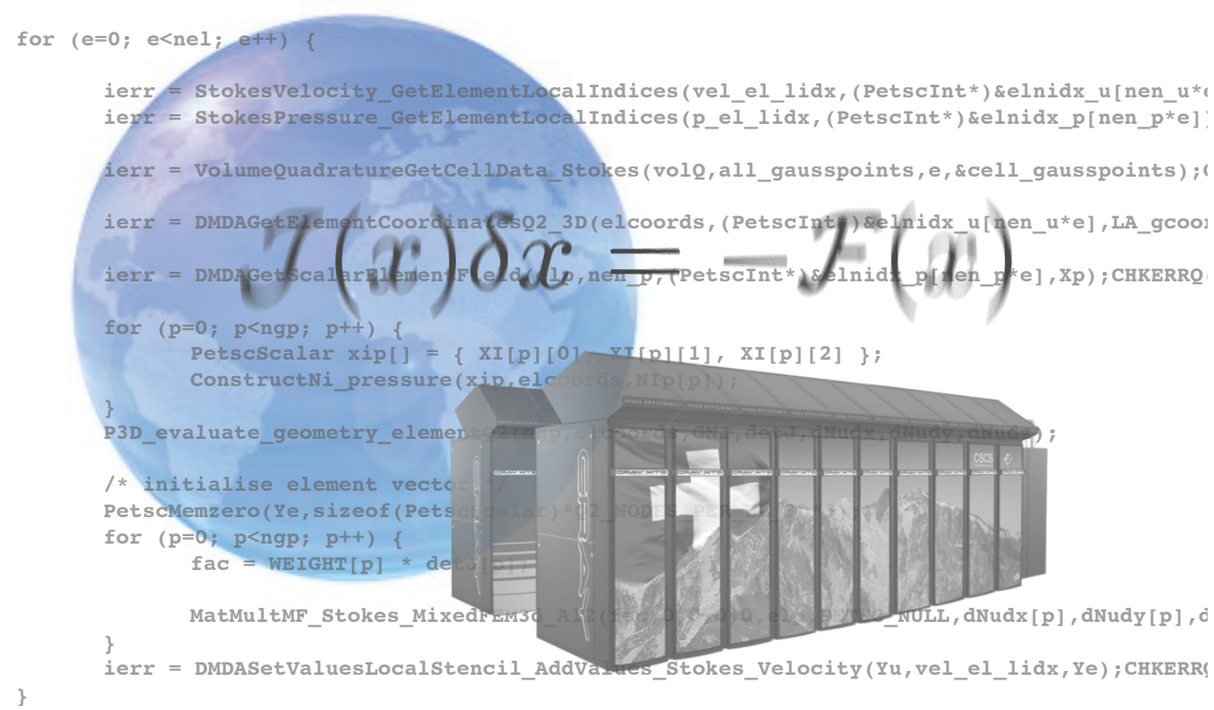
Multi-level Preconditioners

- High resolution, 3D lithospheric dynamics forward models **mandate** the usage of multi-level preconditioners - forget about using sparse direct
- These preconditioners are scalable (algorithmically and parallel)
- Their performance fundamentally governs our scientific throughput
- Making them robust is non-trivial, however there is an ever increasing volume of research from both the math and geodynamic fields to improve this situation

Fundamental component for ALL 3D lithospheric dynamics applications

Conclusion



extensibility to new physics
works with new applications (same physics)
boundary conditions / rheology permitted

Thanks for your attention... questions?