Tightly Coupled Geodynamic Systems: Software, Implicit Solvers & Applications

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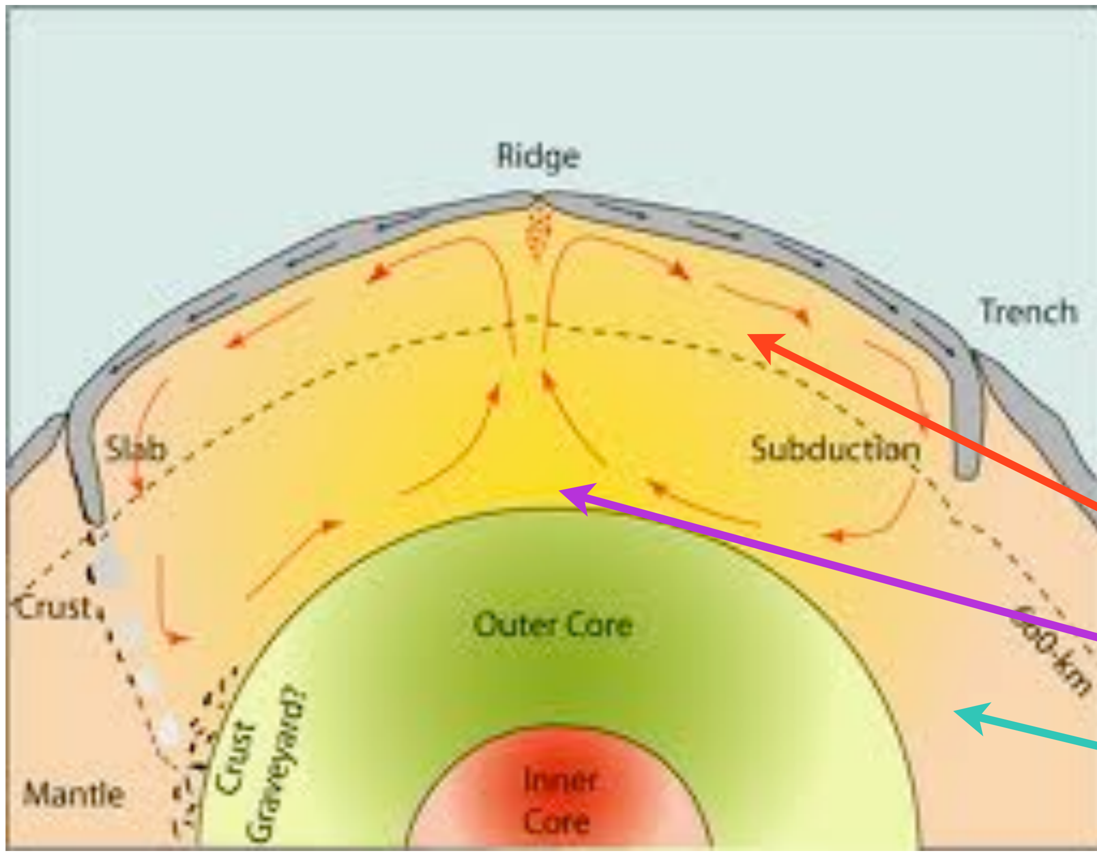
Outline

- Geodynamic examples.
- Current practices.
- Solvers & Software.
- Example: Visco-elasticity.
- Example: Visco-plasticity.
- Example: Free surface evolution.
- Summary.

Motivation(s)

Even with a simplified view of the Earth, when considering the governing dynamics of the entire system, many forms of nonlinearities and coupling between different physical processes are apparent.



viscous flow

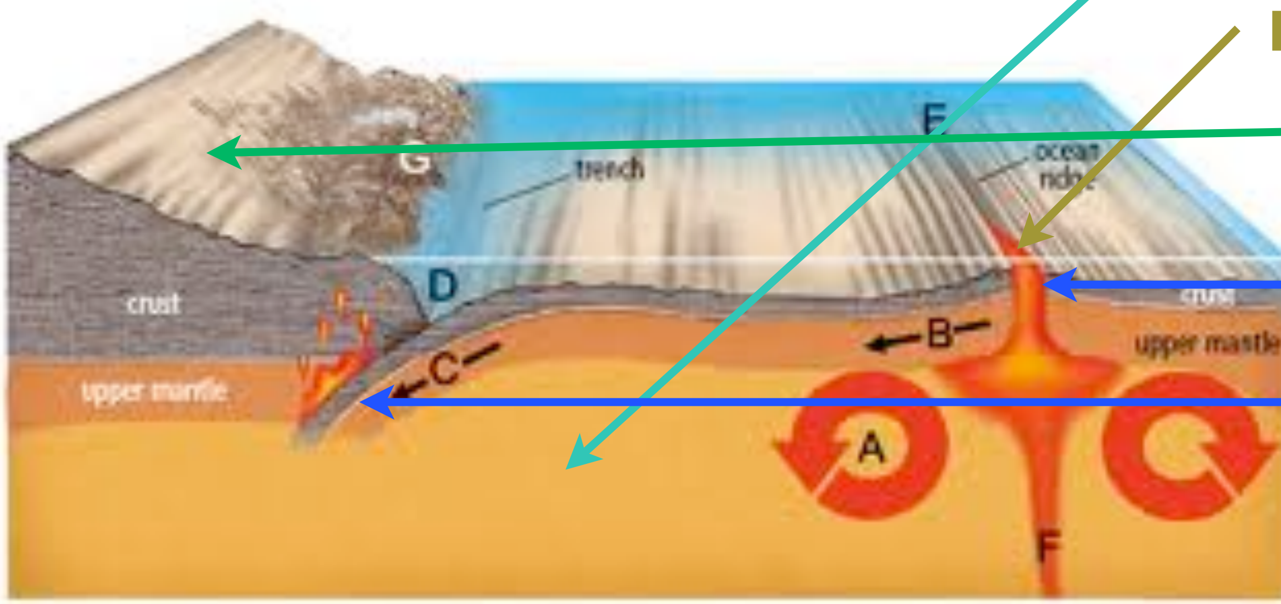
heat transport

thermo-mechanical coupling

rheology

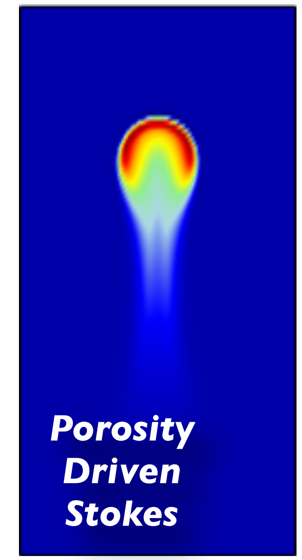
surface processes

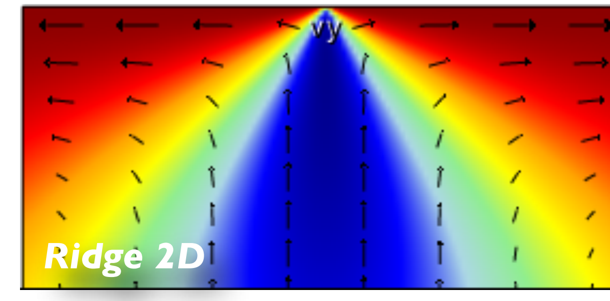
melting / fluid migration

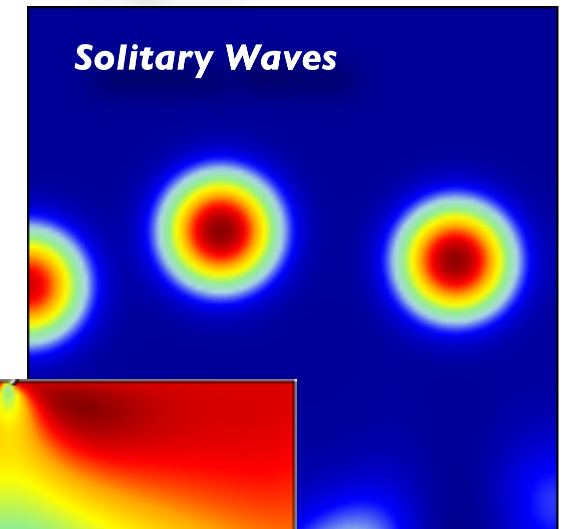


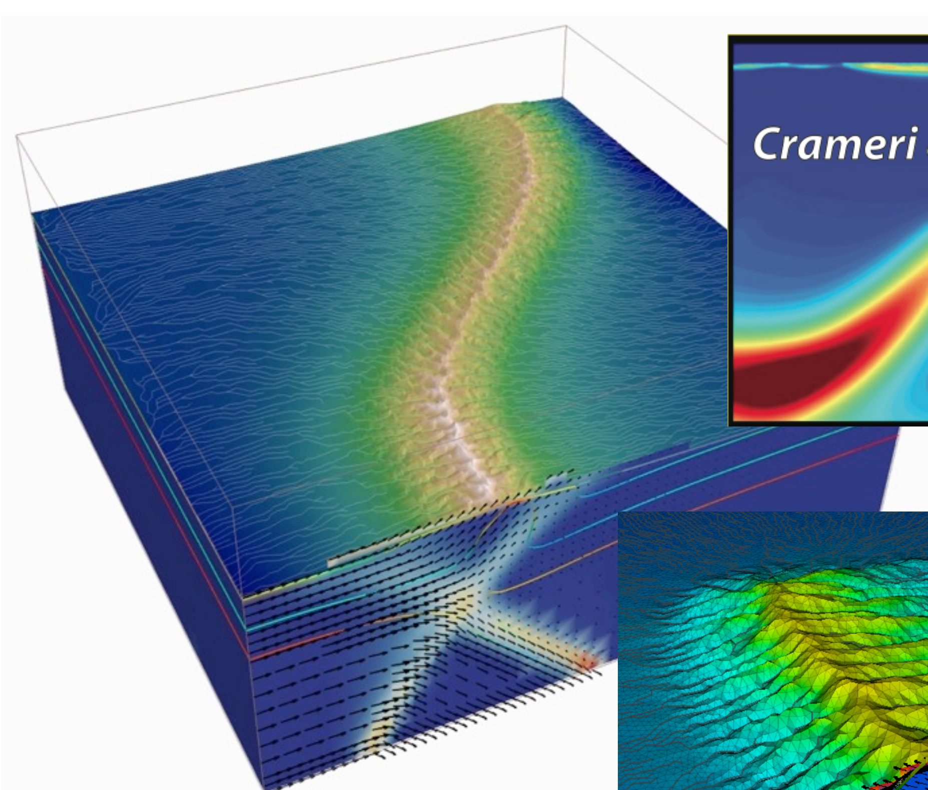
Specific Physical Processes

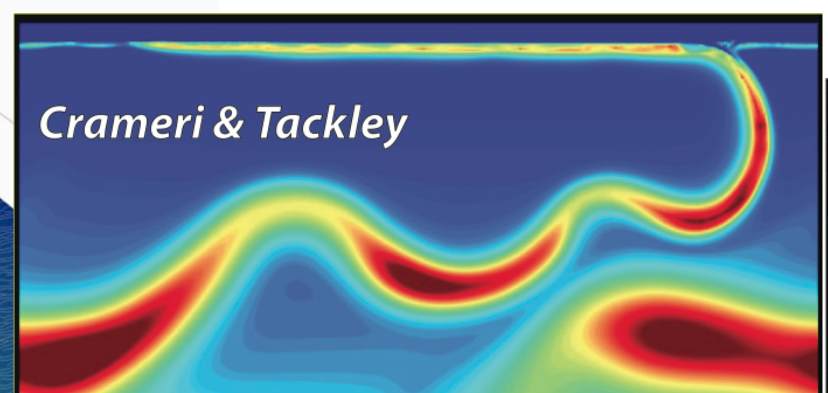
- Mantle convection
- Dynamics of the lithosphere
- Diapirism
- Two phase flow
- Landscape evolution

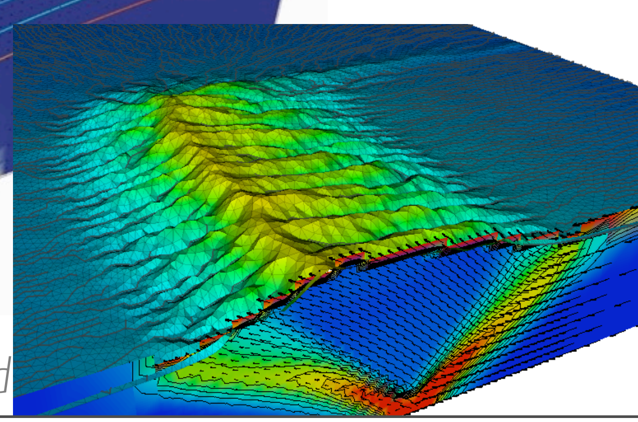


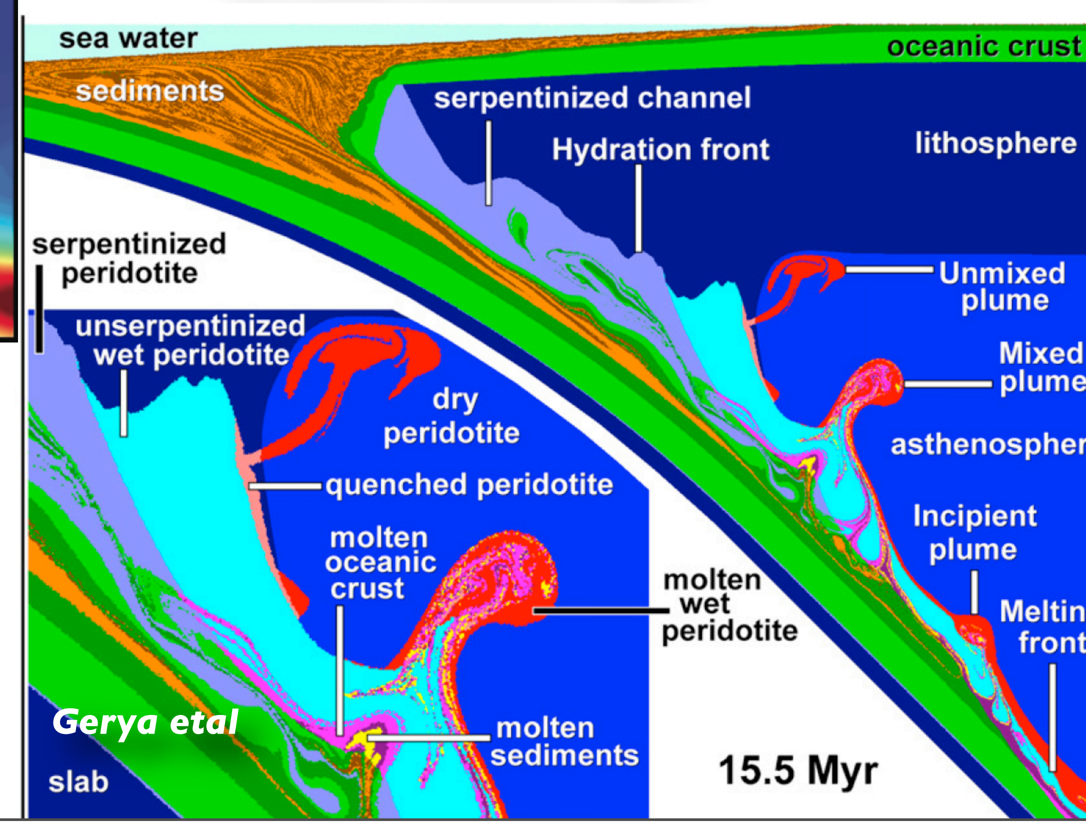












Our Focus

- Effective solution methods for studying dynamical systems described by very viscous, creeping flow, i.e.

  Stokes flow

  and in which nonlinearities arise due to either:

  1) implicit treatment of visco-elastic effects,

  2) inclusion of a visco-plastic rheology,

  3) implicit treatment of the evolution equation describing the motion of a free surface.

Current Practices

- Explicit decoupling of the physics:
  - E.g. in mantle dynamics the energy is solved independently of the momentum balance, even though the buoyancy force and viscosity are both functions of temperature.
- Code coupling via different executables:
  - E.g. CitcomS (spherical mantle convection model) + SNAC (crustal scale elasto-visco-plastic model).
    - No means to evaluate the nonlinear residual.
    - No access to robust nonlinear solvers.
- Use small timesteps:
  - Possibly no nonlinear solver is employed.
    - No means to control or measure the nonlinear residual.

What are the consequences?? Results may be wrong

- importance of coupling w.r.t free surface dynamics [Kaus, et al. 2010, Duretz, et al. 2011]

What is needed...

- A mechanism to compose coupled systems of partial differential equations in a memory efficient and time (programming time) efficient manner.
- A robust, scalable solution algorithm which enables solutions to both linear and nonlinear problems to be obtained.

- If the coupled problem is nonlinear, we need:
  - A method to solve the set of nonlinear equations.
  - A measure of how close we are to the obtaining the nonlinear solution.
  - A robust, scalable preconditioner for each solve of the linearised problem.

- If the coupled problem is linear, we need
  - A robust, scalable preconditioner for the linear solve.

Solution: **PETSc $\longrightarrow$ MatNest + FieldSplit**

Solvers

$$F(x) = 0$$

$$x = [x_a, x_b, x_c]$$ Three different physics, *a,b,c*

$$J := \frac{\partial F}{\partial x} \qquad J = \begin{bmatrix} J_{aa} & J_{ab} & J_{ac} \\ J_{ba} & J_{bb} & J_{bc} \\ J_{ca} & J_{cb} & J_{cc} \end{bmatrix}$$

while not converged

Solve

$$J(x^k)\delta x = -F(x^k)$$

Update

$$x^{k+1} = x^k + \delta x$$

[1] JFNK

$$Jy \approx \frac{F(x+\epsilon y) - F(x)}{\epsilon}$$

[2] Assembled Jacobian (exact)

[3] Picard linearisation

Preconditioning

Solving

$$J(x)\delta x = -F(x)$$

via an iterative method requires a preconditioner *P*, i.e. we actually solve

$$P^{-1}J(x)\delta x = -P^{-1}F(x)$$

EXPLOIT KNOWN "PHYSICS" BASED PRECONDITIONERS WITHIN THE COUPLED SYSTEM

E.g. Use robust saddle point preconditioners on Stokes blocks (yellow)

Mantle Dynamics (temperature dep. viscosity) + Energy

$$J = \begin{bmatrix} A & B & C \\ B^T & 0 & 0 \\ D & 0 & E \end{bmatrix} \quad P = \begin{bmatrix} \begin{bmatrix} \hat{A} & B \\ 0 & M_\eta \end{bmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} \hat{D} & 0 \end{matrix} & \hat{E} \end{bmatrix}$$

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Multi-physics in PETSc

- Package each "physics" independently.
- Solve single-physics and coupled problems.
- Semi-implicit and fully implicit.
- Reuse residual and Jacobian evaluation unmodified.
- Direct solvers, fieldsplit inside multigrid, multigrid inside fieldsplit without recompilation.
- Use the best possible matrix format for each physics (e.g. symmetric block size 3).
- Matrix-free anywhere.
- Multiple levels of nesting.

Demonstrators

Stokes

PDE

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

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

Momentum

Pressure

"Stokes"

Prototype two "physics" system with non-trivial preconditioner

NONLINEAR RESIDUALS

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

$$F_c := u_{k,k}$$

NONLINEAR UPDATE

$$\begin{bmatrix} A+\delta A & B+\delta B \\ B^T+\delta B^T & 0 \end{bmatrix}\begin{bmatrix} \delta u \\ \delta p \end{bmatrix} = -\begin{bmatrix} F_u \\ F_c \end{bmatrix}$$

JACOBIAN

$$\mathcal{J}_s = \begin{bmatrix} A+\delta A & B+\delta B \\ B^T+\delta B^T & 0 \end{bmatrix}$$

PRECONDITIONER (ELMAN STYLE)

$$\mathcal{P}_s = \begin{bmatrix} A' & B \\ 0 & -S \end{bmatrix}$$

Stokes (visco-elastic)

a) Introduce evolution equation for the stress

$$\frac{1}{2\mu}\left(\frac{D\tau_{ij}}{Dt} + \mathcal{L}(\tau_{ij}, u_i)\right) + \frac{1}{2\eta}\tau_{ij} = D_{ij}$$

b) Discretise in time, eliminate stress as independent unknown

$$F_{u_i} := \left[\eta_e D_{ij}(\boldsymbol{u})\right]_{,j} - p_{,i} - \rho g_i - \left[\chi_e \tau_{ij}^{t-\Delta t} - \chi_e \Delta t \mathcal{L}\left(\tau_{ij}, \boldsymbol{u}\right)\right]_{,j}$$

[stress history]

c) Stable time integration (e.g. backward Euler) results in a nonlinear problem when objective derivatives are considered

$$\mathcal{L}\left(\tau_{ij}, \boldsymbol{u}\right) := 0$$

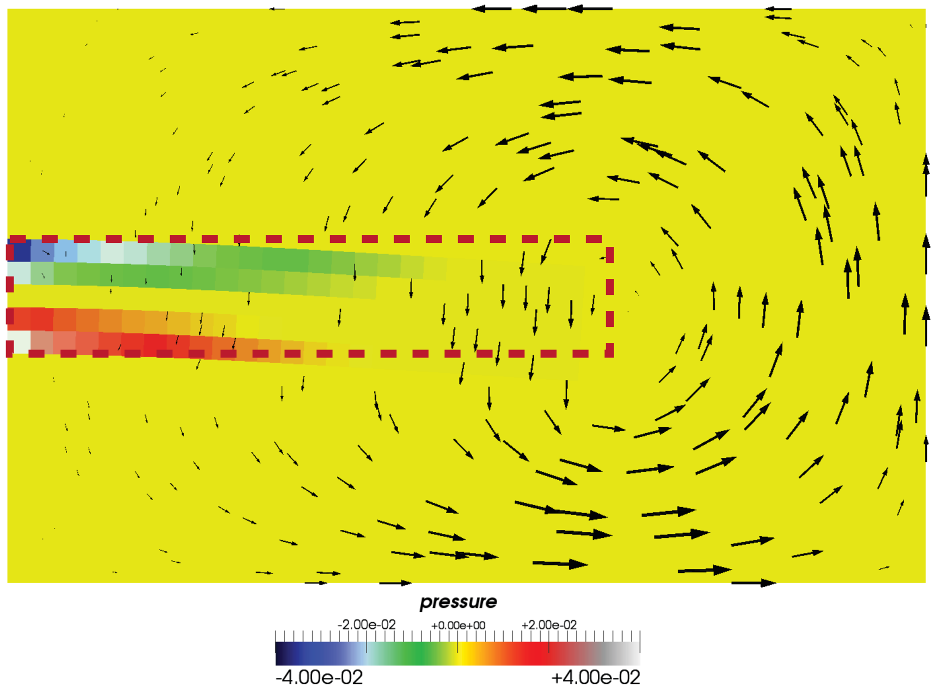
$$\mathcal{L}\left(\tau_{ij}, \boldsymbol{u}\right) := \tau_{ik} W_{kj} - W_{ik}\tau_{kj} \qquad \text{(Jaumann)}$$

$$\mathcal{L}\left(\tau_{ij}, \boldsymbol{u}\right) := -\alpha\left(L_{ik}\tau_{kj} + \tau_{ik}L_{jk}\right) \qquad \text{(Oldroyd-A)}$$

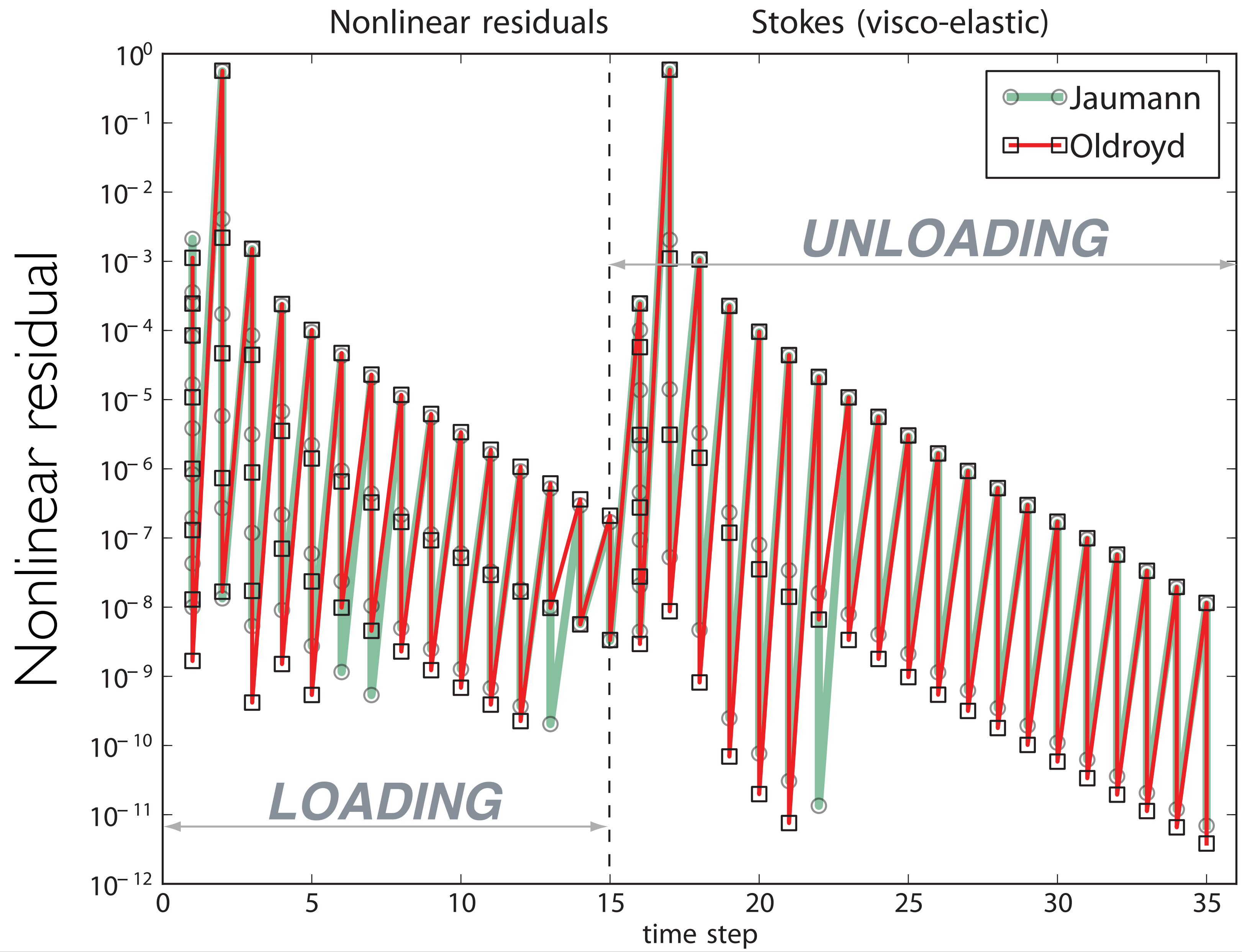
W: vorticity tensor

L: deformation tensor

Stokes (visco-elastic)



"Viagra" test case.
Nearly perfectly elastic bar, loaded under gravity, embedded within a viscous background medium.
Initial bar position indicated via red dashed line.
Loading is removed at step 15.



* Nonlinear residual jumps at each time step. Jump is proportional to dt.

* Picard linearisation is extremely effective.

Stokes (visco-plastic)

von Mises, J2 plasticity

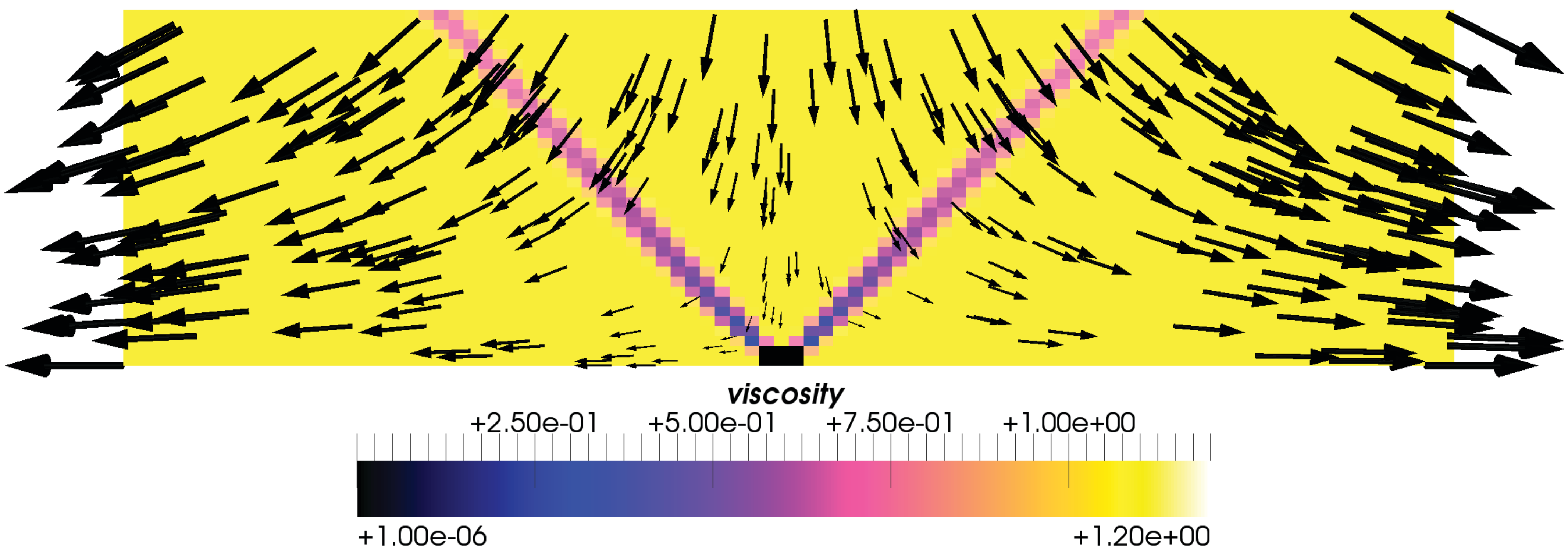
$\eta := \eta_{vp}(\boldsymbol{u}, p)$ (effective viscosity)

$f := \tau_{II} - \tau_y \leq 0$ (stress limiter)

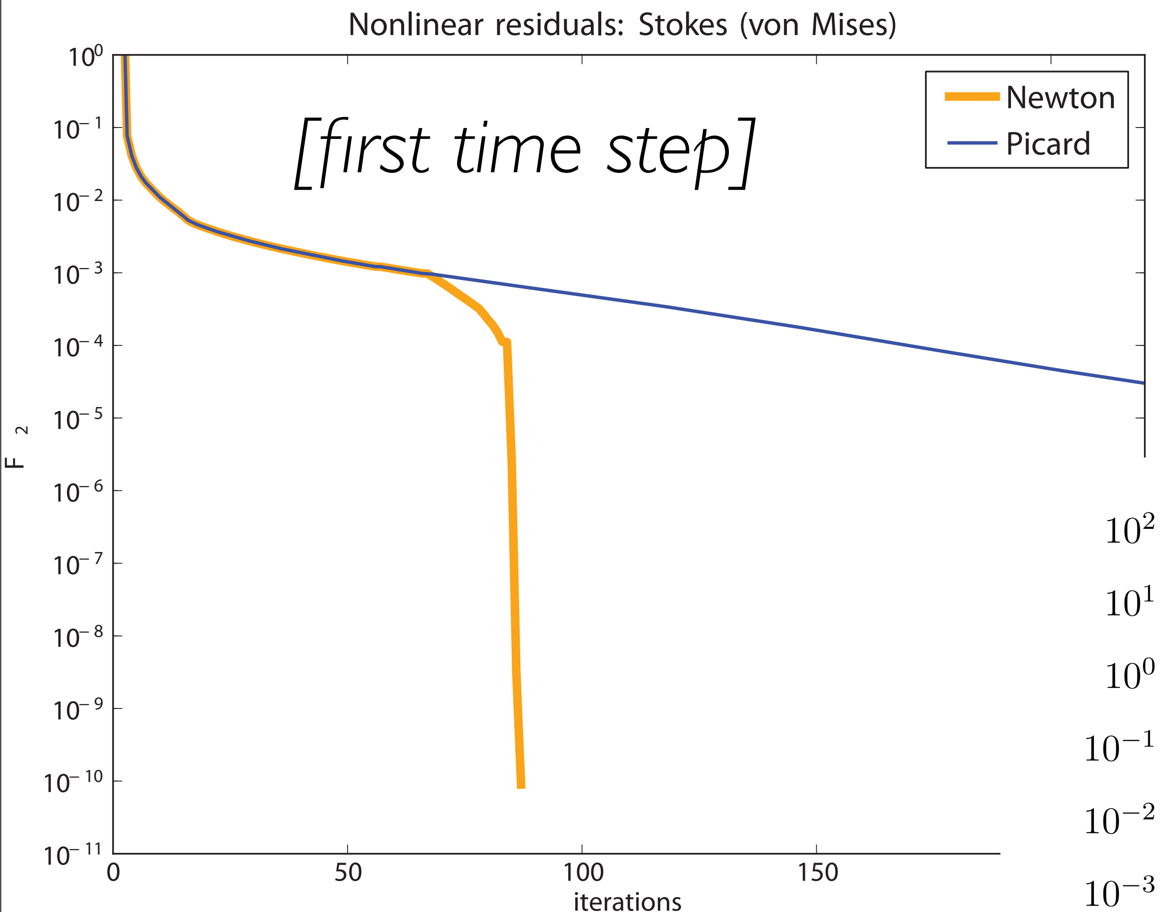
$$\tau_{II} := \sqrt{\tfrac{1}{2}\tau_{ij}\tau_{ij}}$$

$$\eta_{vp} = \begin{cases} \dfrac{\tau_y}{\sqrt{2\epsilon_{ij}\epsilon_{ij}}} & \text{if } \tau_{II} > \tau_y \\ \eta & \text{otherwise} \end{cases}$$

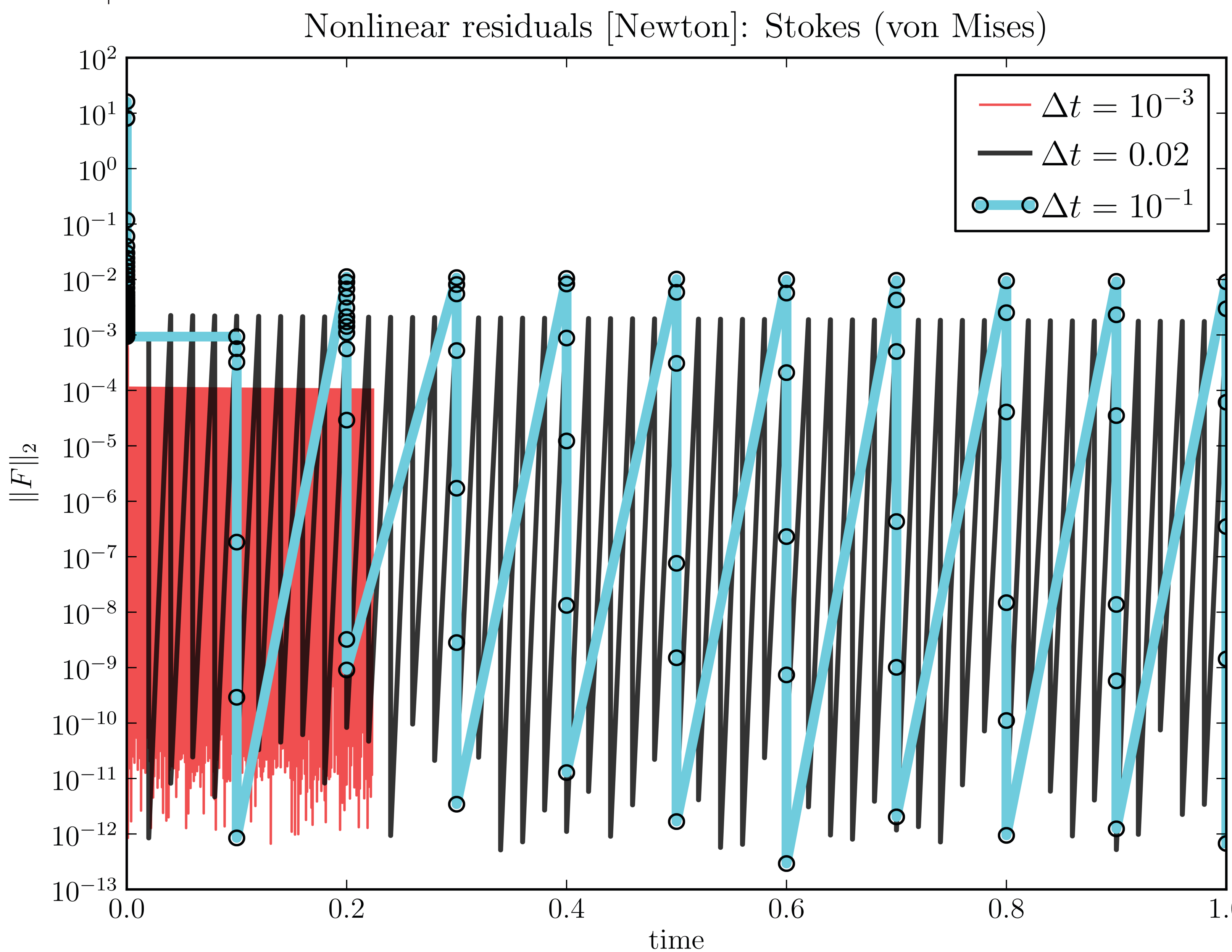
Notched bar, tension experiment with a free surface. The bar is composed of a Mises material.



Stokes (visco-plastic)



* JFNK + Picard linearisation is robust.



* Small time steps reduce nonlinear residual on the subsequent time step.

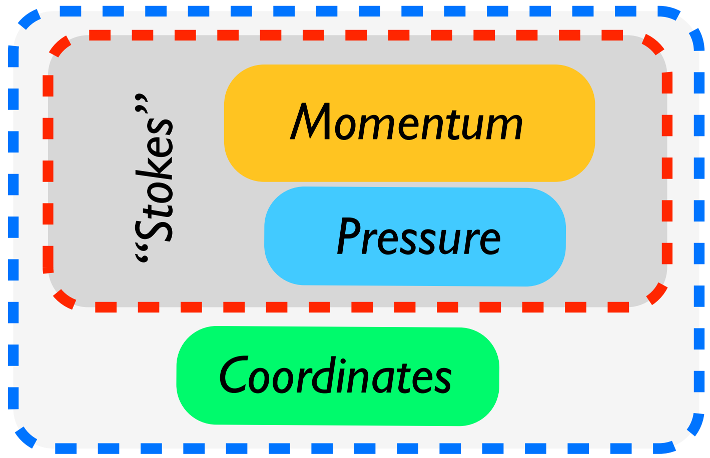
* Still require 5-7 Newtons iterations to reduce *F*, even when dt is small.

Stokes + Implicit Free Surface

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

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

$$\hat{x}_i = \hat{x}_i^{t-\Delta t} + \Delta t\, u_i(\hat{x}_i)$$



COORDINATE RESIDUALS

$$F_x := -u_i + \frac{\hat{x}_i}{\Delta t} - \frac{\hat{x}_i^{t-\Delta t}}{\Delta t}$$

[We use a full Lagrangian update of our mesh, with no remeshing]

JACOBIAN

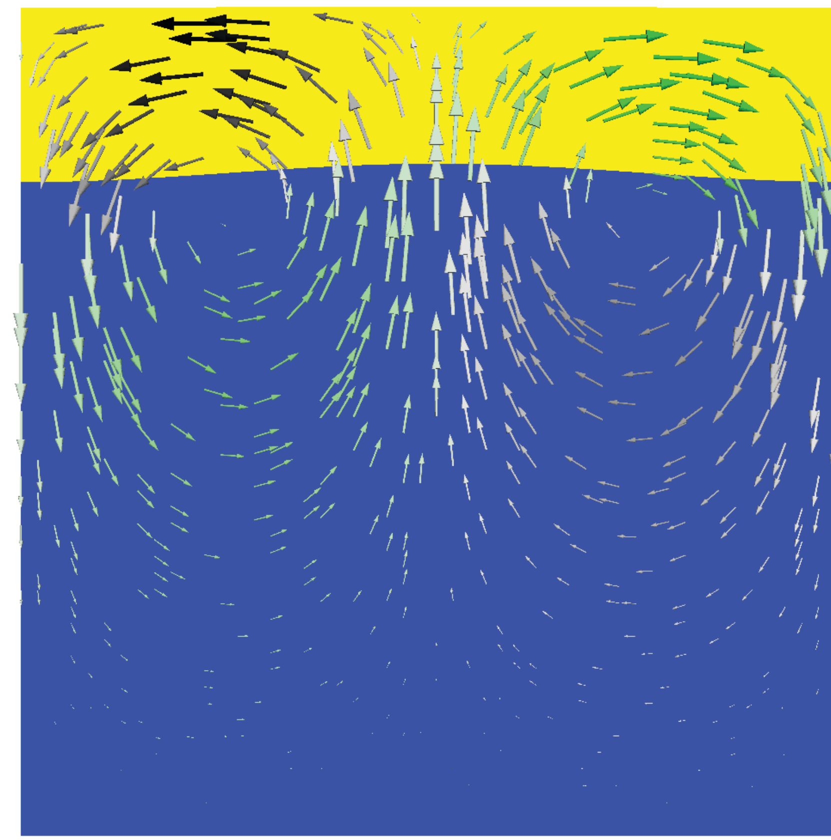
$$\mathcal{J}_{si} = \begin{bmatrix} A + \delta_{\hat{x}} A & B + \delta_{\hat{x}} B & J_{ac} \\ B^T + \delta_{\hat{x}} B^T & 0 & J_{bc} \\ -I & 0 & \frac{I}{\Delta t} \end{bmatrix}$$

Reuse stokes operators and saddle point preconditioners

NESTED PRECONDITIONER

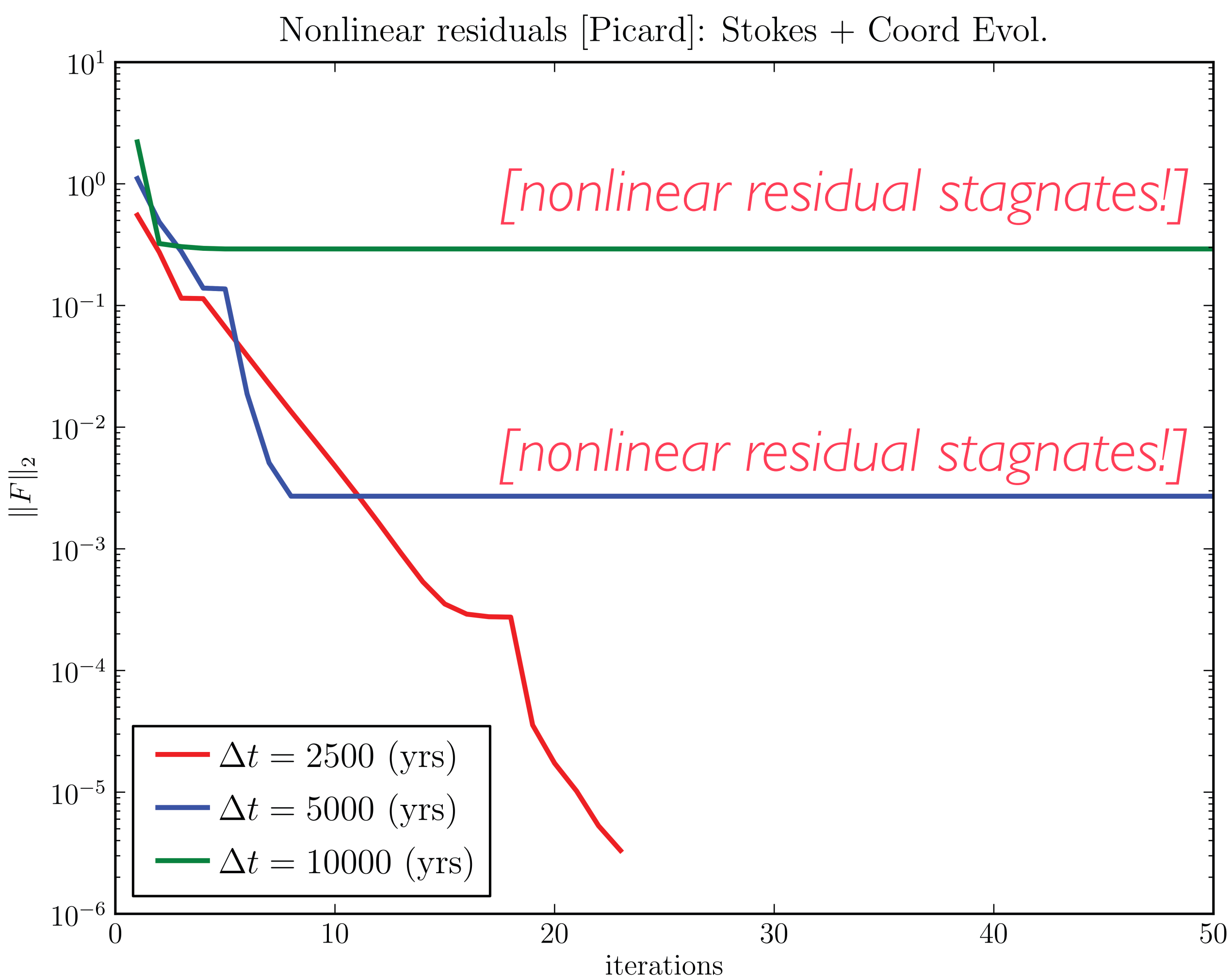
$$\mathcal{P}_{si} = \begin{bmatrix} \left[\ \mathcal{P}_s^l\ \right] & \\ \left[\ I\ \right] & \left[\ -\frac{I}{\Delta t}\ \right] \end{bmatrix}$$

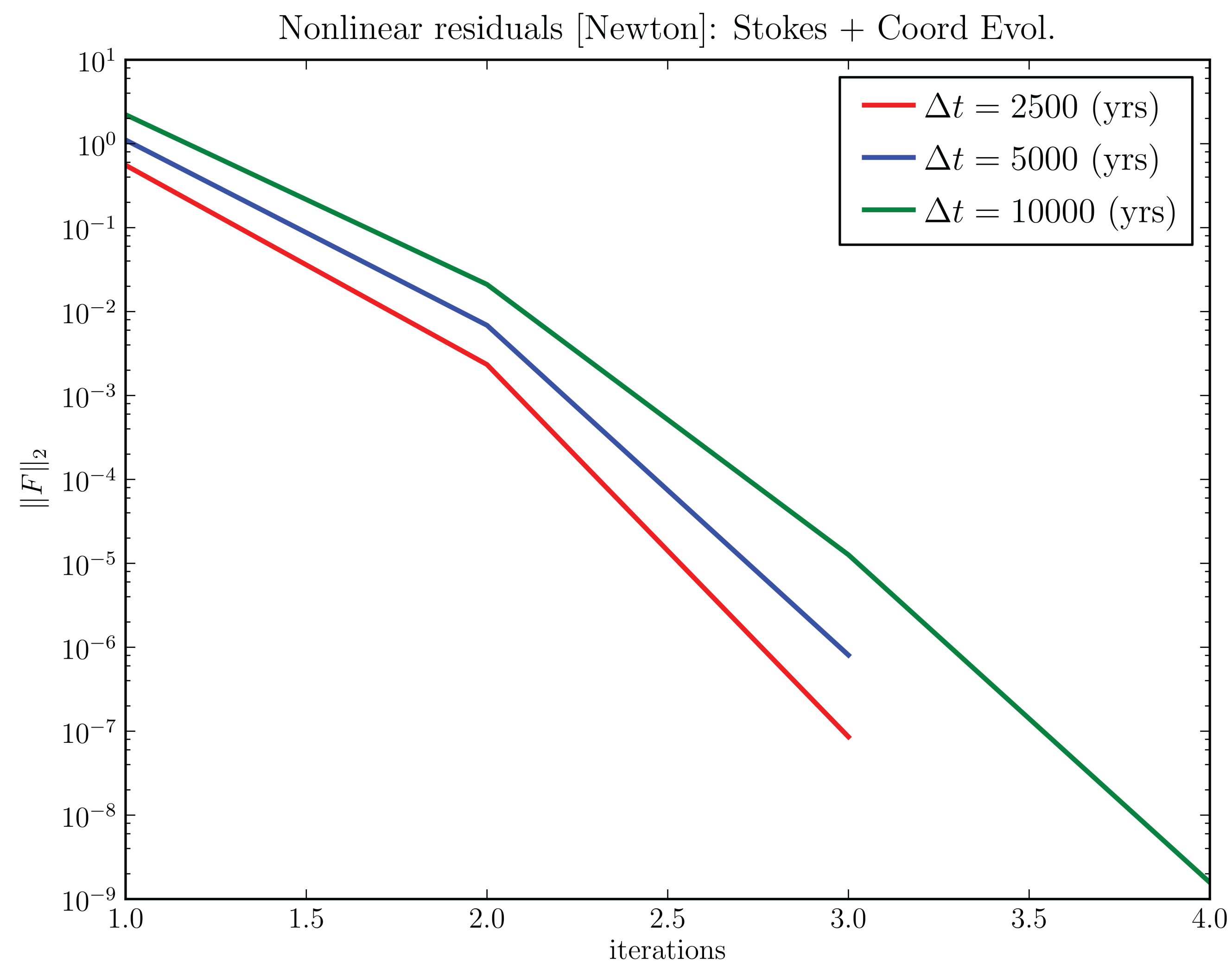
$$\mathcal{P}_s^l = \begin{bmatrix} A & 0 \\ B^T & -S \end{bmatrix}$$



"Drunken seaman", Rayleigh Taylor instability test case from Kaus et al., 2010. Dense, viscous material (yellow) overlying less dense, less viscous material (blue).

Stokes + Implicit Free Surface

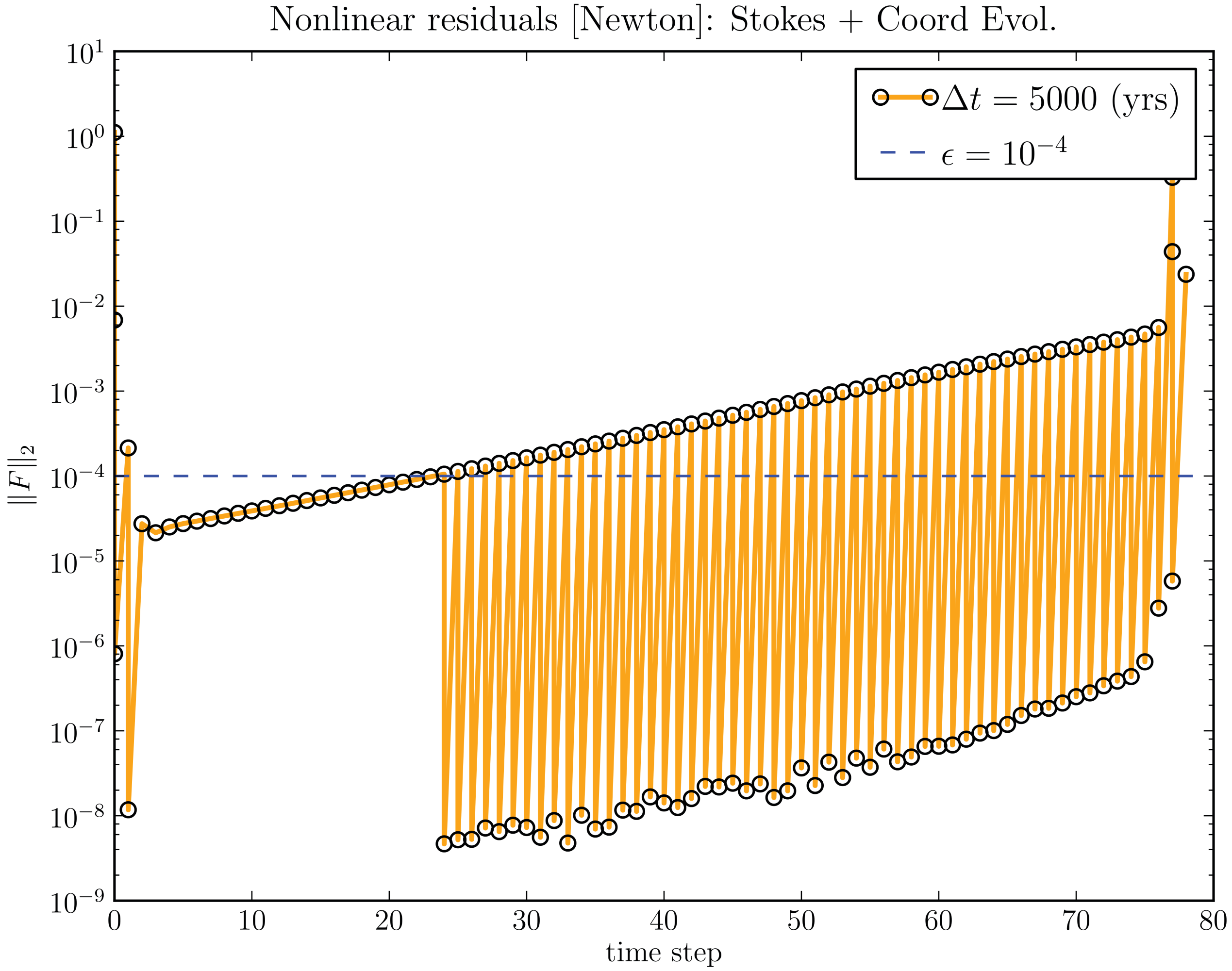


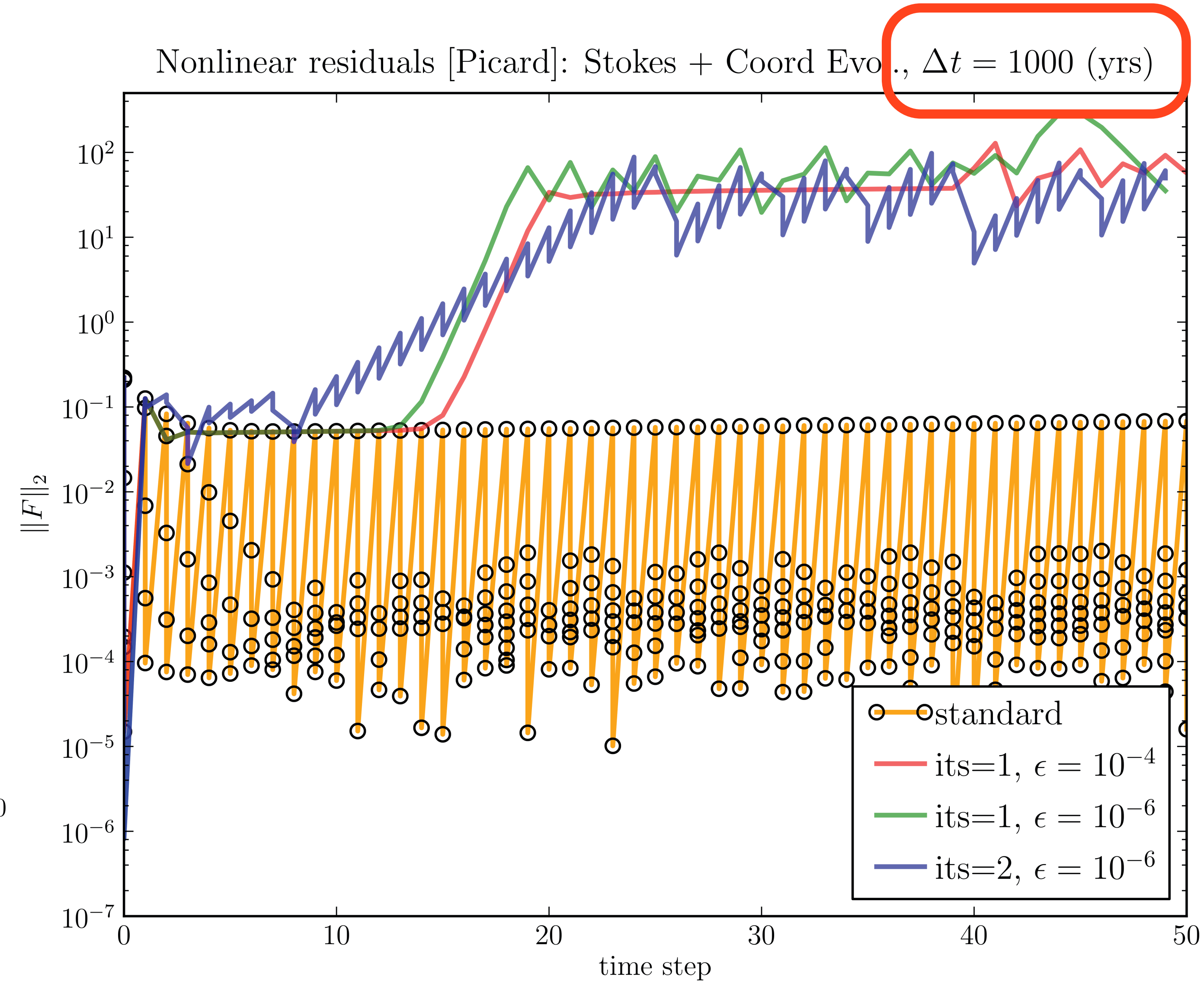


* Picard fails to converge for large time steps sizes.

* Newton is robust for a wide range of time step sizes.

Stokes + Implicit Free Surface





* The nonlinear residual *ALWAYS* increases from one step to the next.

* A nonlinear solve is required to control the error.

* An accurate nonlinear solve on the first time step, combined with 1 or 2 nonlinear iterations on subsequent steps still results in severe errors. *This is true even when dt is small.*

Summary

- Correct treatment of multi-physics coupling is needed to both understand complex geodynamic processes and to produce stable and reliable numerical solutions.

- Picard is not effective for Mises plasticity or implicit surface evolution. Efficient solution methods for these applications are essential to study lithospheric dynamics in 3D.

- The PETSc - MatNest - Fieldsplit framework demonstrated here enables new physics to be introduced with minimal code changes and maximal software re-use of residual evaluation routines and any existing preconditioners.

- Additional benefits of this infra-structure are:

  - Always have access to the nonlinear residual.
  - Always solve in defect correction form.
  - Use either Picard or Newton.
  - Use matrix free methods anywhere.
  - Multiple nesting within preconditioners is possible with little memory overhead.
  - Re-use existing physics based preconditioners.