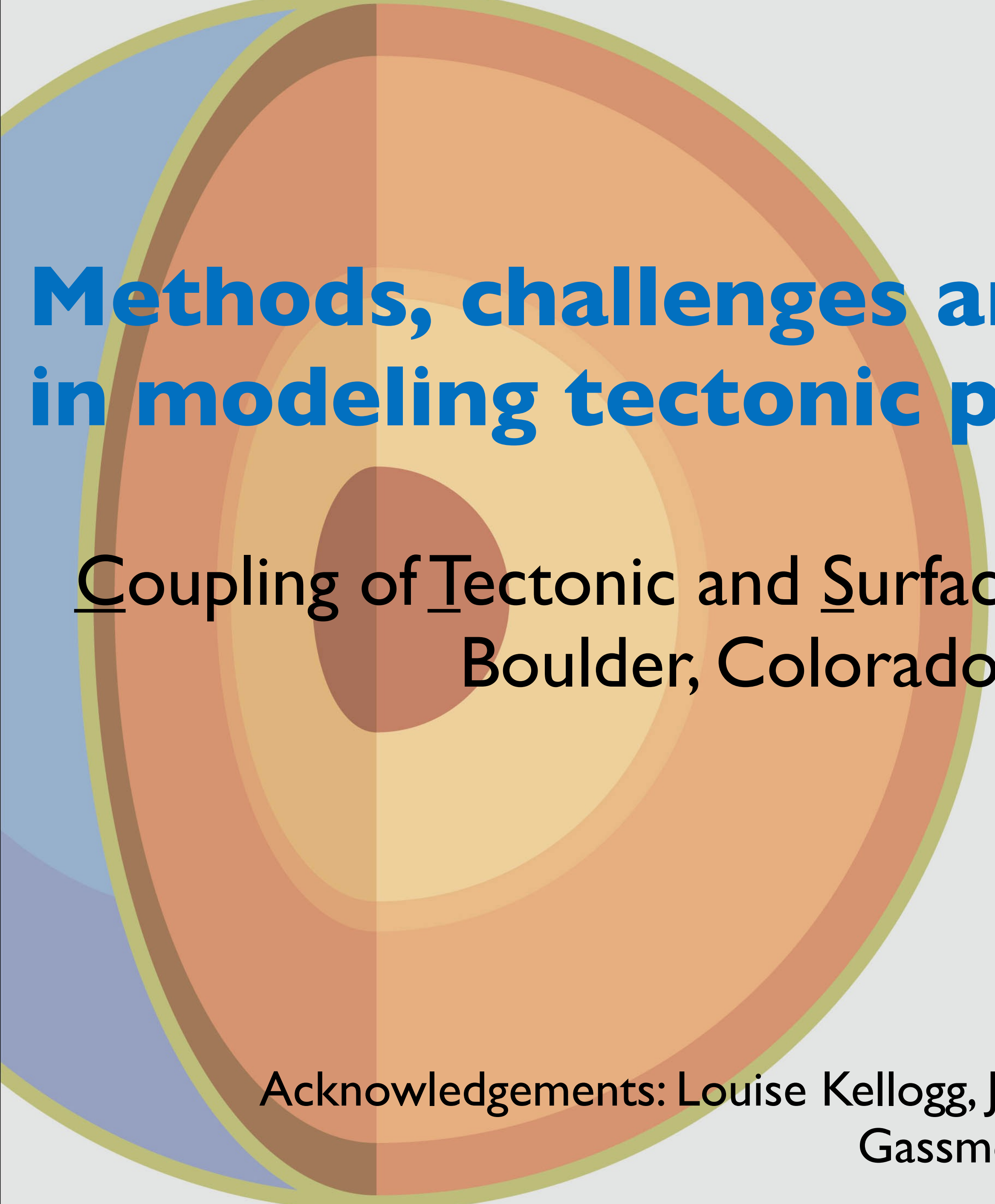


Methods, challenges and uncertainty in modeling tectonic processes

Coupling of Tectonic and Surface Processes Meeting
Boulder, Colorado (2018)

John Naliboff
UC Davis, CIG

Acknowledgements: Louise Kellogg, Juliane Dannberg, Rene Gassmöeller, Lorraine Hwang

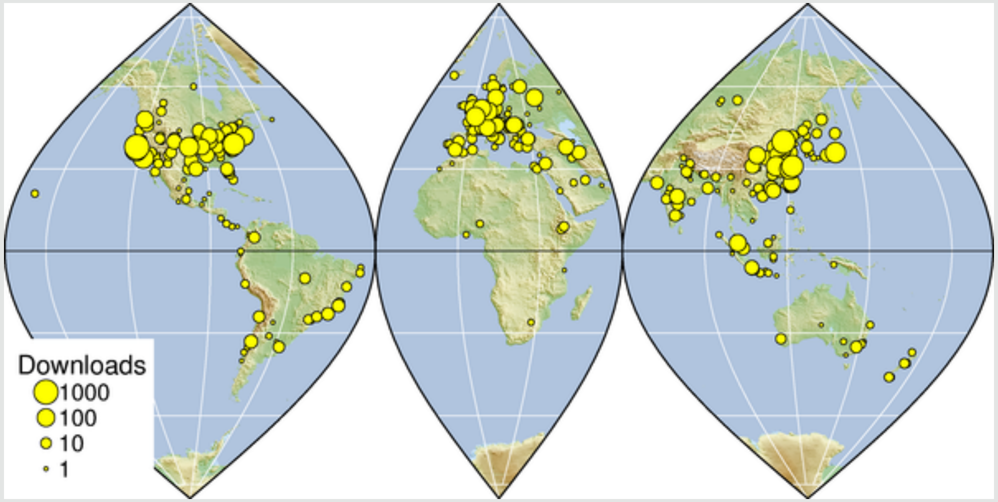
Computational Infrastructure for Geodynamics

Our Mission: advance Earth science by **developing and disseminating software** for geophysics and related fields.

33 codes

Primary Scientific domains:

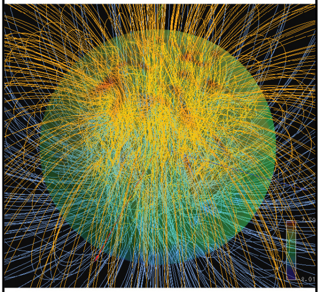
- Geodynamo
- Mantle convection
- Long-term tectonics
- Seismology
- Short term crustal dynamics
- Computational science
- Fluid migration/multiphysics



Community

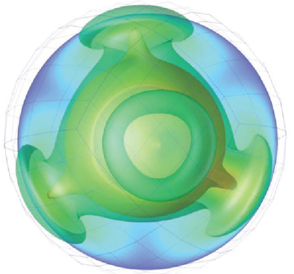
- •75+ institutional members: universities, government labs & agencies
- •900+ participants
- •20 countries

Calypso

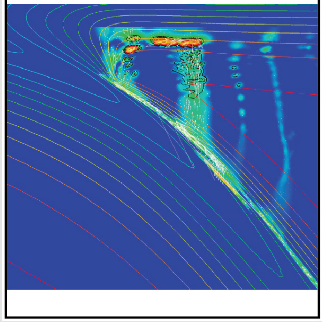


Rayleigh

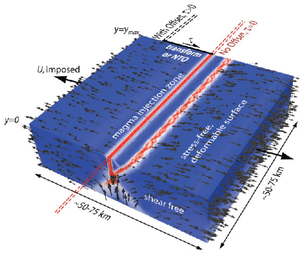
CitcomS



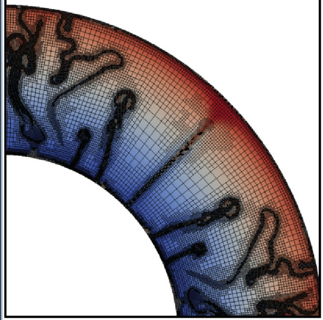
TerraFERMA



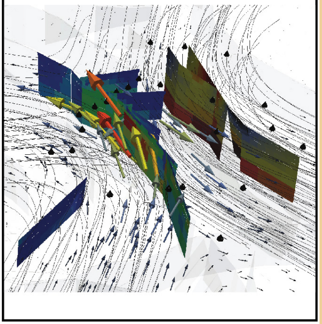
Gale



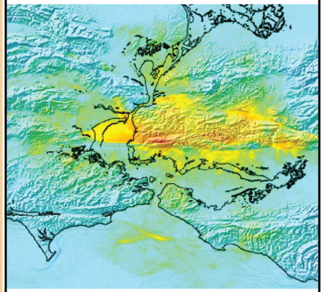
ASPECT



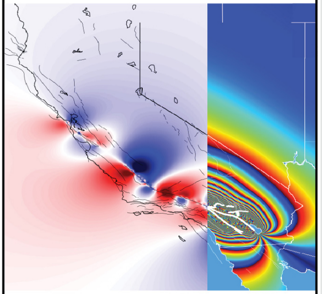
Relax



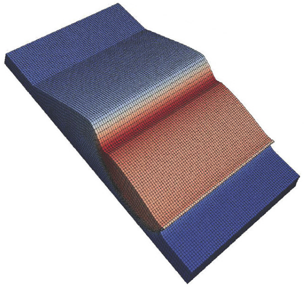
SW4



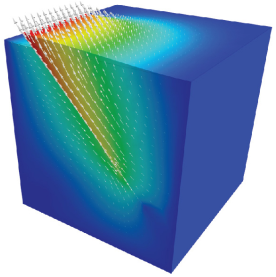
Virtual Quake



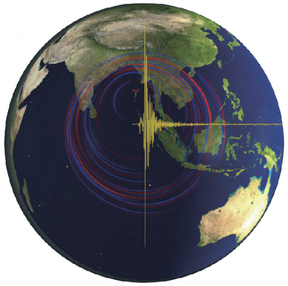
SPECFEM 3D Geotech



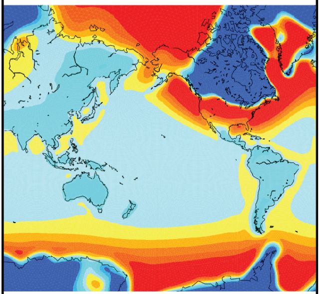
PyLith



SPECFEM 3D Globe



SELEN



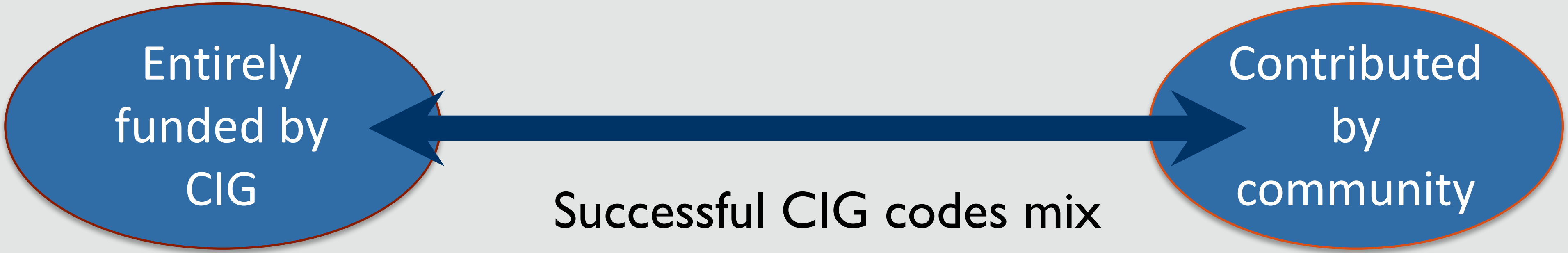
BurnMan

CitcomCU

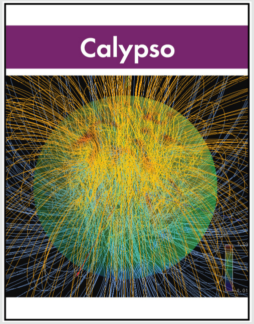
CIG
COMPUTATIONAL
INFRASTRUCTURE
for GEODYNAMICS

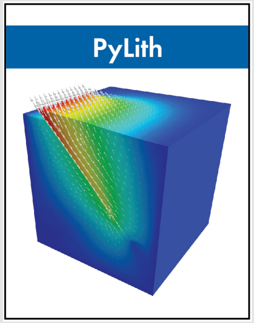
+ 18 more

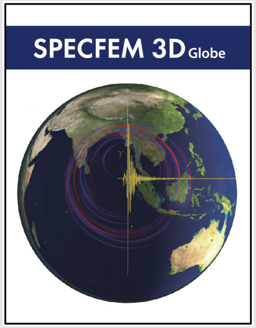
Software development

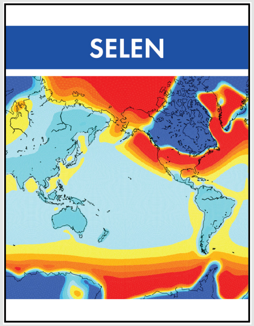


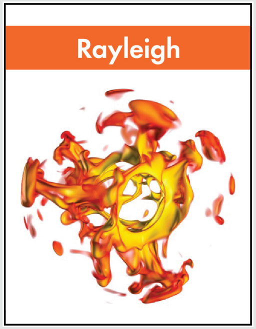
Successful CIG codes mix
Community and CIG development and support

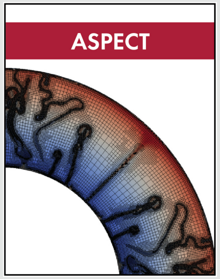


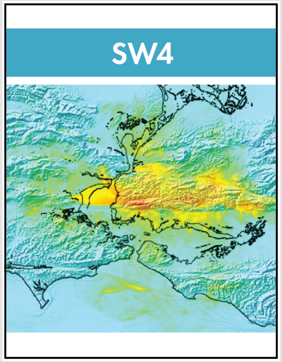




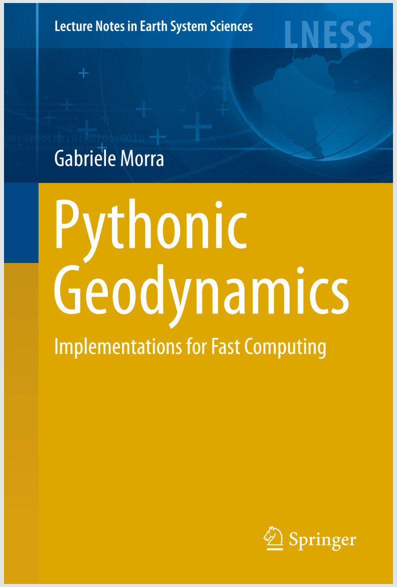








Educational Resources



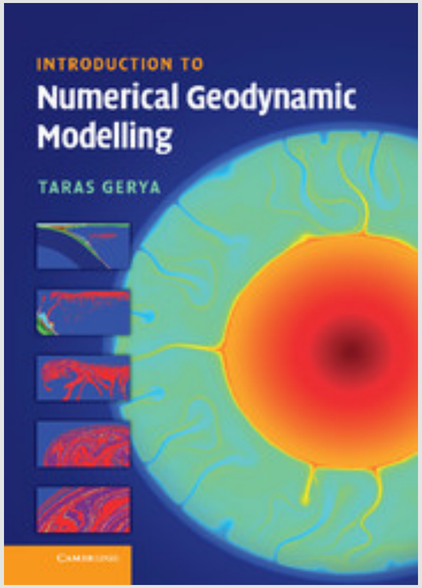
Lecture Notes in Earth System Sciences LNESS

Gabriele Morra

Pythonic Geodynamics

Implementations for Fast Computing

Springer

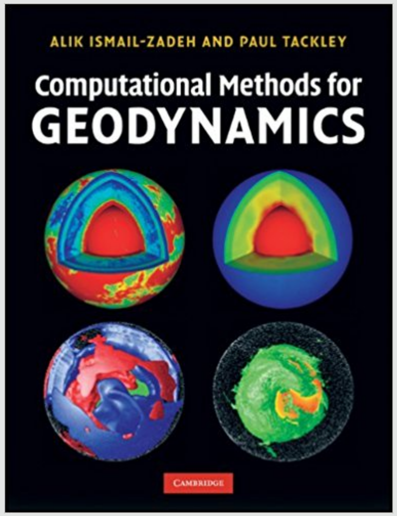


INTRODUCTION TO

Numerical Geodynamic Modelling

TARAS GERYA

CAMBRIDGE



ALIK ISMAIL-ZADEH AND PAUL TACKLEY

Computational Methods for GEODYNAMICS

CAMBRIDGE

Numerical Modeling of Earth Systems

An introduction to computational methods with focus on
solid Earth applications of continuum mechanics

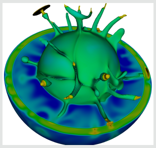
Lecture notes for USC GEOL557, v. 1.2

Thorsten W. Becker
Department of Earth Sciences,
University of Southern California, Los Angeles CA, USA

and

Boris J. P. Kaus
University of Mainz, Germany

April 16, 2016



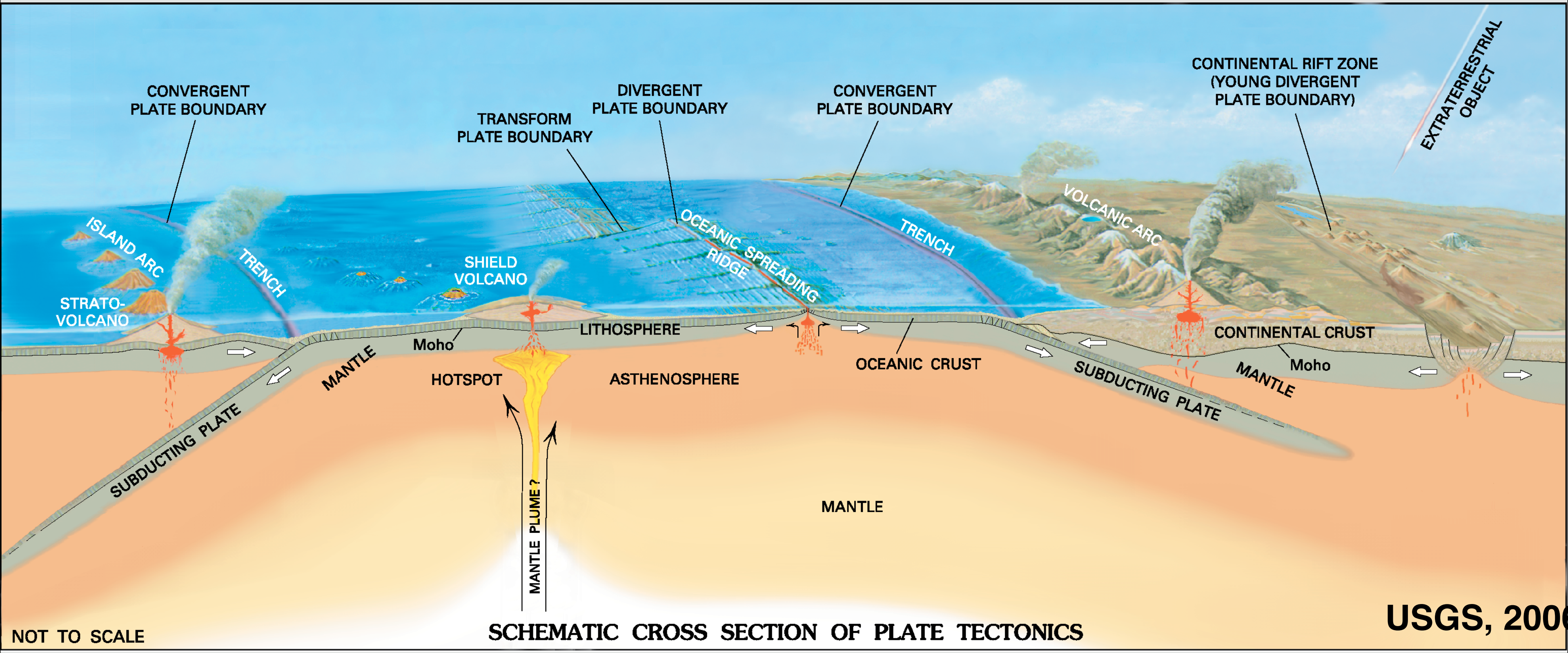
Outline

1. <u>Overview and numerical methods</u>

2. Challenges
   - Verification
   - Sensitivity Analysis
   - Validation
   - Resources

- Summary and Outlook

Long-Term Tectonic Processes



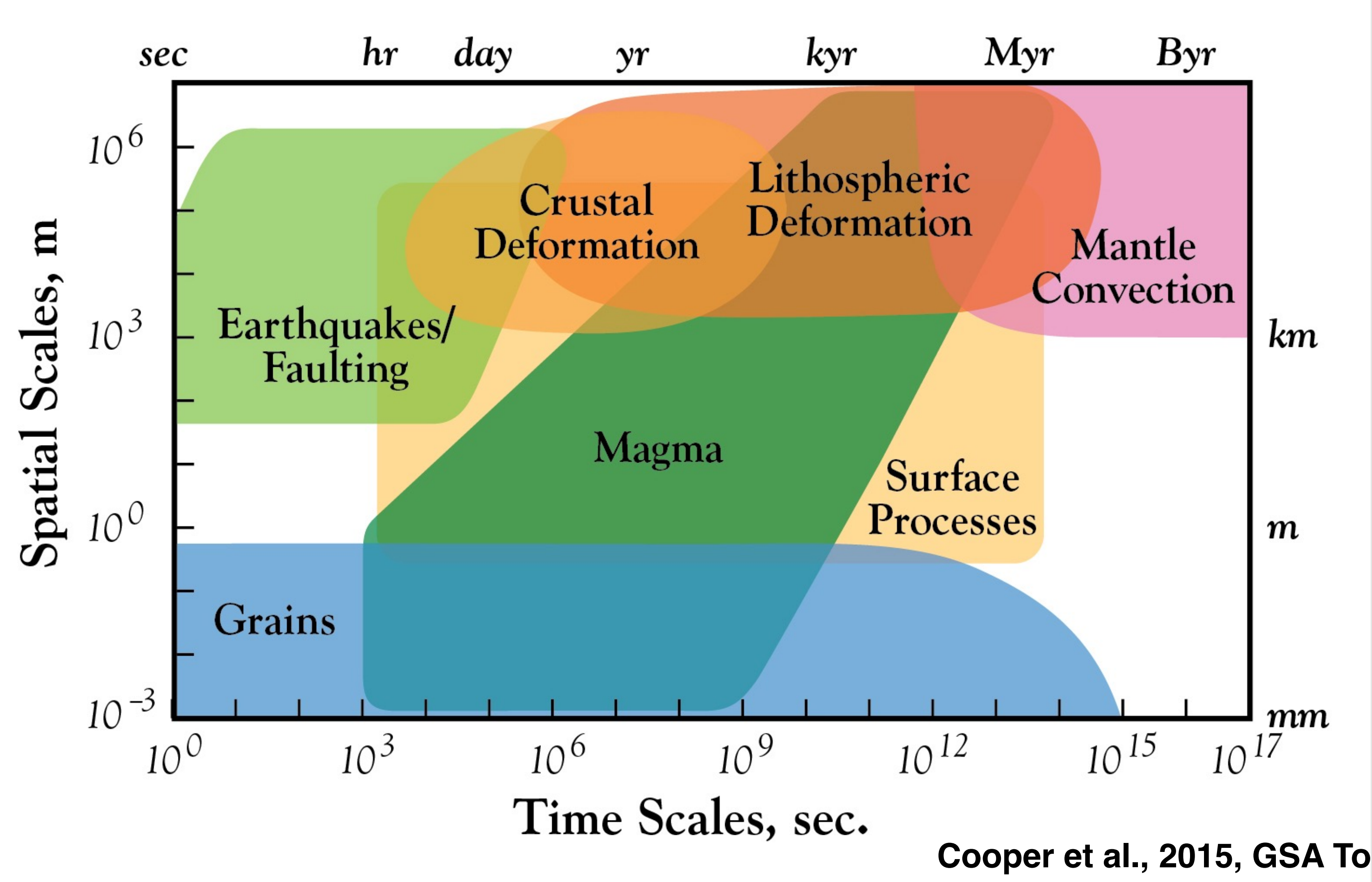
SCHEMATIC CROSS SECTION OF PLATE TECTONICS

USGS, 200

Crustal Deformation, Lithospheric Deformation, Mantle Convection

Spatial and temporal scales?

The challenge: modeling processes at vastly varying scales of space and time



Cooper et al., 2015, GSA Today

Long-Term Tectonics

10^4 to 10^7 years, 10’s to 1000’s of km

Basic Physical Approximations

Conservation equations for incompressible viscous flow

$$\nabla \bullet u = 0$$ **Mass**

$$\nabla \bullet \sigma' - \nabla P + \rho g = 0$$ **Force Balance**

$$\rho c \left(\frac{\partial T}{\partial t} + u \bullet \nabla T \right) = \nabla \bullet k \nabla T + H$$ **Energy**

Additional terms: adiabatic & viscous heating, phase changes

Basic Physical Approximations

Constitutive behavior (rheology)

$$\sigma_{eff} = A^{-1/n}\dot{\varepsilon}^{1/n} d^{p/m} e^{\frac{Q+PV}{nRT}}$$

Non-linear viscous flow

$$\eta_{eff} = \frac{\eta\mu dt}{\eta + \mu dt}$$

Viscoelasticity*

$$\sigma_{eff} = P\sin\theta + C\cos\theta$$

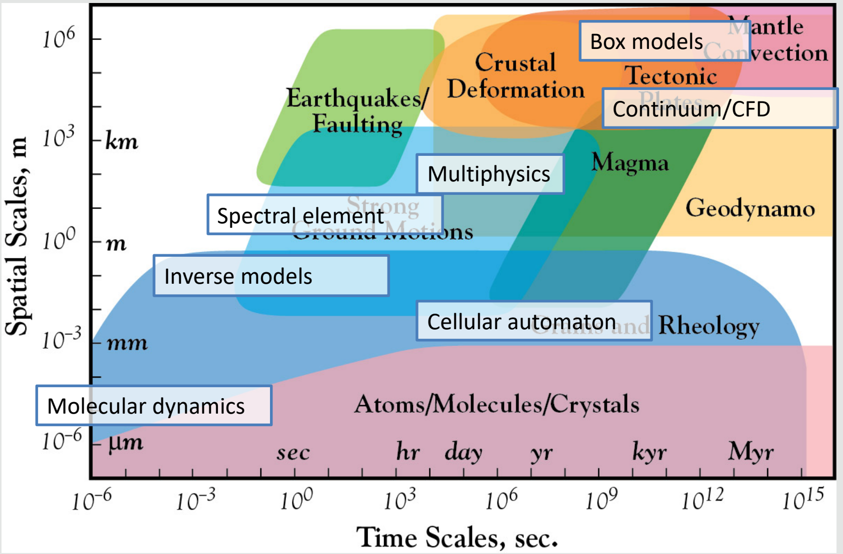
Brittle Failure (Plasticity)

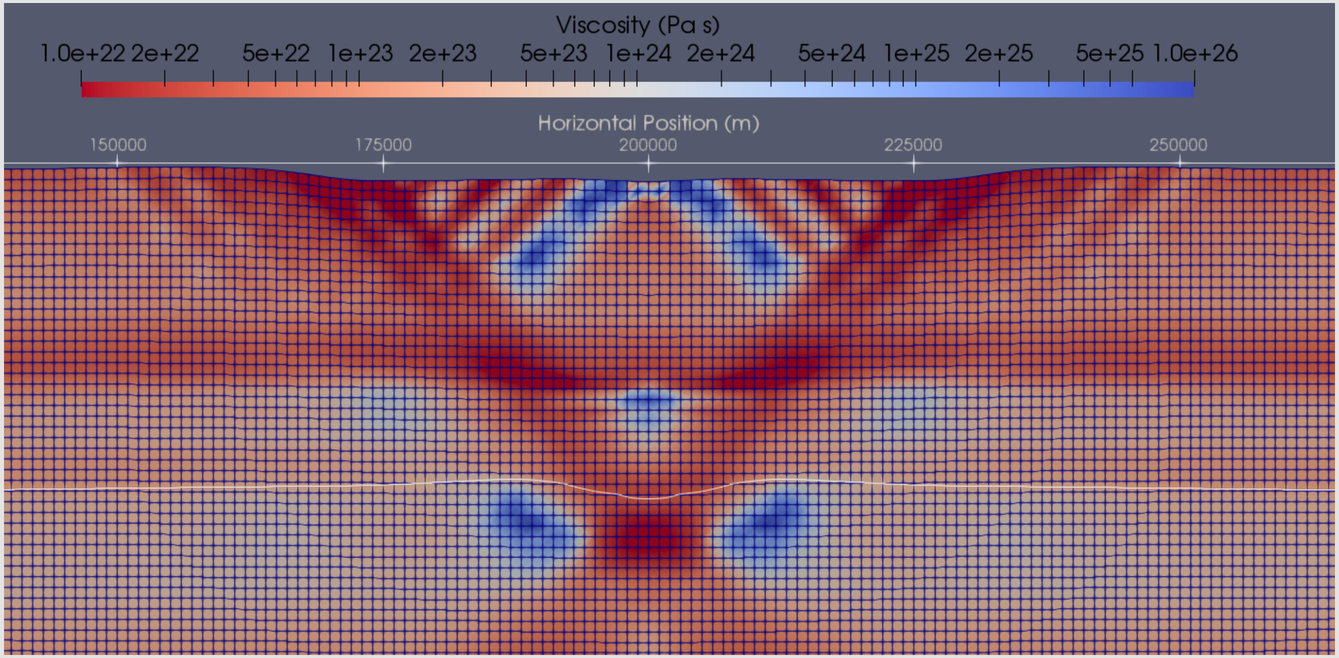
Additional processes: strain-weakening, grain-size evolution, …

Numerical Methods

General procedure example

1. Choose a numerical method
2. Rewrite PDE's as algebraic eqns.
3. Specify boundary & initial conditions
4. Solve for velocity (non-linear iterations?)
5. Solver for temperature (+/- composition)
6. Advect free surface* and tracers





Results of numerical simulation (continental extension) with 1 km grid superimposed.

Software Design

Simple Design	Complex Design
100s lines Single file	>100,000 lines 10 - 1000's files Multiple packages
Straightforward physical assumptions	Can model a wide range of physical behavior
Small (2-D) simulations Basic numerical methods Runs in serial (single-cpu)	Small (2-D) or large (3-D) simulations Advanced numerical methods Serial or massively parallel simulations
Interpreted Language (Python, Matlab) Compiled Language (C, C++, Fortran)	Compiled Language (C, C++, Fortran) Interpreted Language (Python) Use of Parallel Processing (MPI)

“Tectonics” Software

ABAQUS

ASPECT*

COMSOL

DOUAR

DynEarthSol2D*

DynEarthSol3D*

ELEFANT

I2ELVIS/I3ELVIS

LaMEM*

MVEP2*

pTatin3D

SLIM3D

SiStER*

SNAC*

SULEC

TerraFERMA*

Underworld2*

Outline

1. Overview and numerical methods

2. <u>Challenges</u>
    - Verification
    - Sensitivity Analysis
    - Validation
    - Resources

- Summary and Outlook

Verification verse Validation

Verification

> “The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.”

Validation

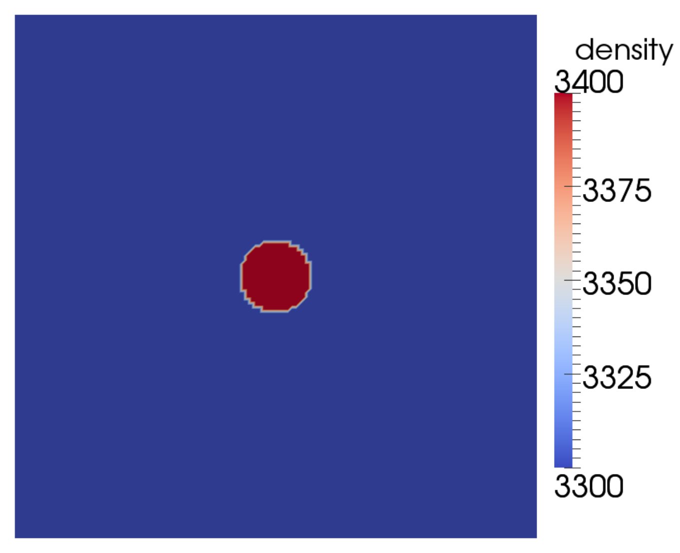
> “The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.”

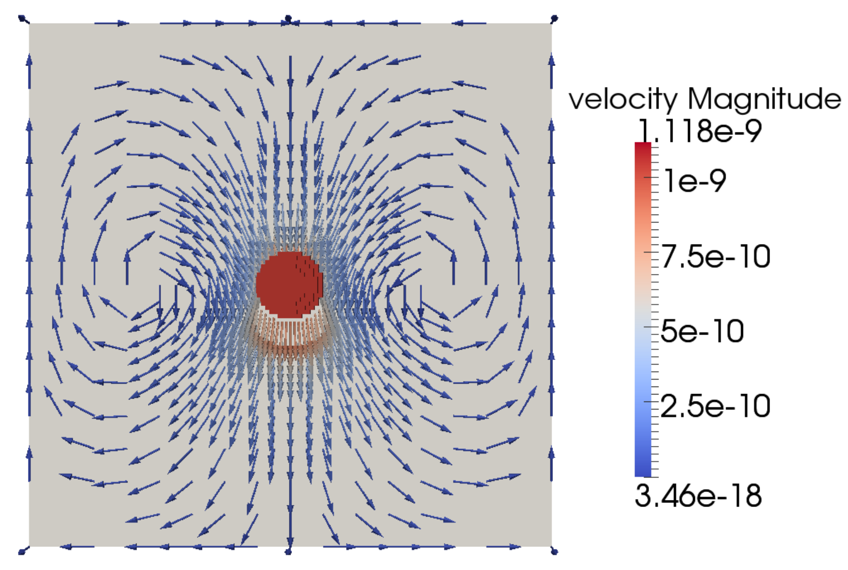
Verification, Validation, and Predictive Capability in Computational Engineering and Physics (Oberkampf et al., 2003); CIG Webinar

Challenges: Verification

How do you know your code is doing what you intended it to do?

1. Numerical Implementation
2. Physics Implementation



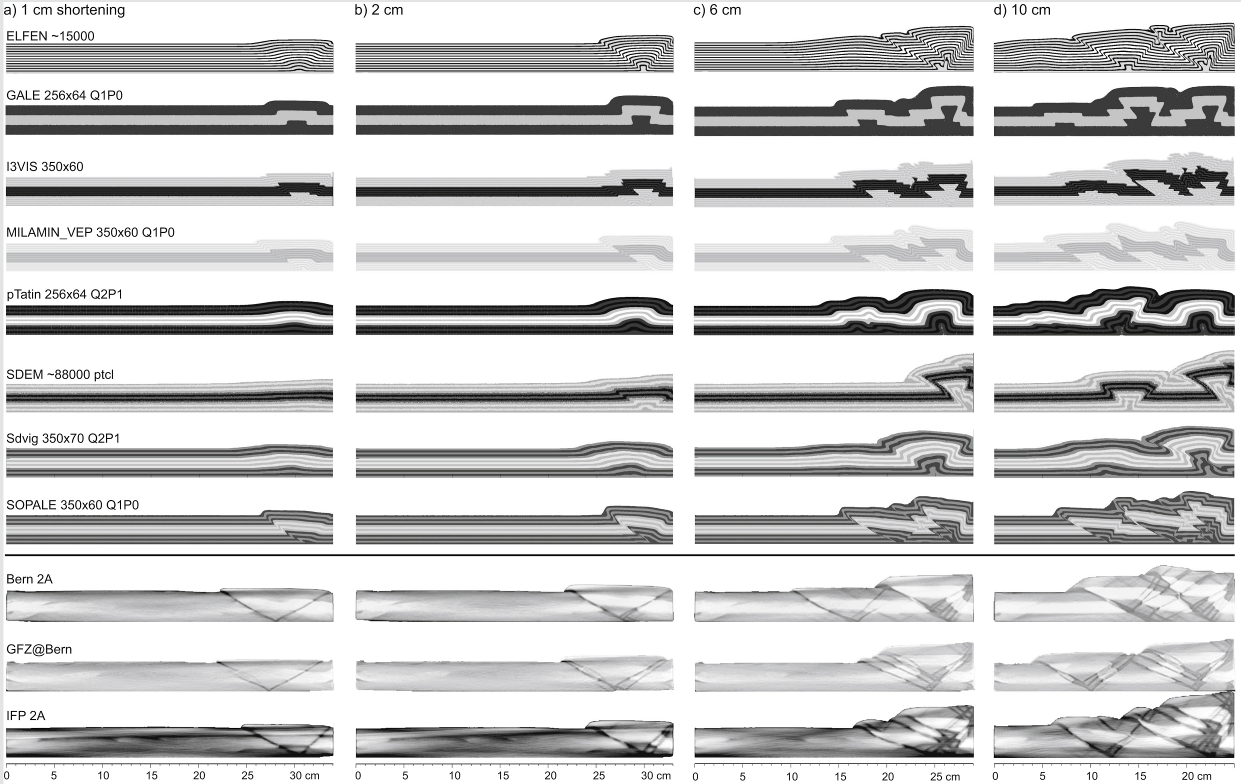


Analytical Stokes solution for a sinking sphere (ASPECT manual)

Challenges: Verification

How do you know your code is doing what you intended it to do?

3. Comparisons to other numerical models (replication) and analogue models



Benchmarking numerical models of brittle thrust wedges (Buiter et al., 2016)

Challenges: Verification

How do you know your code is doing what you intended it to do?

4. Use open-source software and 'best practices' in code design!

'*Best Practices*':

✦Version control (github, bitbucket)

✦Code review (example)

✦Documentation (source code, manual, example problems)

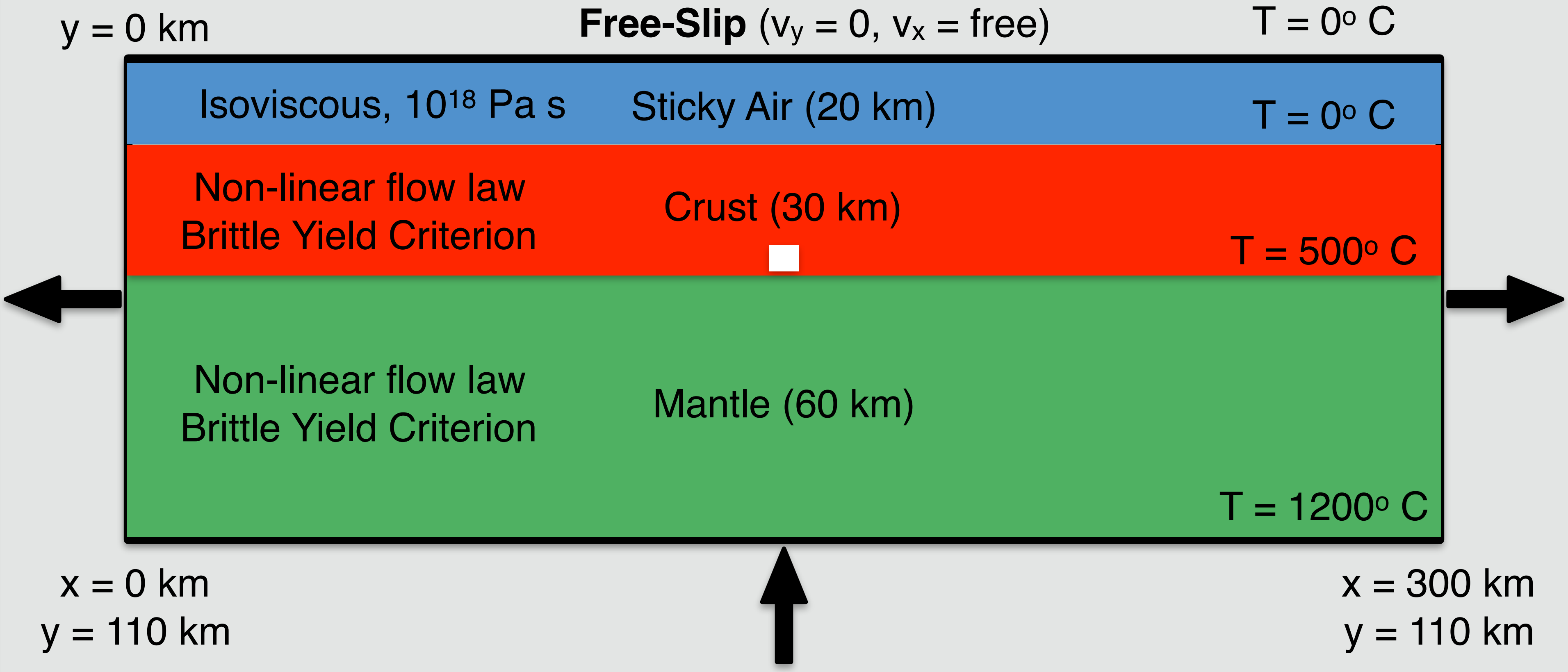
✦More users (more testing, contributors & sustained innovation; 'bus factor')

✦Long-term support for most features

✦Reproducibility and replicability

Challenges: Sensitivity Analysis

“Typical” Numerical Setup



y = 0 km

Free-Slip ($v_y = 0$, v_x = free)

$T = 0^{\circ}$ C

Isoviscous, 10^{18} Pa s

Sticky Air (20 km)

$T = 0^{\circ}$ C

Non-linear flow law
Brittle Yield Criterion

Crust (30 km)

$T = 500^{\circ}$ C

Non-linear flow law
Brittle Yield Criterion

Mantle (60 km)

$T = 1200^{\circ}$ C

x = 0 km
y = 110 km

x = 300 km
y = 110 km

“Typical” Resolution Range (0.1 - 5 km)

Challenges: Sensitivity Analysis

What parameters affect the solution?

Grid Resolution
Particles-Per-Cell
Time-Step Size
Solver Convergence Settings

Model Geometry
Initial Lithology
Initial Temperature
Boundary Conditions

Viscous Flow Law
Brittle Yield Mechanism
Brittle Parameters
Strain-Weakening (magnitude, rate)
Viscoelasticity

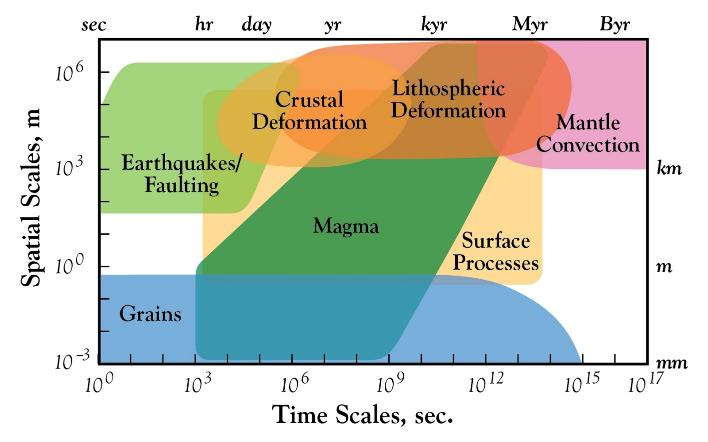
Solution: Lots of sensitivity tests (in 2D if possible).

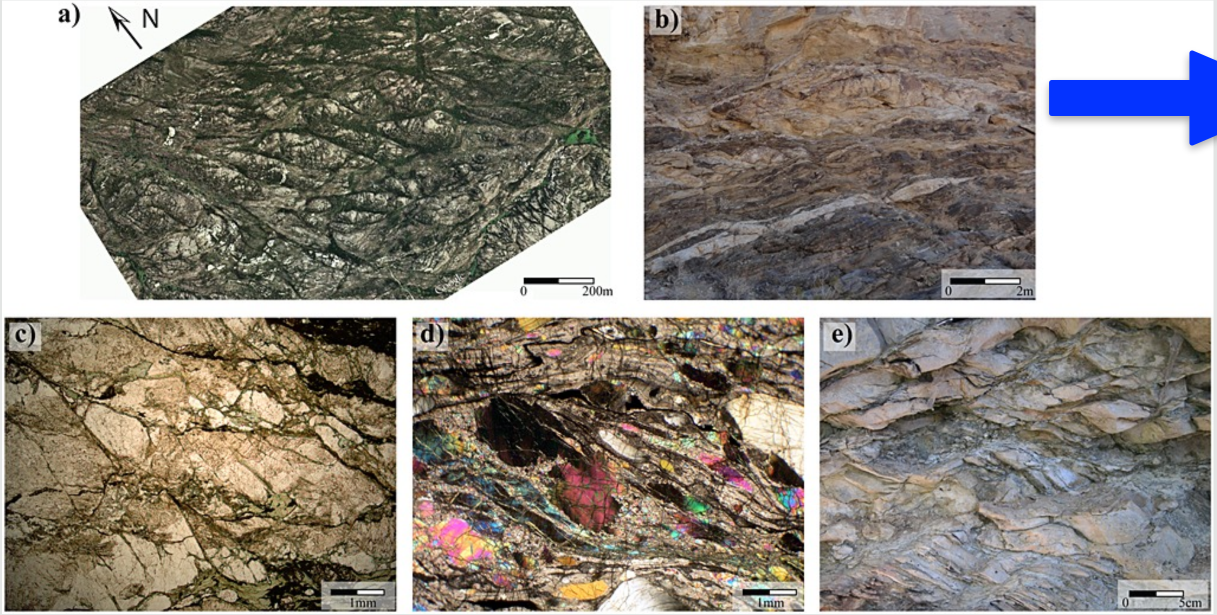
**Please report these tests and all values used in your computations*

Challenges: Validation & Scaling

Challenges arise from …

1. Spatial and temporal scales
2. Rheological uncertainty
3. Solution uniqueness
4. Comparison to natural results





Ductile shear zones at varying scales (1 mm - 200 m)

Observed variations in …

✓ Scales of heterogeneity

✓ Composition

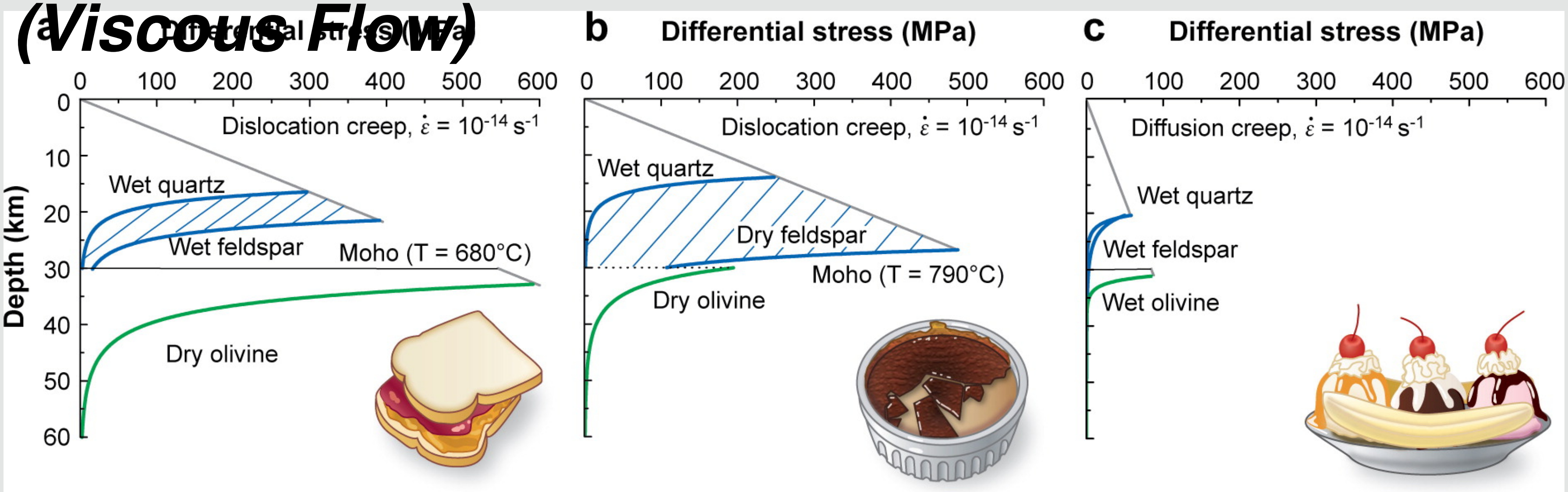
✓ Grain-size

✓ Strength

Localization and delocalization of deformation in a bimineralic material (Jammes et al., 2015)

Challenges: Validation & Scaling

Rheological Uncertainty & Numerical Issues (Viscous Flow)



Bürgmann R, Dresen G. 2008.
Annu. Rev. Earth Planet. Sci. 36:531–67.

Rheology of the Lower Crust and Upper Mantle: Evidence from Rock Mechanics, Geodesy, and Field Observations

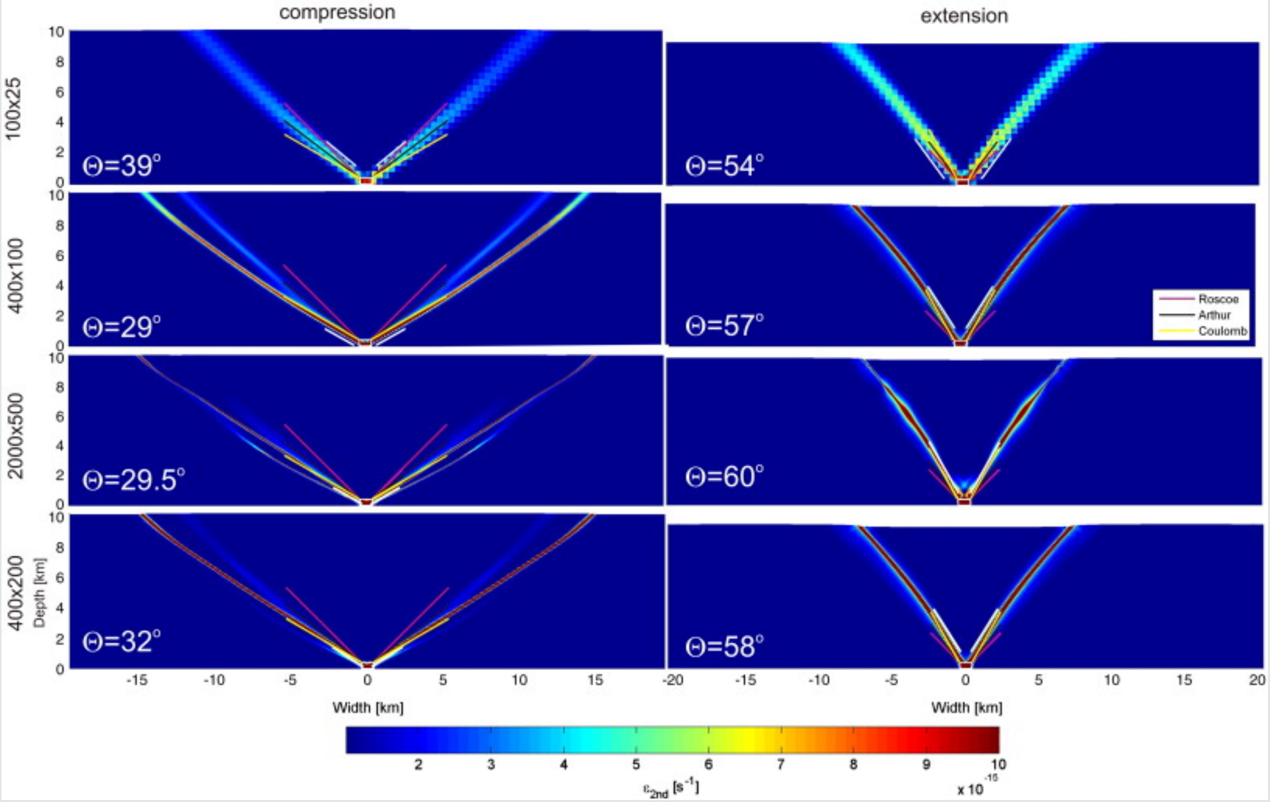
Issues?

1. Scaling of flow laws (experiments done at high strain-rates)
2. Choice of flow laws (wet verse dry, composition, diffusion verses dislocation, etc)
3. Applicability to the lithosphere? (bimineralic material, length-scales of heterogeneity)

Challenges: Validation & Scaling

COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

Rheological Uncertainty & Numerical Issues (Brittle Failure)



Issues?

1. Resolution-dependent

2. Convergence behavior

2. Rates, magnitudes and mechanisms of brittle weakening?

3. Reasonable approximation of integrated seismicity?

Factors that control the angle of shear bands in geodynamic numerical models of brittle deformation (Kaus 2010)

Challenges: Validation & Scaling

Rheological Numerical Issues (Resolution-Dependence)

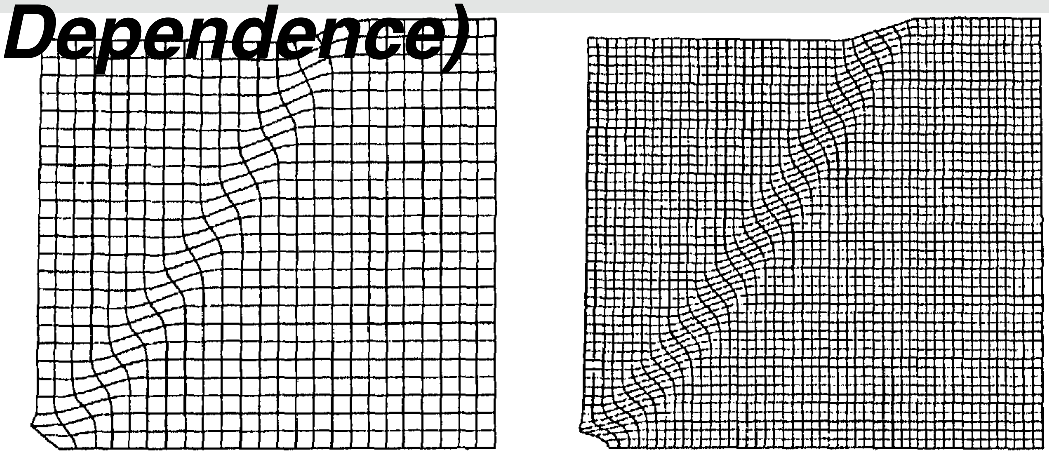


FIG. 13. Incremental deformation patterns for the medium and fine mesh ($l = 0.02$ m).

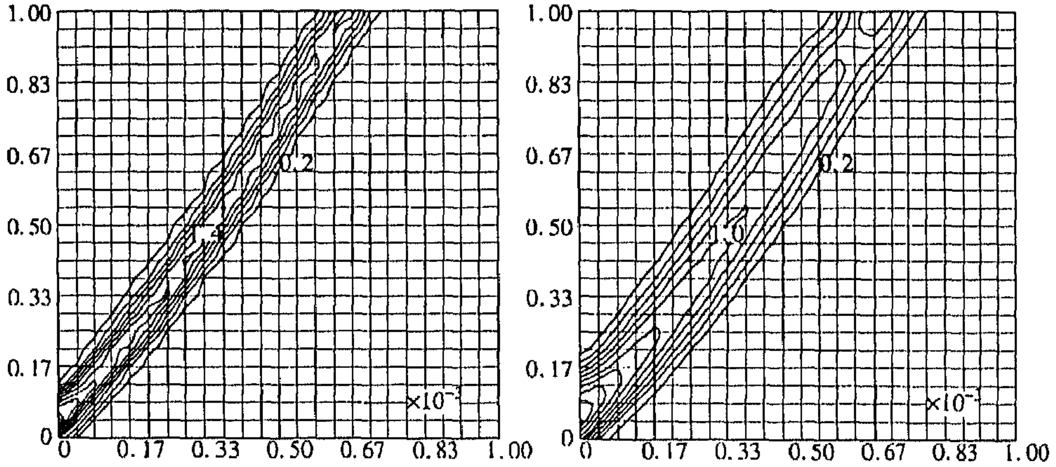
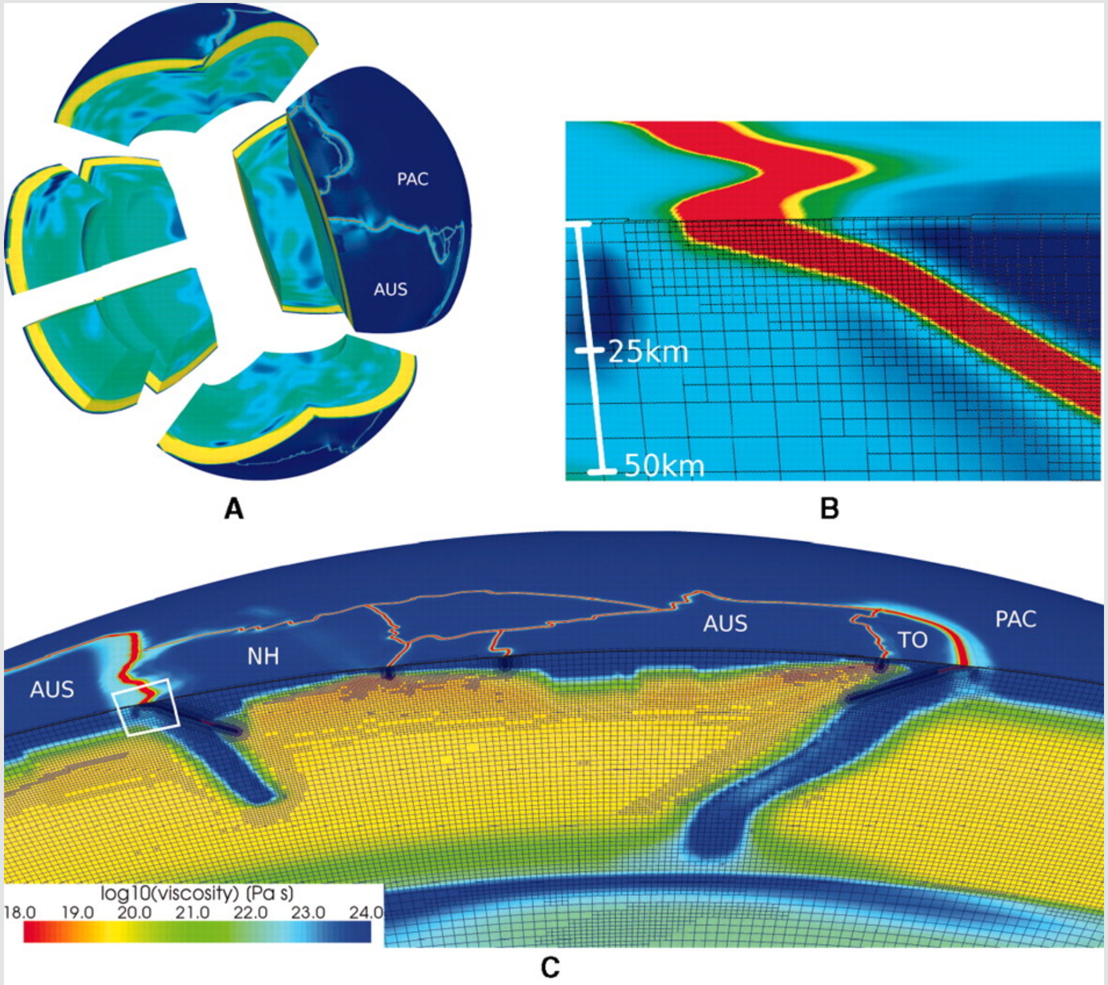


FIG. 14. Contour plots of equivalent plastic strain for $l = 0.02$ m (left) and $l = 0.04$ m (right).

Solution: Introduce a characteristic length-scale!

Pamin and De Borst (1995), *Archives of Mechanics* **45**, p. 353-377

Challenges: Validation & Scaling



Solution: AMR

Adaptive Mesh Refinement

Advantages

- Significantly reduce model size
- Focus on regions of interest

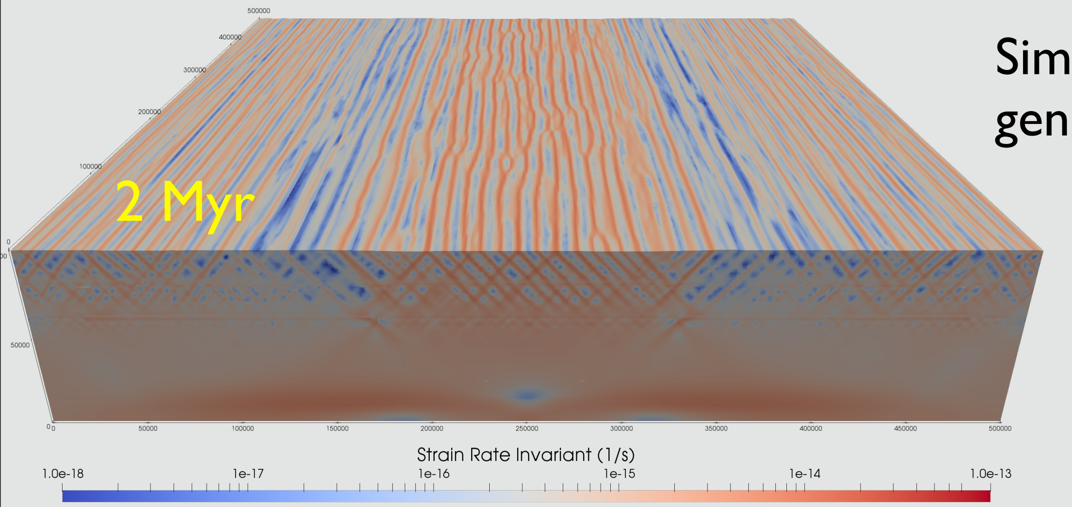
Disadvantages

- Reduced time-step size
- Mesh-dependent rheology?

The Dynamics of Plate Tectonics and Mantle Flow: From Local to Global Scales (Stadler et al., 2010)

Challenges: Validation

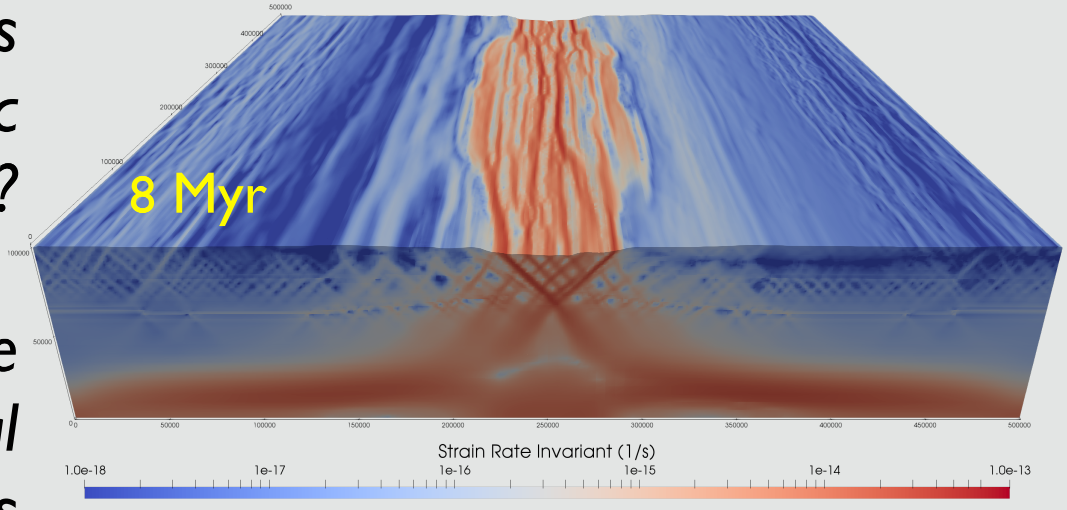
Uncertainty (Interpretation & Uniqueness)



Simulations qualitatively reproduce general observations. However, ….

Model criticisms
- ✓ Low-resolution (2.5 km)
- ✓ Initial conditions play key role
- ✓ ‘Simple’ rheology
- ✓ Simplified boundary conditions

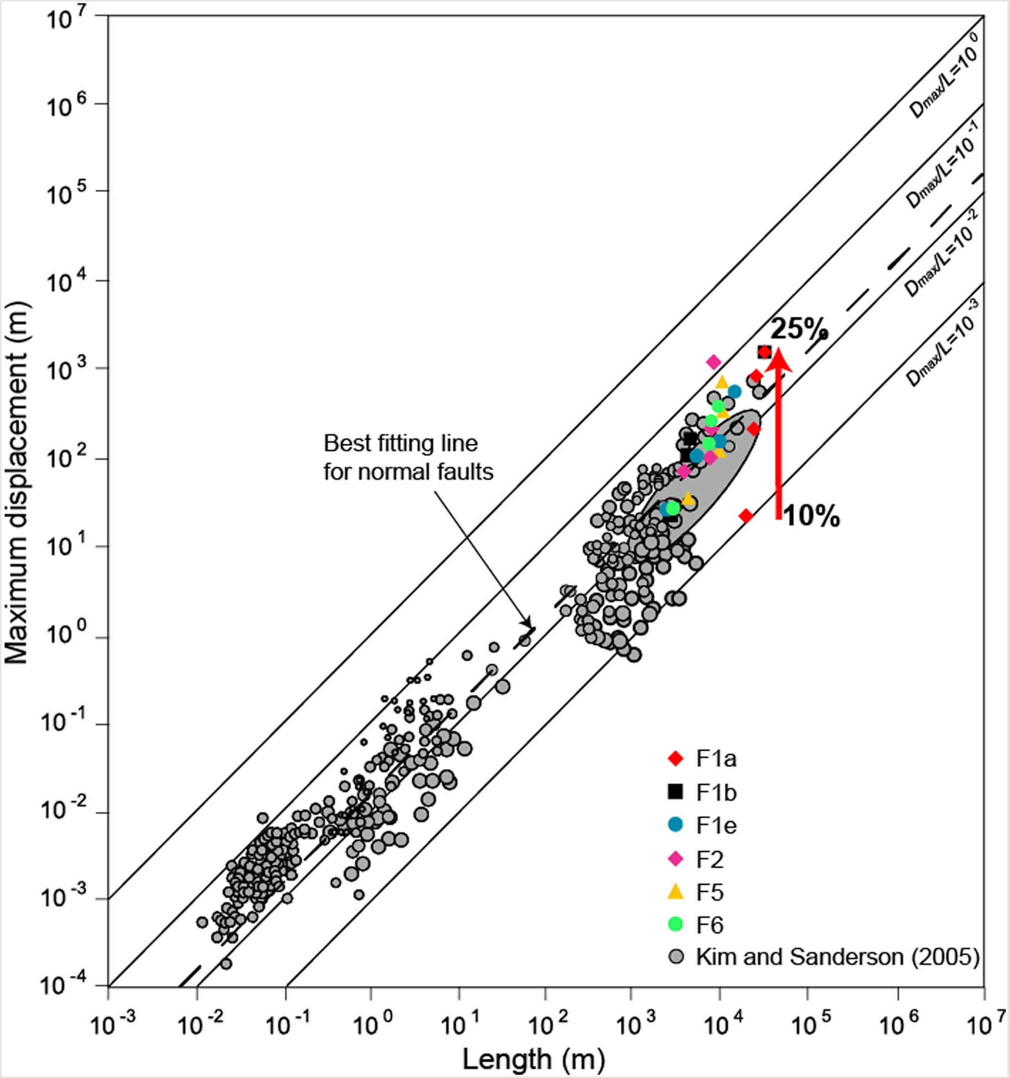
Are these results relevant to lithospheric processes?



… requires quantitative comparisons to natural observations

Challenges: Validation

Solution: Quantitative Comparisons to Natural

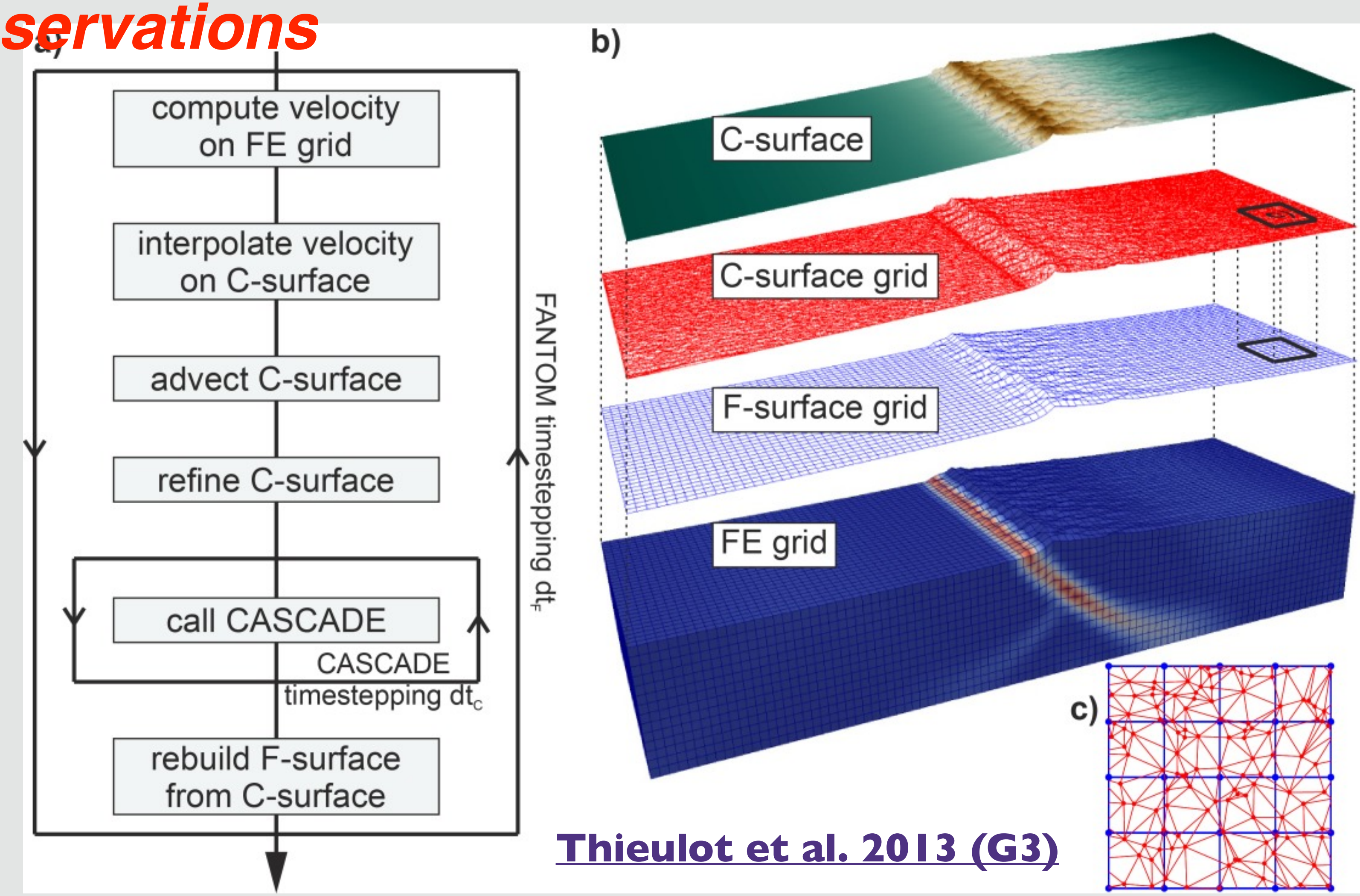


Normal Fault Maximum Displacement verse Length (Modeled & Observed)

[Influence of a pre-existing basement weakness on normal fault growth during oblique extension: Insights from discrete element modeling (Cheng et al., 2017)]

Challenges: Validation

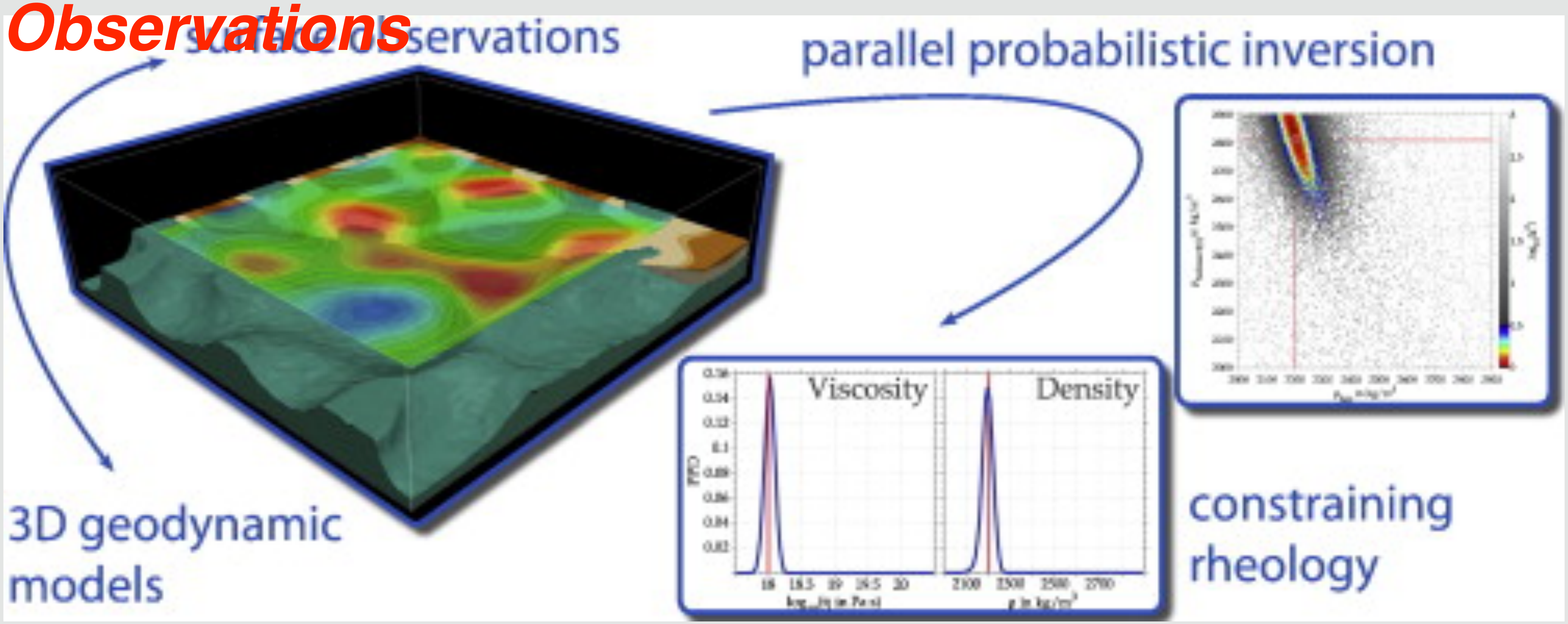
Solution: Quantitative Comparisons to Natural Observations



Thieulot et al. 2013 (G3)

Challenges: Validation

Solution: Quantitative Comparisons to Natural Observations



Baumman, Kaus & Popov:

[Constraining effective rheology through parallel joint geodynamic inversion (2014)]

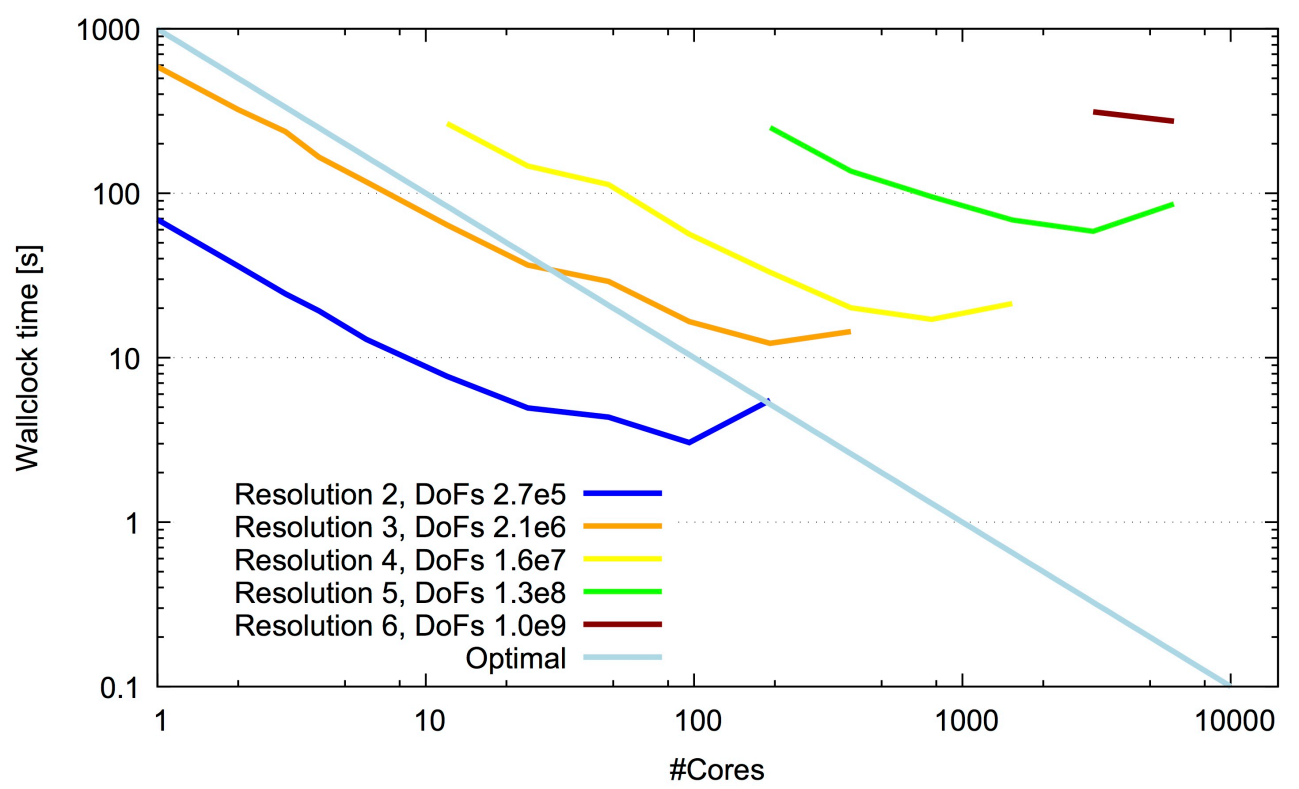
[Geodynamic inversion to constrain the non-linear rheology of the lithosphere (2015)])

Challenges: Computational Resources

<u>High-resolution 3D simulations are computationally expensive</u>

✓One model can require 10^4-10^6 core hours

Solution: Parallelism and Efficient Solvers



<u>Source: CIG software scaling results</u>

Challenges: Computational Resources

High-resolution 3D simulations are computationally expensive

✓One model can require 10^4-10^6 core hours

✓Data processing (visualization, analysis) can require HPC resources

✓Storage requirements: 10^3-10^6 Gigabytes

Solution: NSF Funded HPC Facilities (XSEDE)

❖ Obtain large allocations (computing time) through proposals

❖ Startup allocations provide time for initial testing; CIG Resources

❖ Short-term data storage and visualization (GPU nodes) are available

- Long-term storage and hosting solutions? … TBD

Conclusions and Outlook

- ❖ Multiple open-source and open-access software packages are capable of simulating non-linear lithospheric dynamics in high-resolution 3D models. These models successfully reproduce many commonly observed features and processes.
- ❖ Challenges in <u>validating</u> the numerical models arise from uncertainty in rheological behavior and the scales (time & space) of geologic processes
- ❖ Solution: Quantitative comparisons between model results & observations
  - 3D and time-dependent comparisons are ideal
  - Multi-physics (e.g., surface, igneous & metamorphic processes) simulations enable more detailed comparisons, but also introduce additional uncertainty.