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INTUITIVE NUMERICAL MODELLING IN STRUCTURAL GEOLOGY AND TECTONICS

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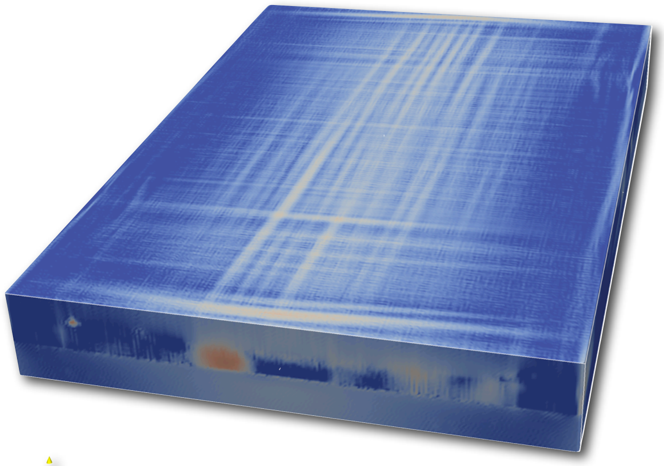
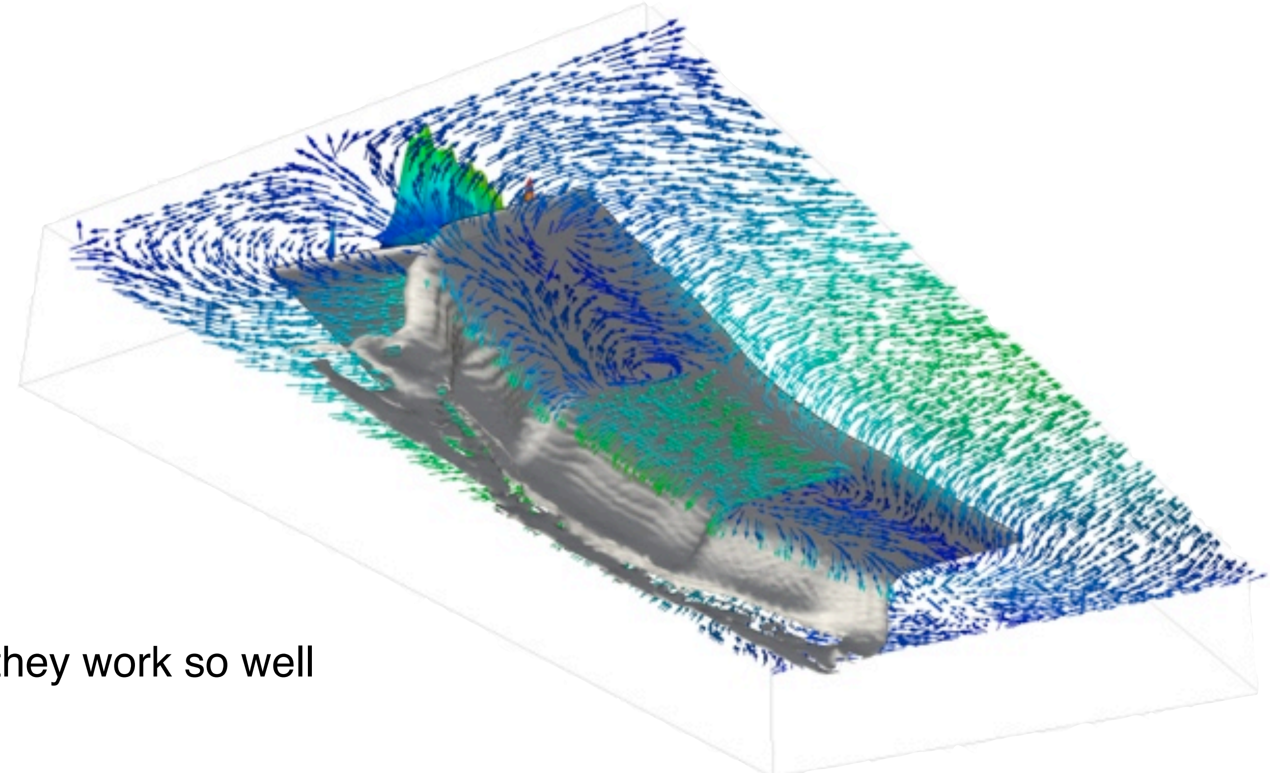
Auscope

Simulation, Analysis, Modelling Group

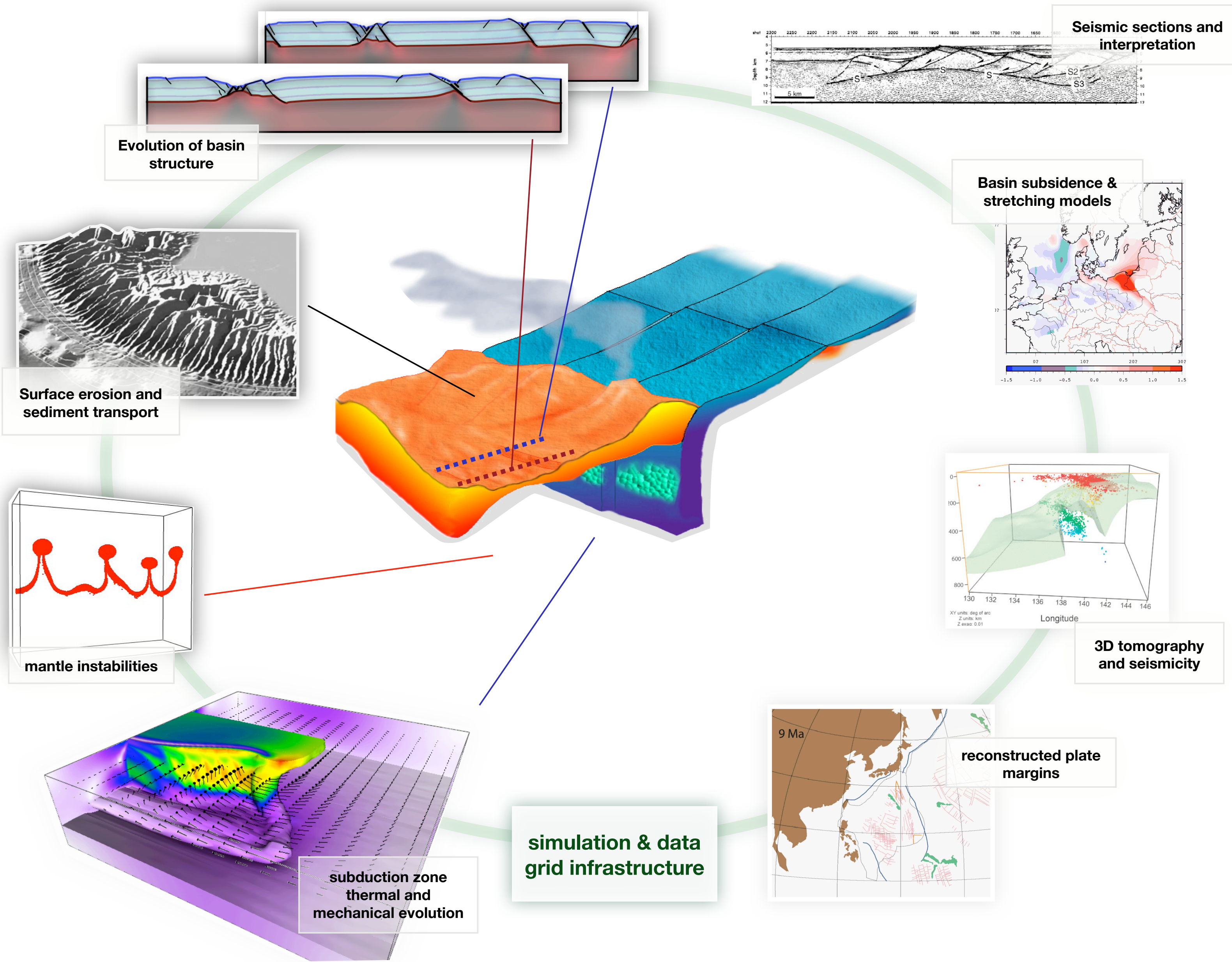


Overview

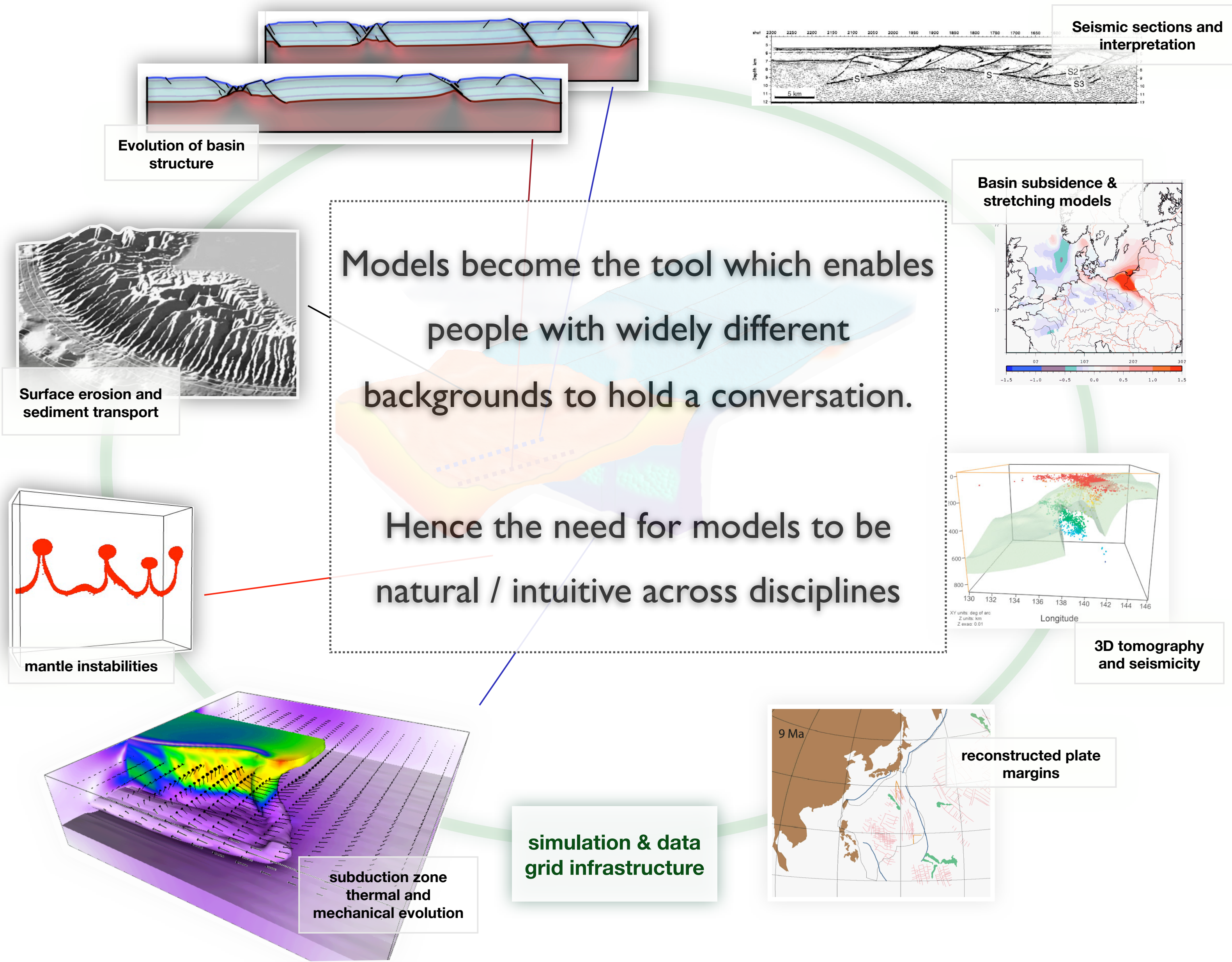


- Intuitive model building
  - Bespoke methods
  - Ease of Use
  - Ease of interpretation
  - Accessibility of HPC
- Particle methods & why they work so well
- Examples
  - Shear banding
  - Thermal mechanical basin scale models
  - Subduction Zones
- Where to from here ?

Vision in 2005 — integrated geodynamic modelling



Vision in 2005 — integrated geodynamic modelling



What is intuitive modelling ?

mental model

simplified conceptual model

model realisation

model analysis

What is intuitive modelling ?

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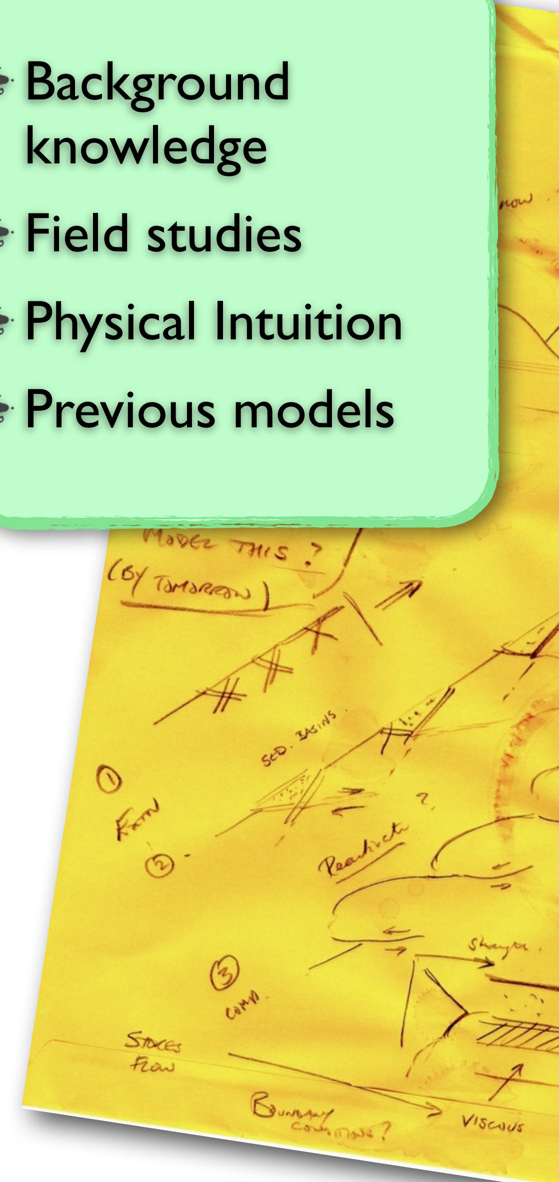
model realisation

model analysis

- Background knowledge
- Field studies
- Physical Intuition
- Previous models



What is intuitive modelling ?

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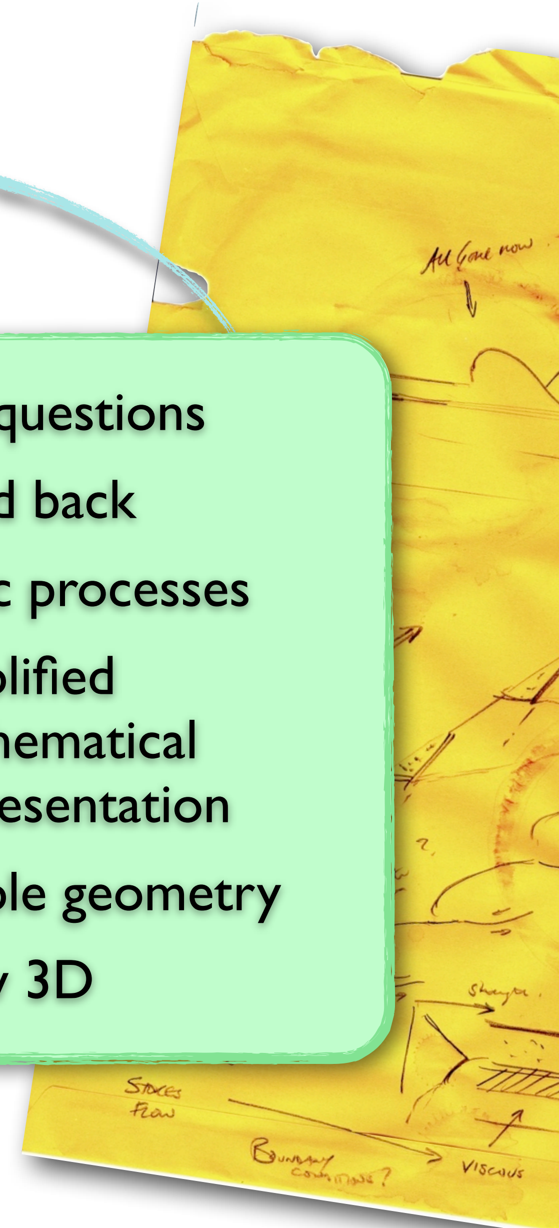
model analysis

- Simple questions
- Stripped back
  - Basic processes
  - Simplified mathematical representation
  - Simple geometry
  - 2D v 3D



What is intuitive modelling ?

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- Faithful to conceptual model
  - Accurate
  - Robust
  - Simple to implement
- Doesn't fight back

What is intuitive modelling ?

mental model

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model realisation

model analysis

- Fit to observations
- Sensitivity to model parameters
- Thought provoking
- Proves you wrong if you are !

Recipe for crust/mantle deformation

Shopping list

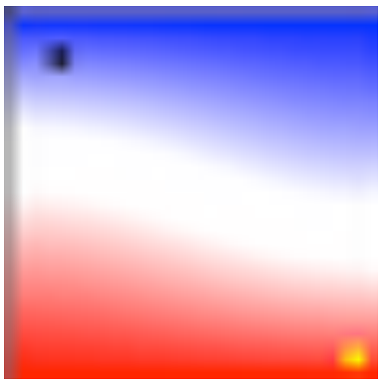
- Rheology
  - Viscoelasticity
  - Plasticity (continuum failure model)
  - Strain history dependence
- Compositional boundaries
- Thermal diffusion and large-scale mantle buoyancy evolution
- Systems evolve over multiple overturn times
- Large scale / high resolution — efficient, robust, fast solvers needed

More usually considered in this context using Lagrangian solid mechanics formulation (deforming grid)

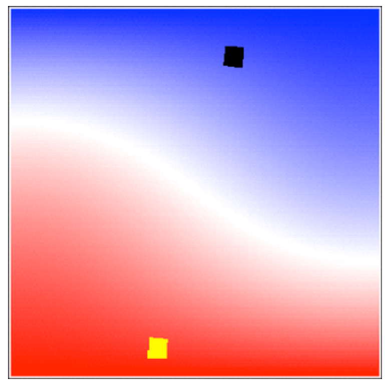
These can be dealt with very naturally if we formulate the problem from an Eulerian incompressible viscous fluid-dynamics perspective (with elasticity as a “correction” ...)

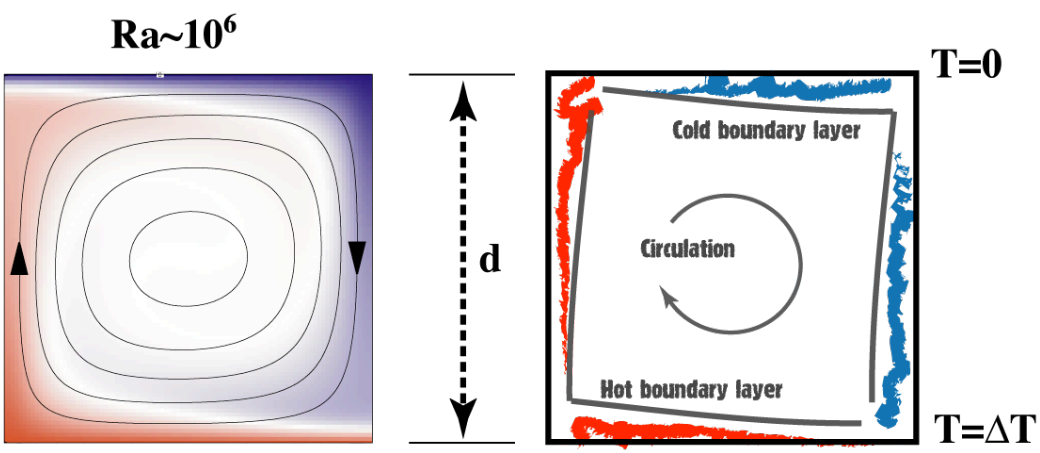
Deformation during fluid-like deformation

$\mathrm{Ra} = 10^5$



$\mathrm{Ra} = 10^7$



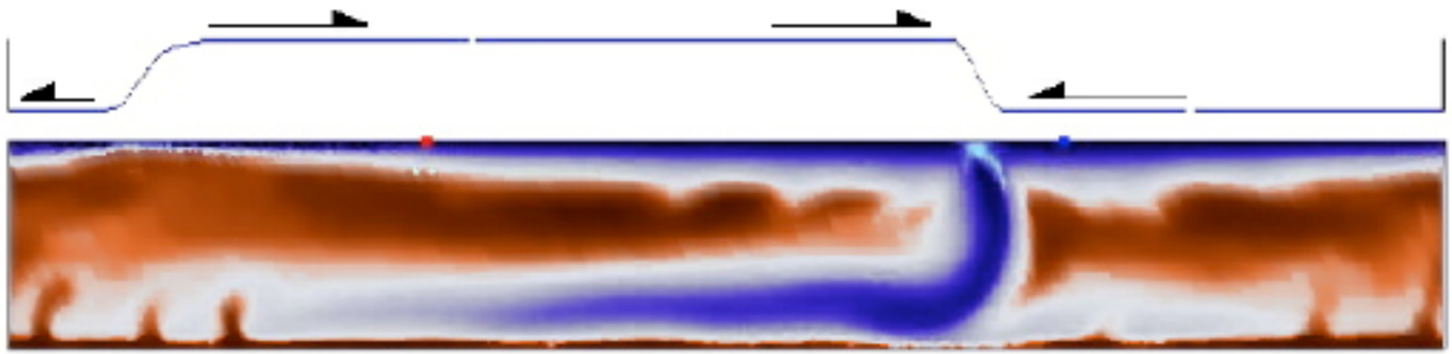


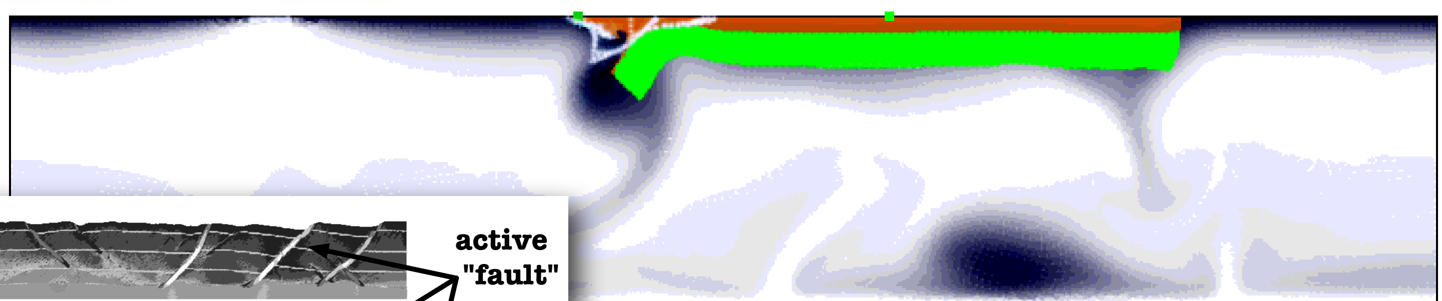
This is a Rayleigh-Bénard convection model which evolves to a straightforward balance between thermal diffusion and thermal advection in narrow boundary layers.

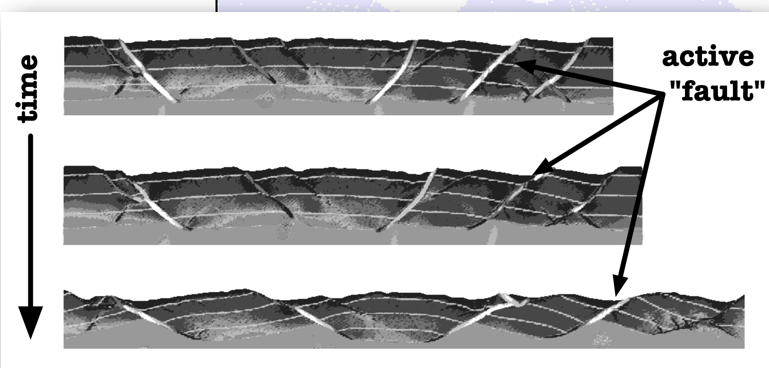
At modest Rayleigh number, the structure which develops is steady despite strongly developed convective flow.

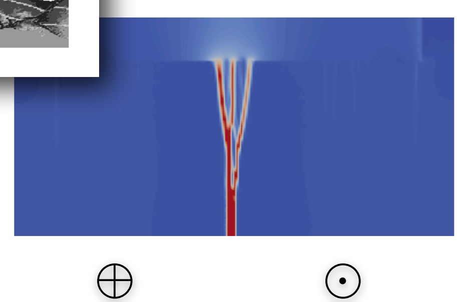
This system can be solved very efficiently on a fixed mesh

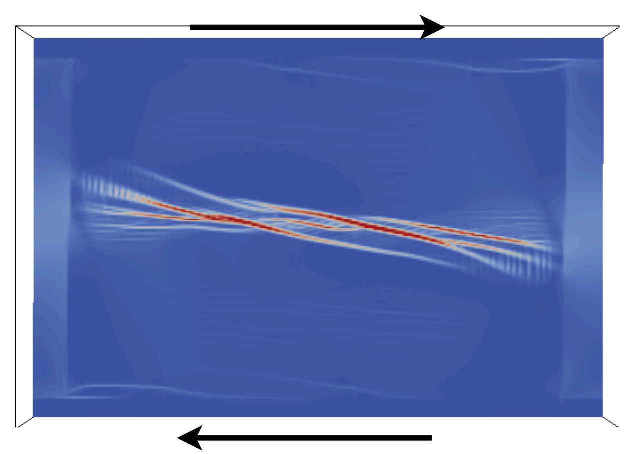
Strain softening plasticity — an example of history dependence











Strain softening plasticity — an example of history dependence

The material weakens locally and carries the history of deformation / softening with it through the fluid flow

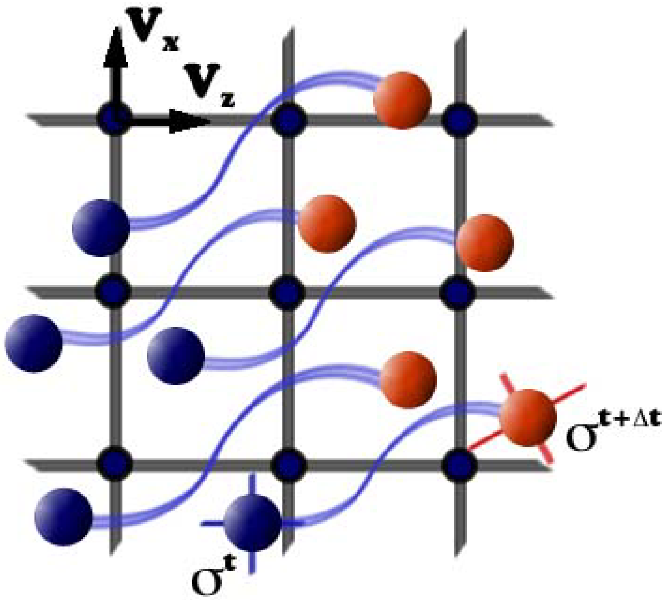
Generally:

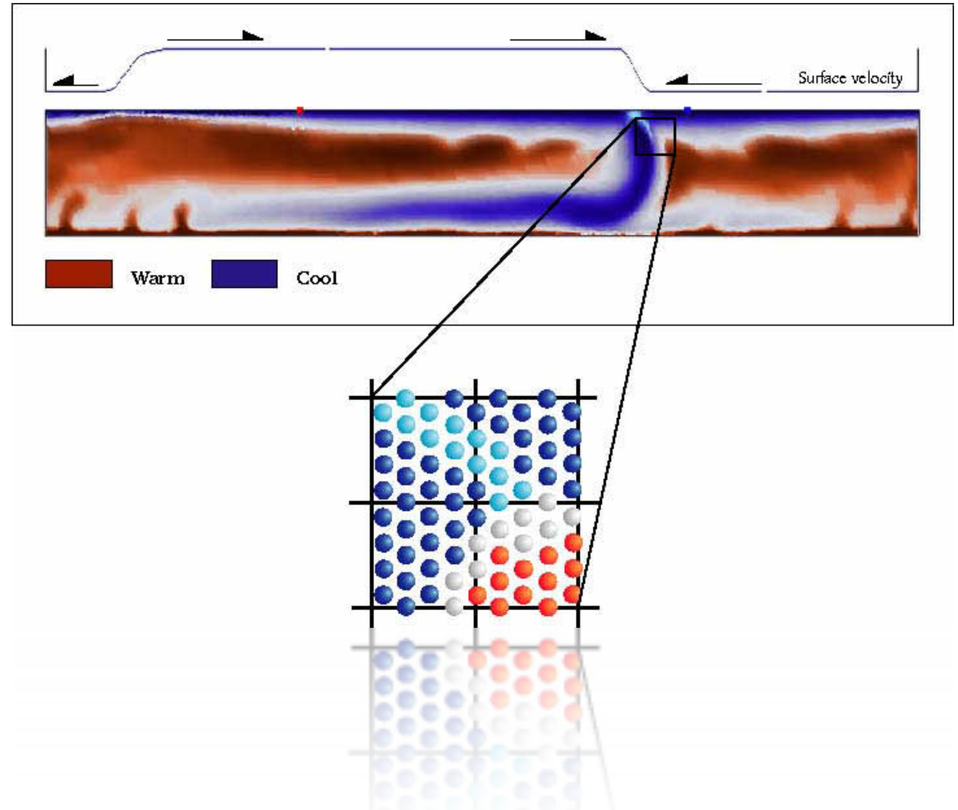
Material interfaces and stresses are carried / rotated by the broad scale flow and deformed by the local flow gradients

Material properties are often history dependent — we need to be able to track individual parcels of material as they deform.

Structure is emergent and complicated — meshing / remeshing based methods are not ideal

A solution – keep both views of the problem

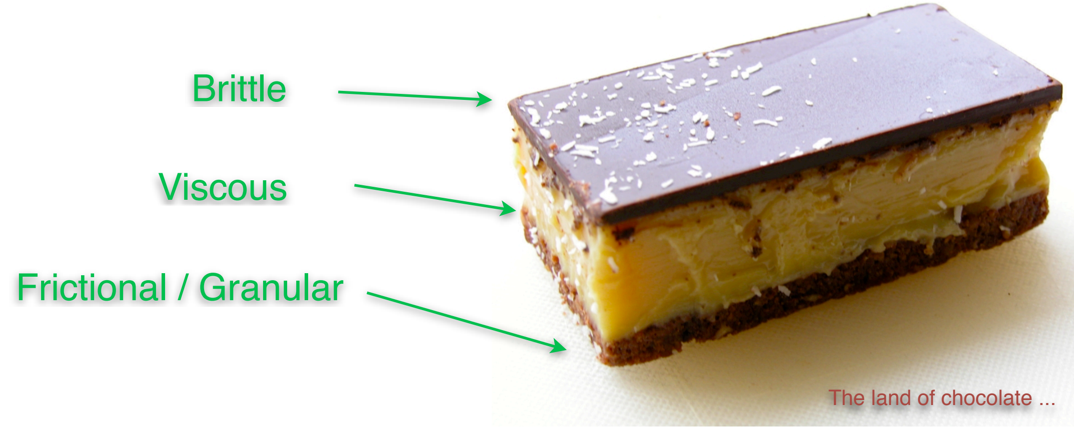




In the **material point method** we can keep a mesh which is computationally efficient for diffusion-dominated problems (including Stokes flow) and material points — a.k.a. particles — for tracking history variables.

This is the technique implemented in Underworld / Gale and leads to a very natural approach to many “difficult” issues in geological thermal / mechanical models (www.underworldproject.org)

Recipe for crust/mantle deformation — part 2



$$\nabla \boldsymbol{\tau} - \nabla p = \boldsymbol{g}\rho(C, T, \boldsymbol{\varepsilon}, \ldots) - \nabla f^{\Delta t}$$

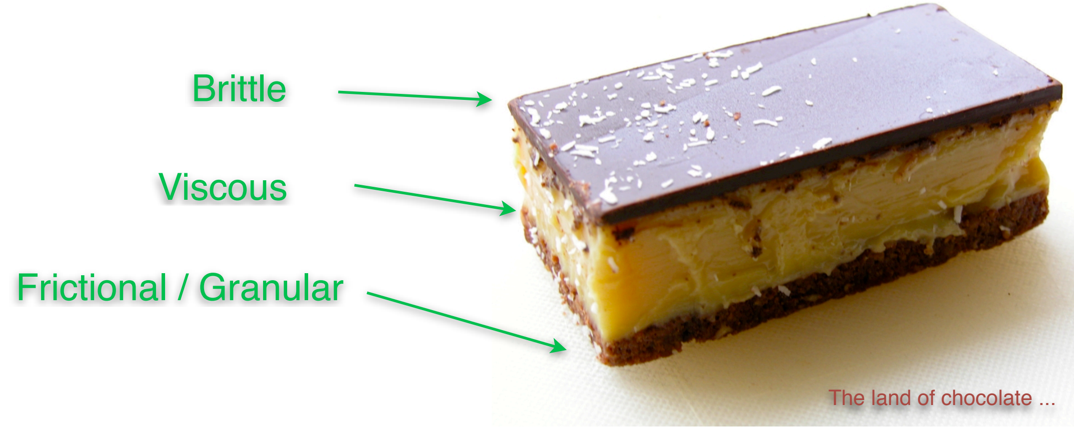
$$\nabla \cdot \boldsymbol{u} = 0$$

Balance viscous / visco-elastic stresses with buoyancy forces

Slow flow: Quasi-static approximation — no acceleration terms

Prescribed volume / density changes

Recipe for crust/mantle deformation — part 2

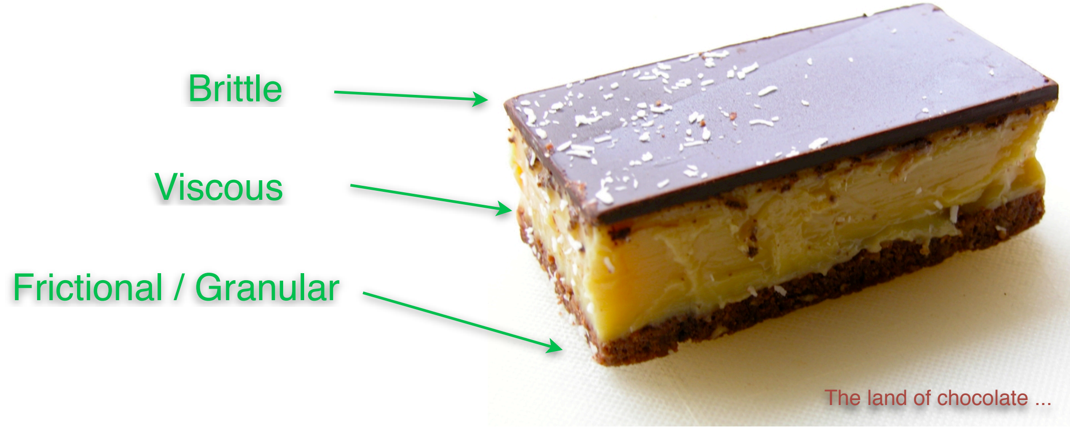


$$\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T = \kappa \nabla^2 T + Q + \ldots$$

Thermal evolution

- balance heat transport, thermal diffusion, heat production
- time dependence of buoyancy in force balance equation

Recipe for crust/mantle deformation — part 2

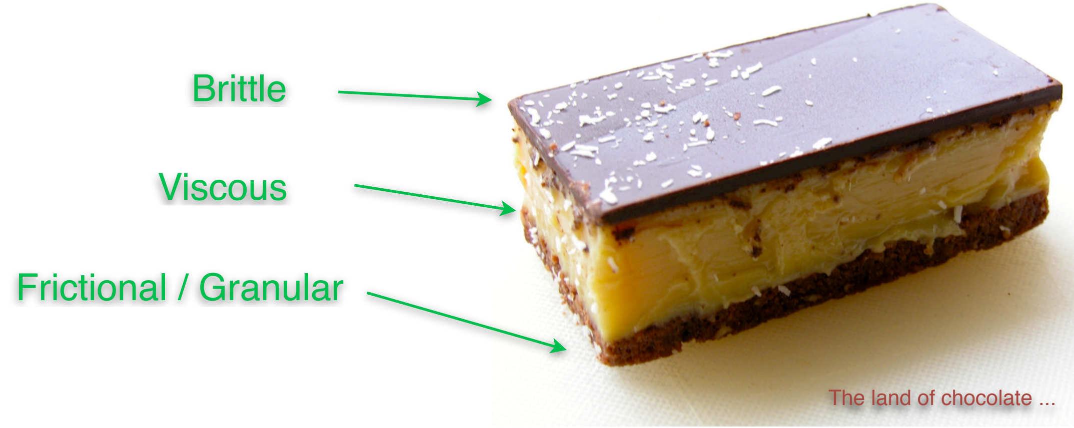


$$\frac{\overset{\triangledown}{\tau}_{ij}}{\mu} + \frac{\tau_{ij}}{\eta} + \alpha \Lambda_{ijkl} \tau_{kl} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}$$

Constitutive law — viscoelastic / plastic (fluid dynamics approach)

- Time dependence: stress history and strain history
- Anisotropic — plasticity (and fabric development)

Recipe for crust/mantle deformation — part 2



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Constitutive law — viscoelastic / plastic (fluid dynamics approach)

- Time dependence: stress history and strain history
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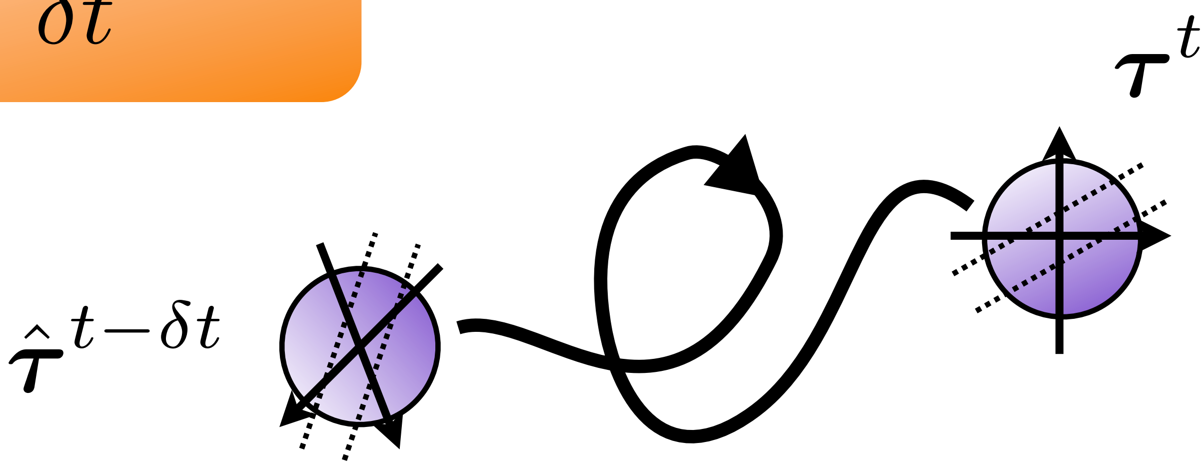
Example: A "natural" way to deal with stress rate

$$\overset{\triangledown}{\boldsymbol{\tau}} = \lim_{\delta t \to 0} \frac{\boldsymbol{\tau}^{t} - \hat{\boldsymbol{\tau}}^{t-\delta t}}{\delta t}$$



Two ways to deal with this term

- Mathematical expansion followed by complicated numerical implementation
- Physically intuitive approach and simple numerical implementation

Viscoelasticity — stress rate

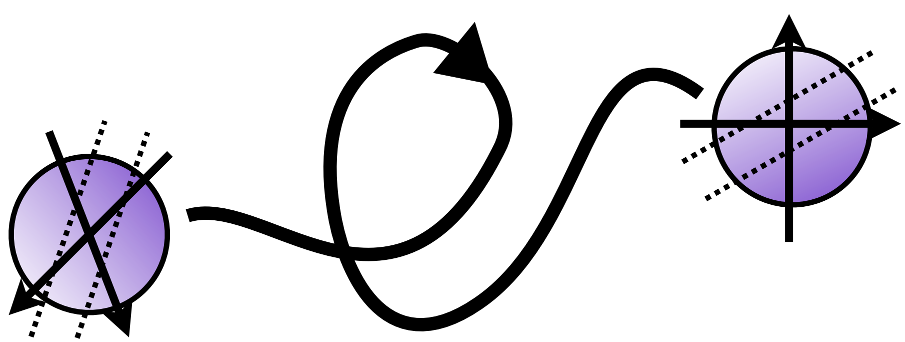
$$\overset{\triangledown}{\boldsymbol{\tau}}_{ij} = \frac{\partial \tau_{ij}}{\partial t} + \tau'_{ij}$$

$$\tau'_{ij} = u_k \frac{\partial \tau_{ij}}{\partial x_k} + \tau_{ik} W_{kj} - W_{ik} \tau_{kj} + a(\tau_{ik} D_{kj} + D_{ik} \tau_{kj})$$

Translation of stress along the flow path

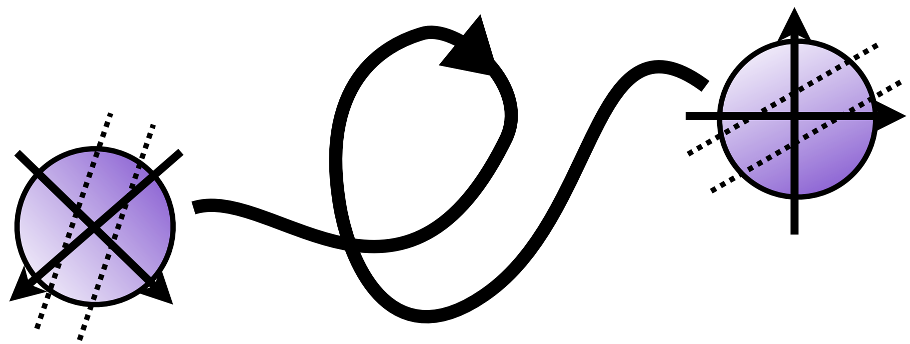
Rotation of the stress along the flow path

Changes in stress due to shearing along flow path (*a* is a constitutive parameter)



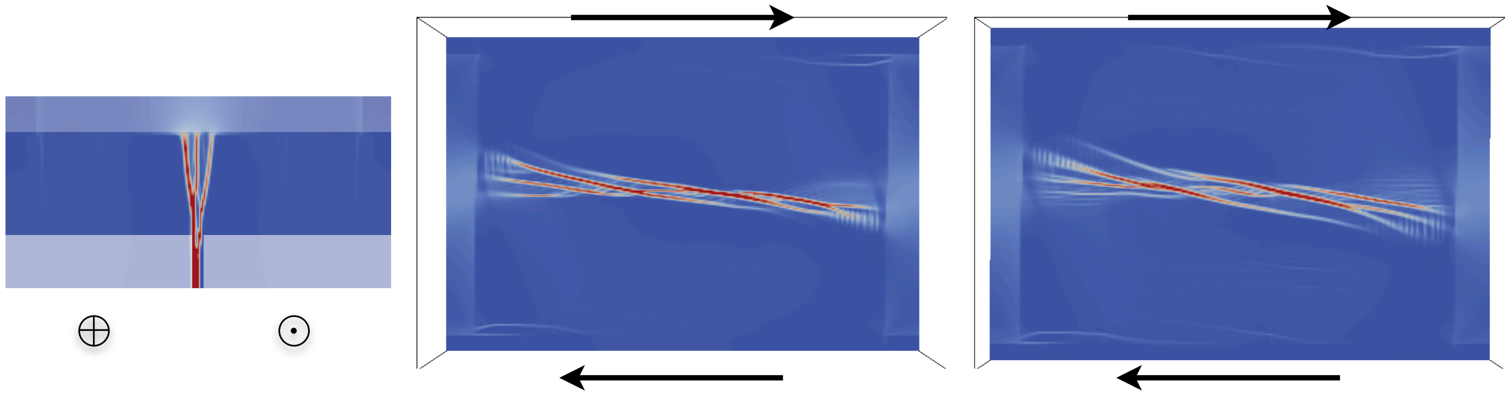
Jaumann derivative in difference form

$$\overset{\triangledown}{\boldsymbol{\tau}} = \lim_{\delta t \to 0} \frac{\boldsymbol{\tau}^{t} - \hat{\boldsymbol{\tau}}^{t-\delta t}}{\delta t} \approx \frac{\boldsymbol{\tau}^{t} - \boldsymbol{\tau}^{t \hat{-} \Delta t}}{\Delta t}$$



Where the difference is now between a **stored stress on the particle from a previous time with the coordinates appropriately rotated and translated** (tracked particle motion) to the local current coordinates of the particle

Example 1 – shear banding



Examples of strong localization requiring large deformation and high resolution

- Shear banding in 2D and 3D as an analogue for localisation in the crust and lithosphere
- Poorly understood mapping from mathematical description to numerical outcome (orientations,
- Viscoelastic/plastic material under simple shear velocity boundary conditions
  - driven by a “fault” in the basement & side boundary conditions
  - free upper surface
  - strain-softening plasticity

Analogue Models for comparison

Schellart & Nieuwland
Geological Society, London
Special Publications 2003
v. 212; p. 169-179

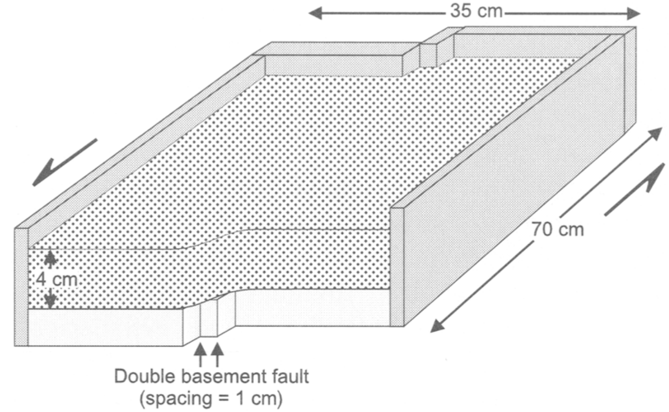
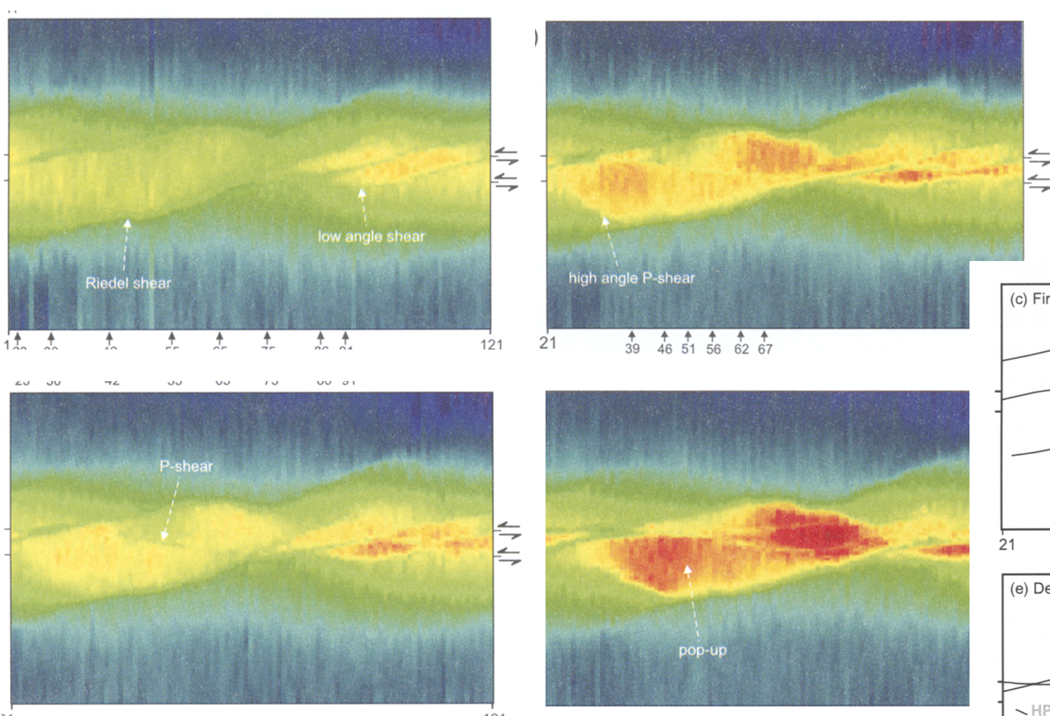
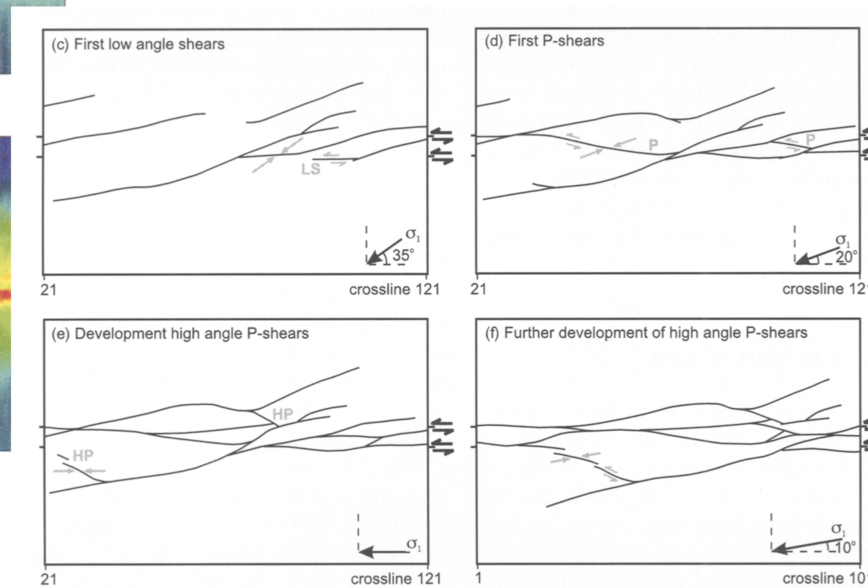


Fig. 1. Model configuration of strike-slip faulting above a double basement fault. Horizontal dimensions are 70 by 35 cm, sediment thickness is 4 cm, sediment used is fine sand (0.075–0.125 mm), double basement fault spacing is 1 cm and sense of shear is sinistral.





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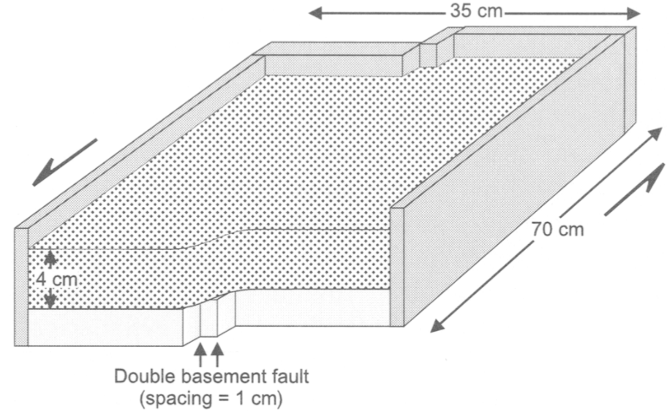
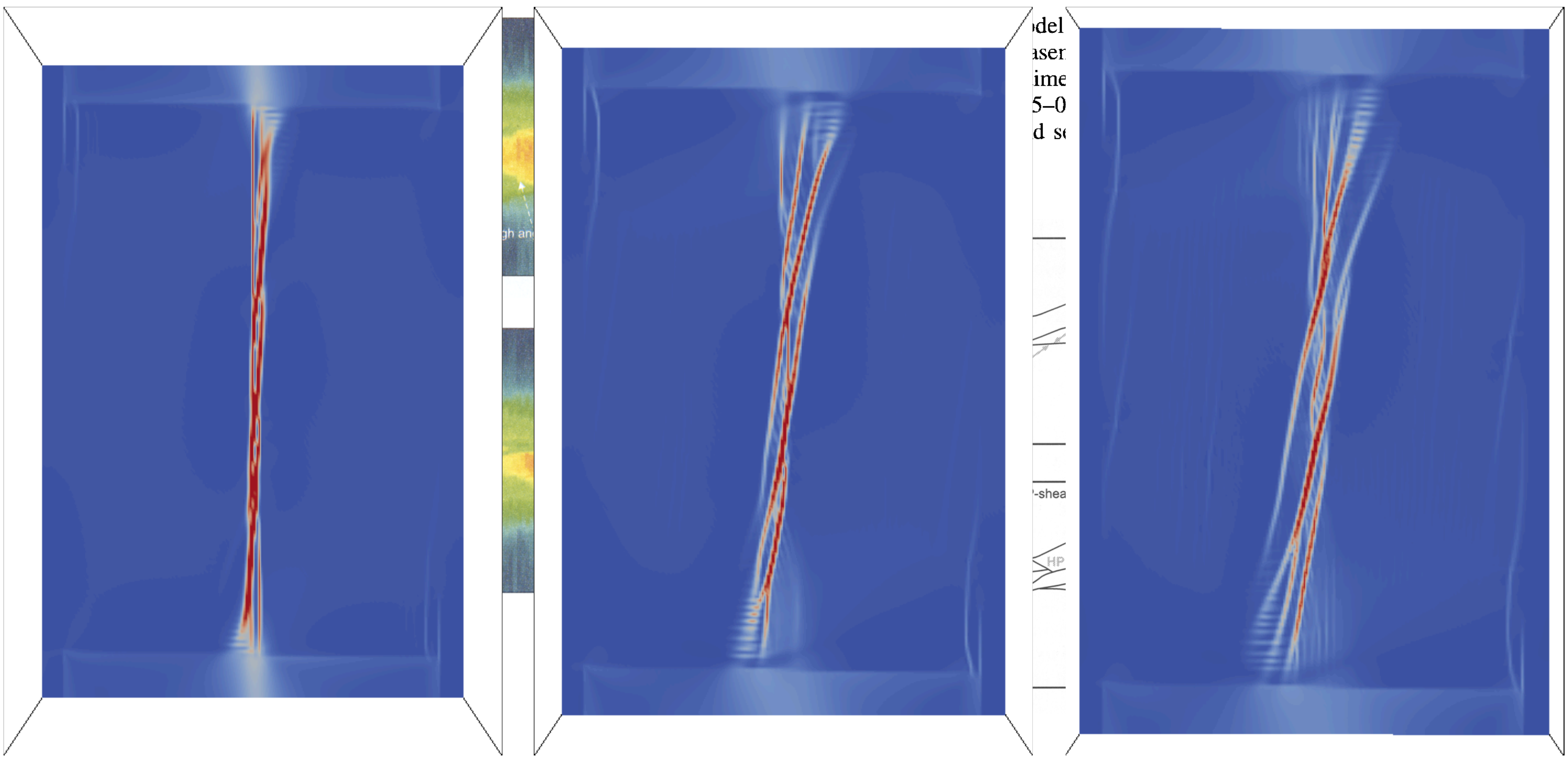
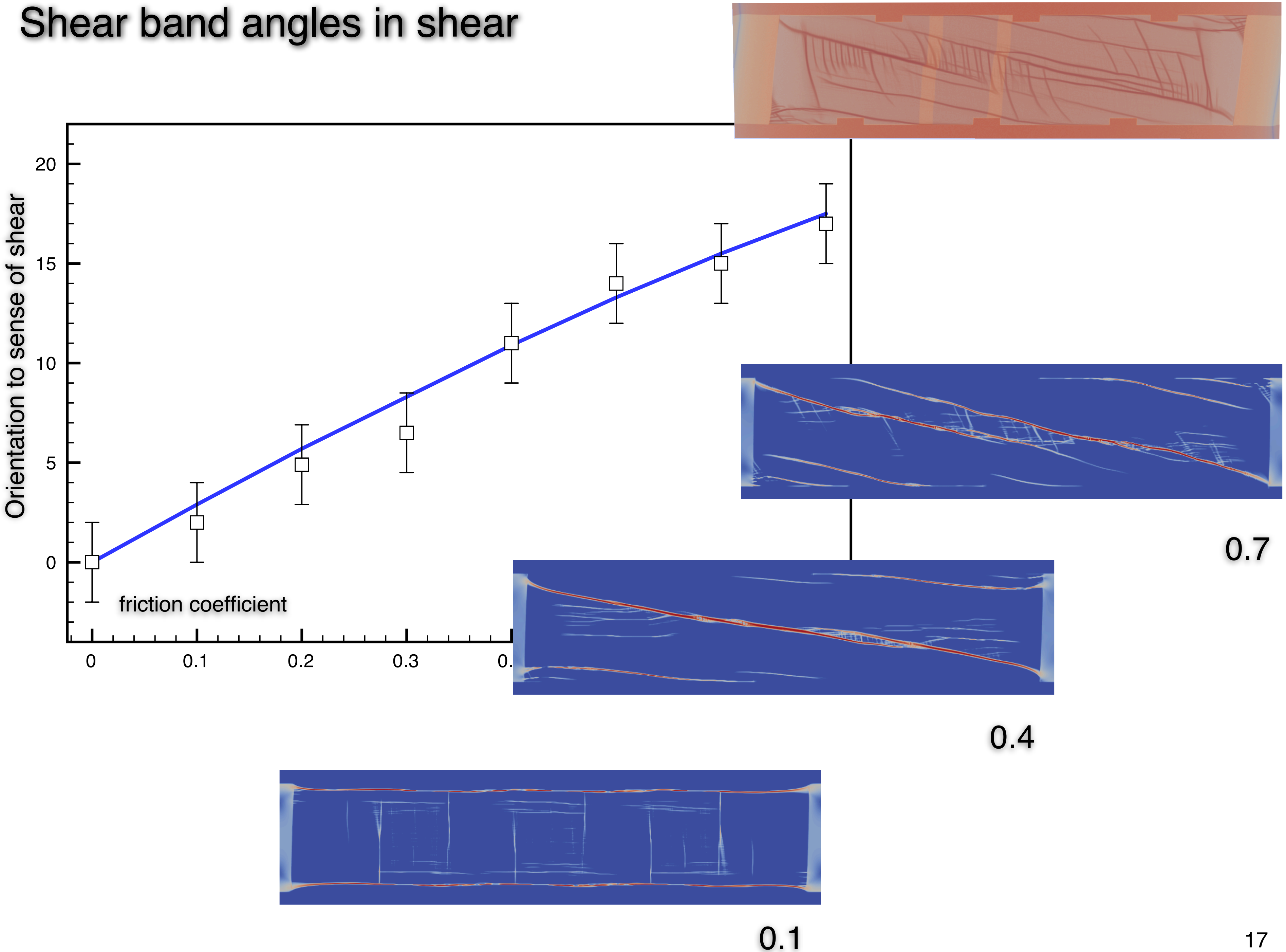




Shear band angles in shear



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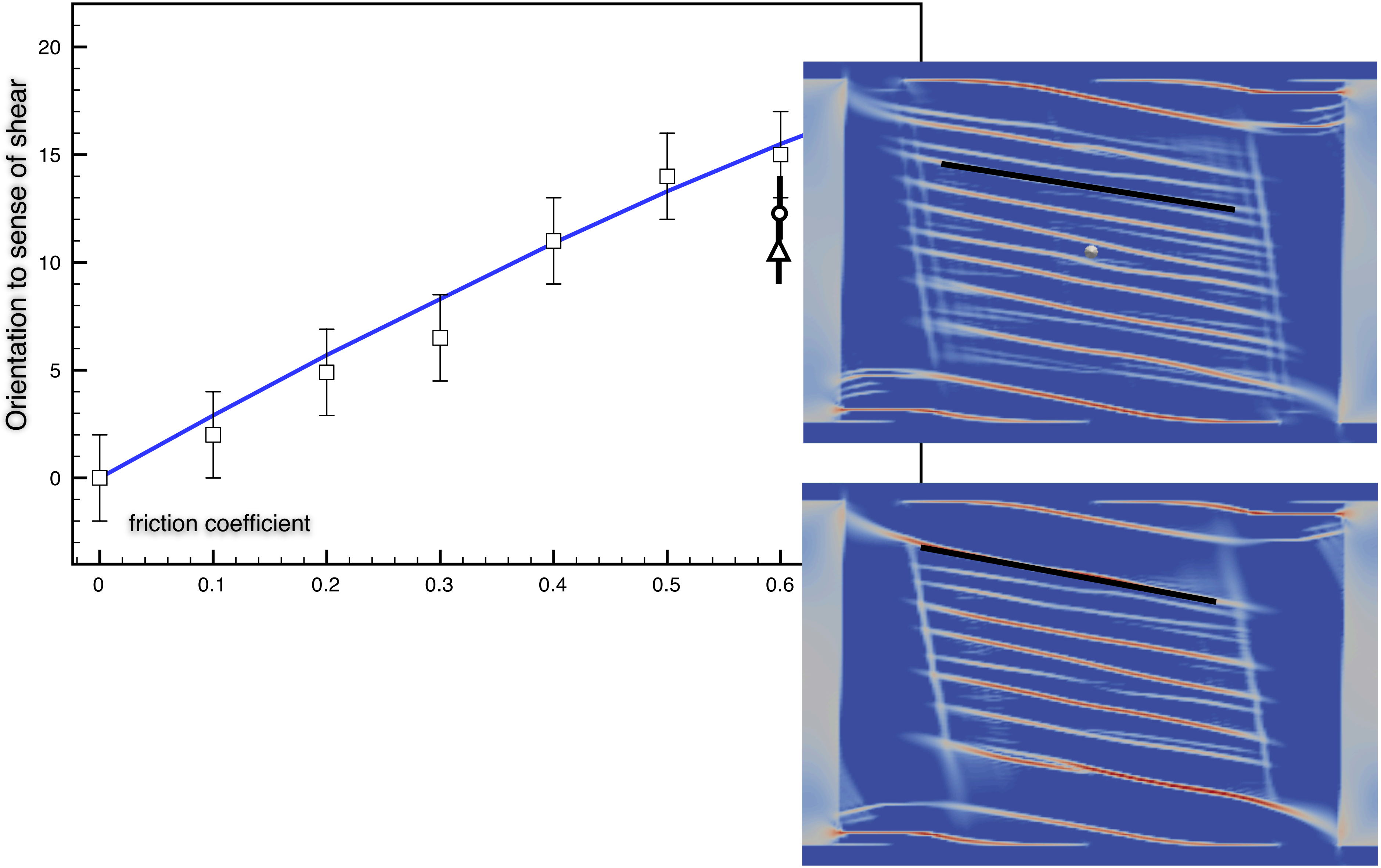
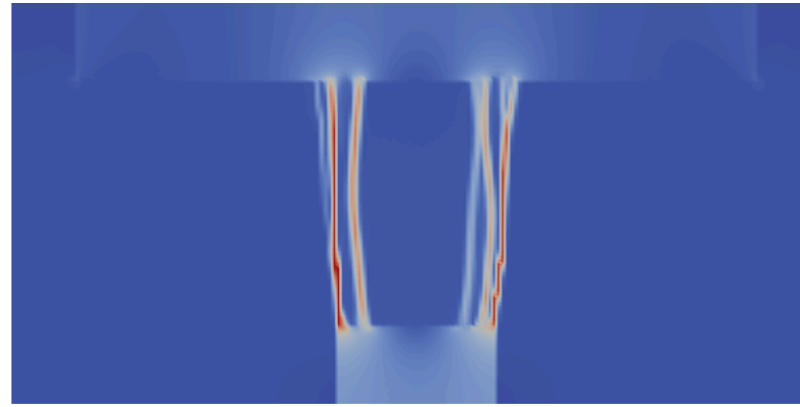
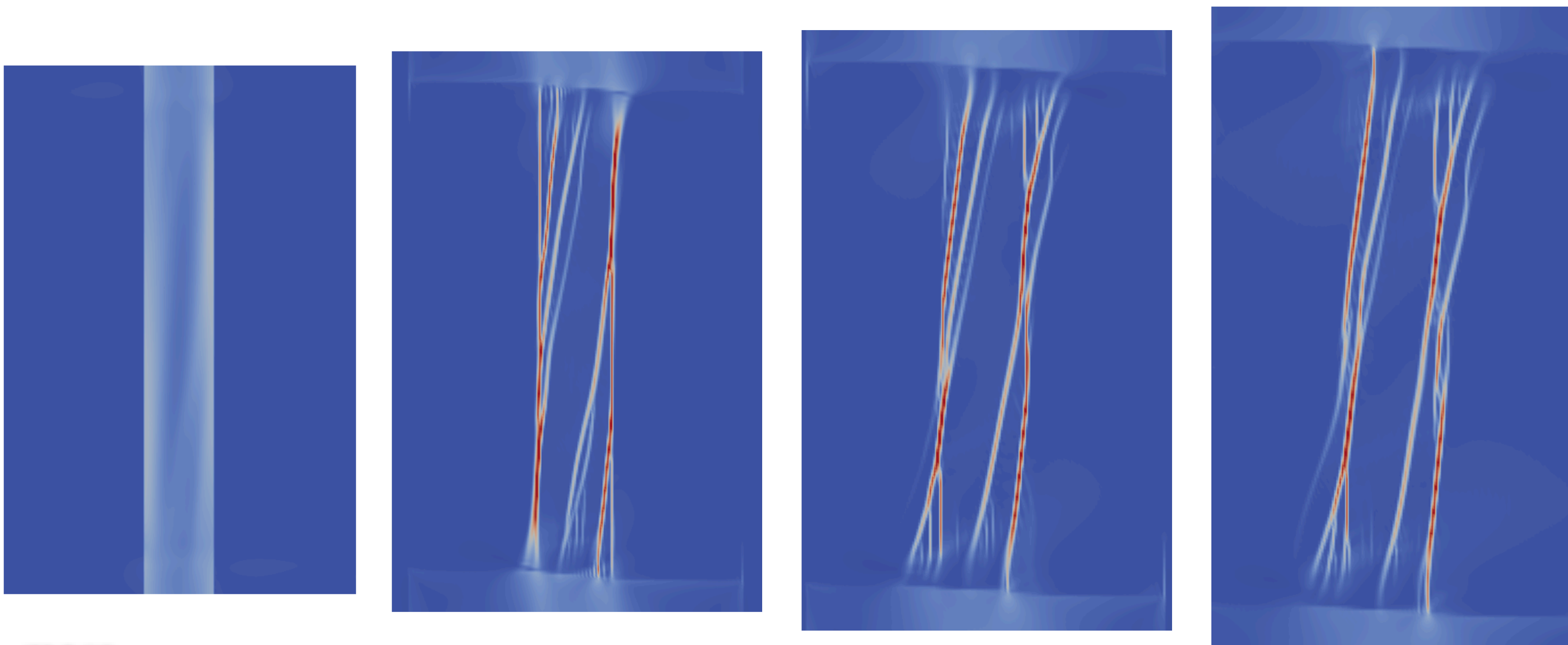


Numerical models with underlying structure

Similar to analogue models

Can we tell what is happening at depth if we look at the surface ?





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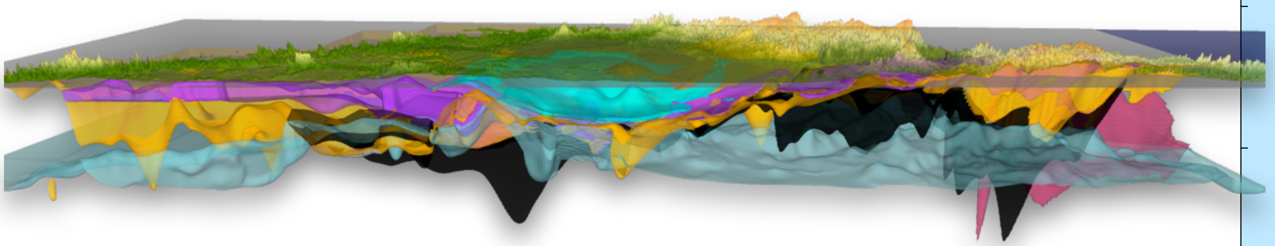
Example 2 – “continent” scale geothermal models



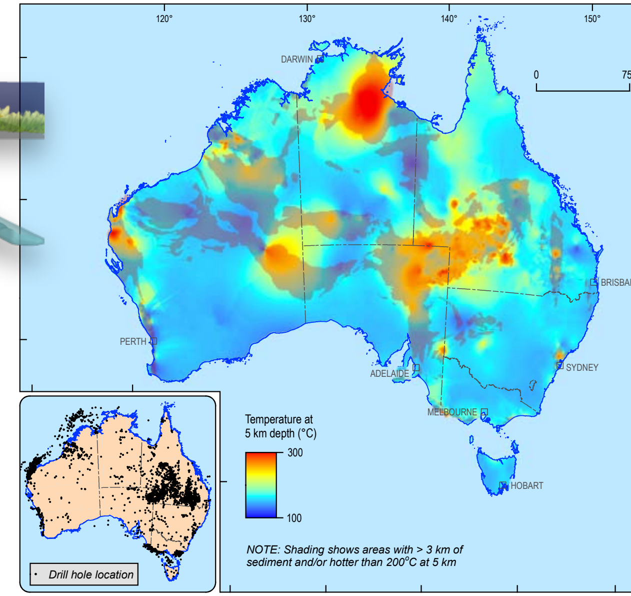
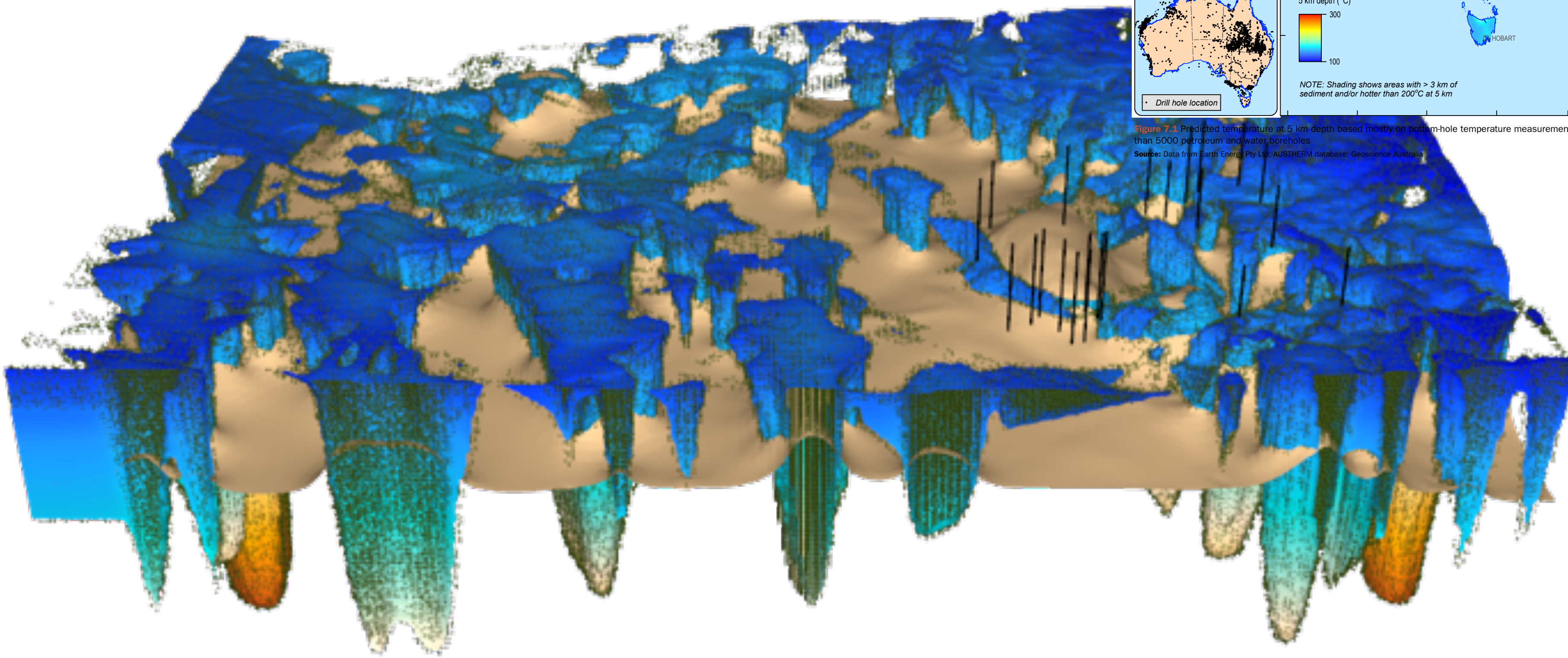


Figure 7.1 Predicted temperature at 5 km depth based mostly on bottom-hole temperature measurements than 5000 petroleum and water boreholes
Source: Data from Earth Energy Pty Ltd; AUSTHERM database; Geoscience Australia

Heat flow models at the 1000km scale

- Current Australian deep-temperature assessment based on horizontally interpolating **2-layer models** from individual sites
  - Assumes 2 layered crustal structure everywhere in Australia
  - Extrapolation to depth (poor choice in heavily insulated basins)
- Incorporating 3D structure — ingest 3D structural models from geophysical interpretation
- Constraints from temperature measurements in drill-holes
- Energy-content assessments for geothermal startup companies
- Risk analysis for management of basins with competing uses (groundwater, geothermal, CO_2 storage, petroleum extraction)

Cooper basin



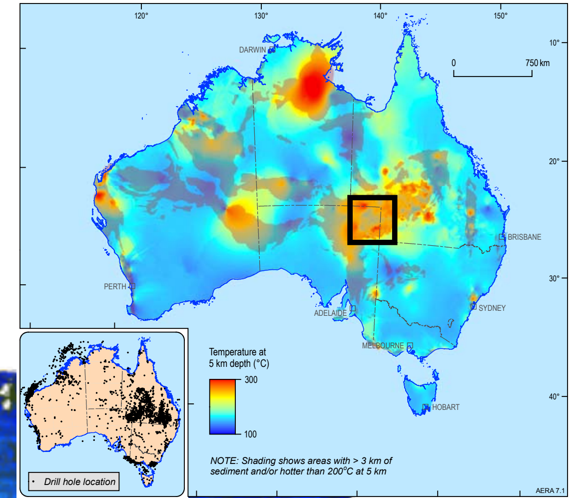
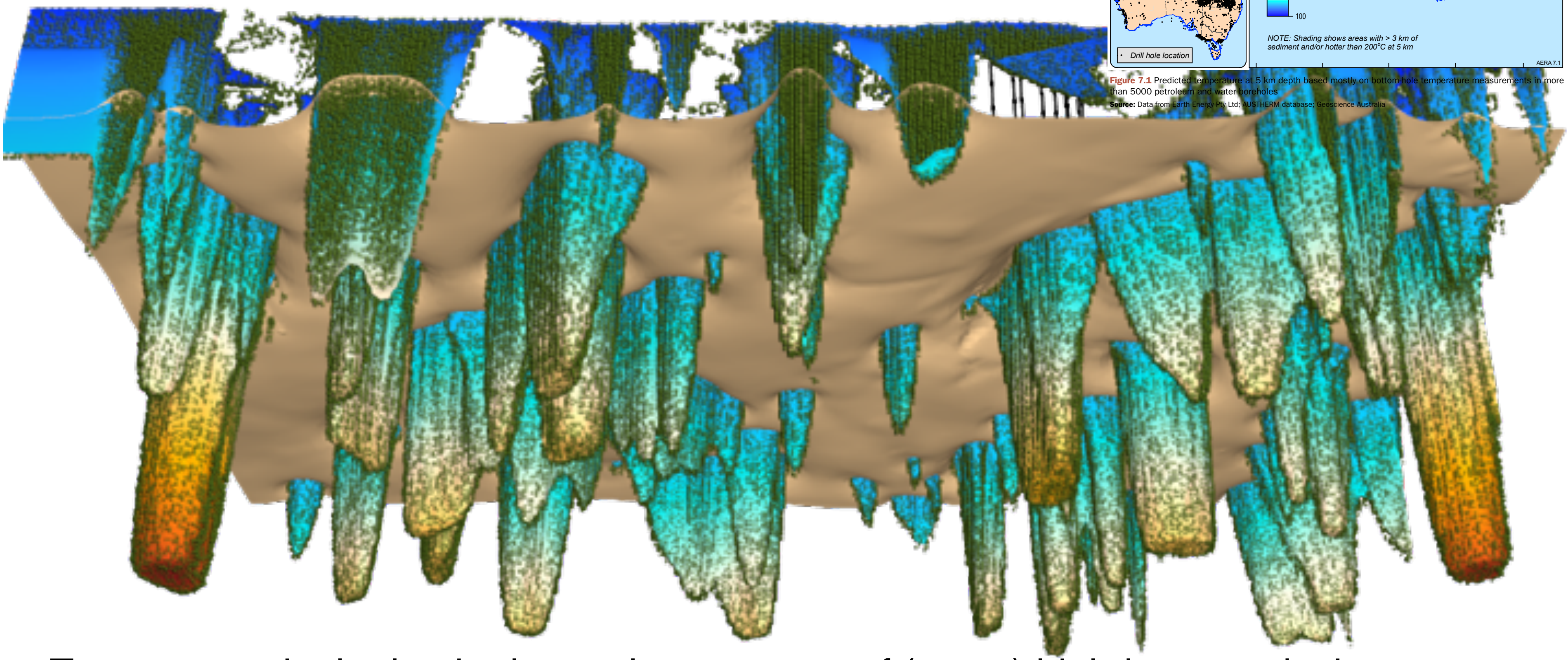


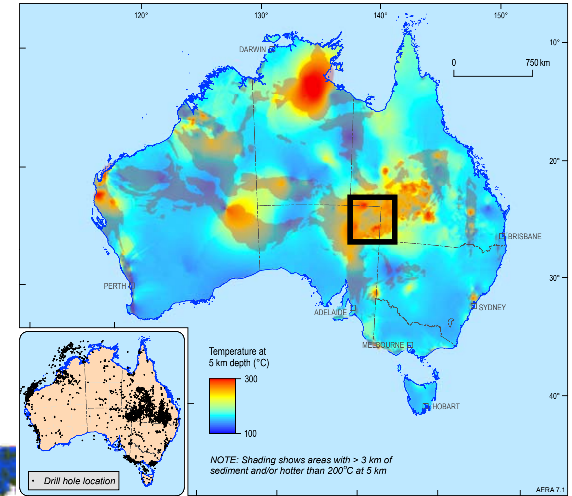
Figure 7.1 Predicted temperature at 5 km depth based mostly on bottom-hole temperature measurements in more than 5000 petroleum and water boreholes

Source: Data from Earth Energy Pty Ltd; AUSTHERM database; Geoscience Australia

Temperature in the basin due to the presence of (some) high-heat producing granites. *Architecture model: Meixner 2009 - https://www.ga.gov.au/products/servlet/controller?event=GEOCAT_DETAILS&catno=68832*

Cooper basin





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FYI: Basin-scale mechanical models

Otway basin

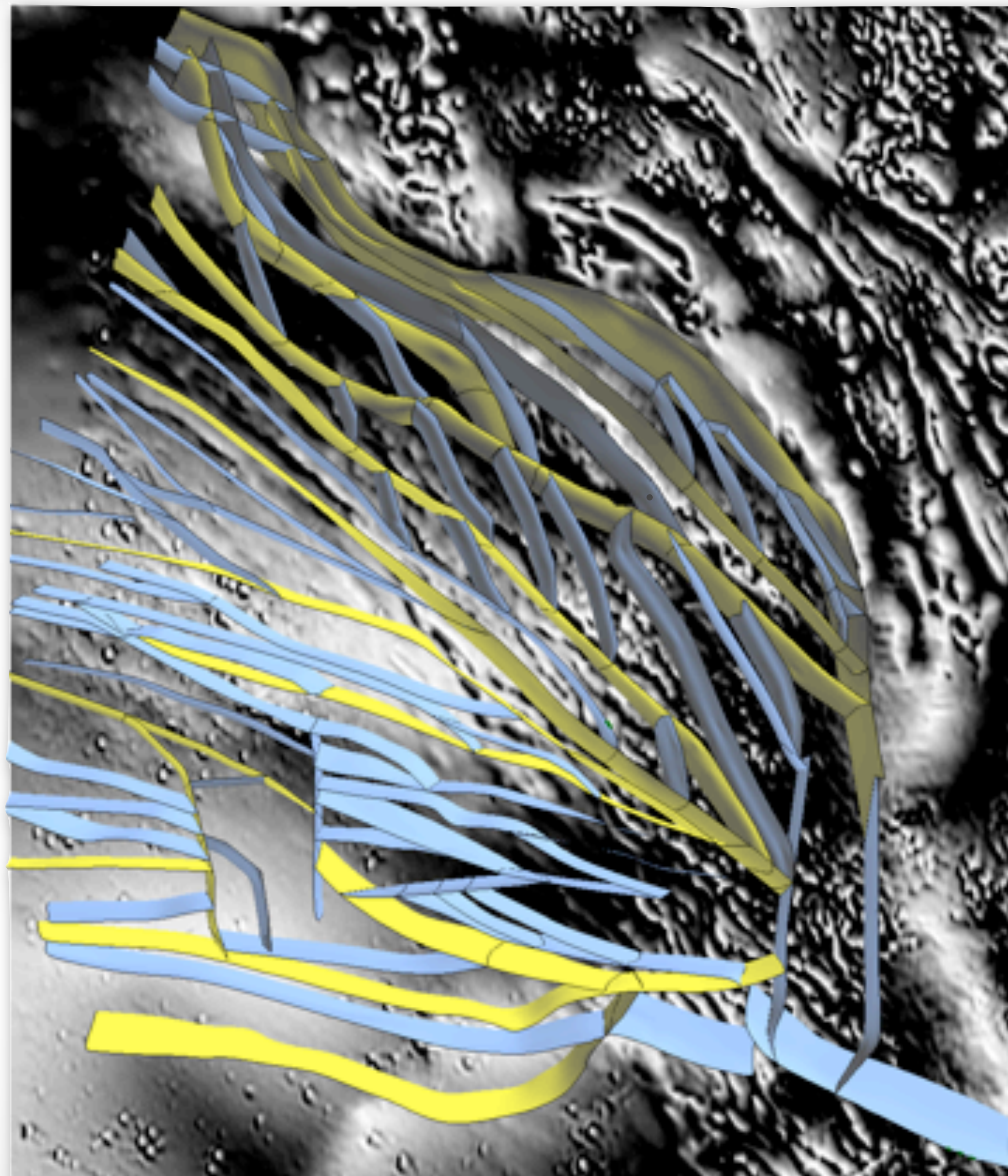
Structural *interpretation* of geophysics:

- Yellow - primary
- Blue - secondary

?

Developed with GoCAD

David Willis (Honours thesis, Monash University, 2011)



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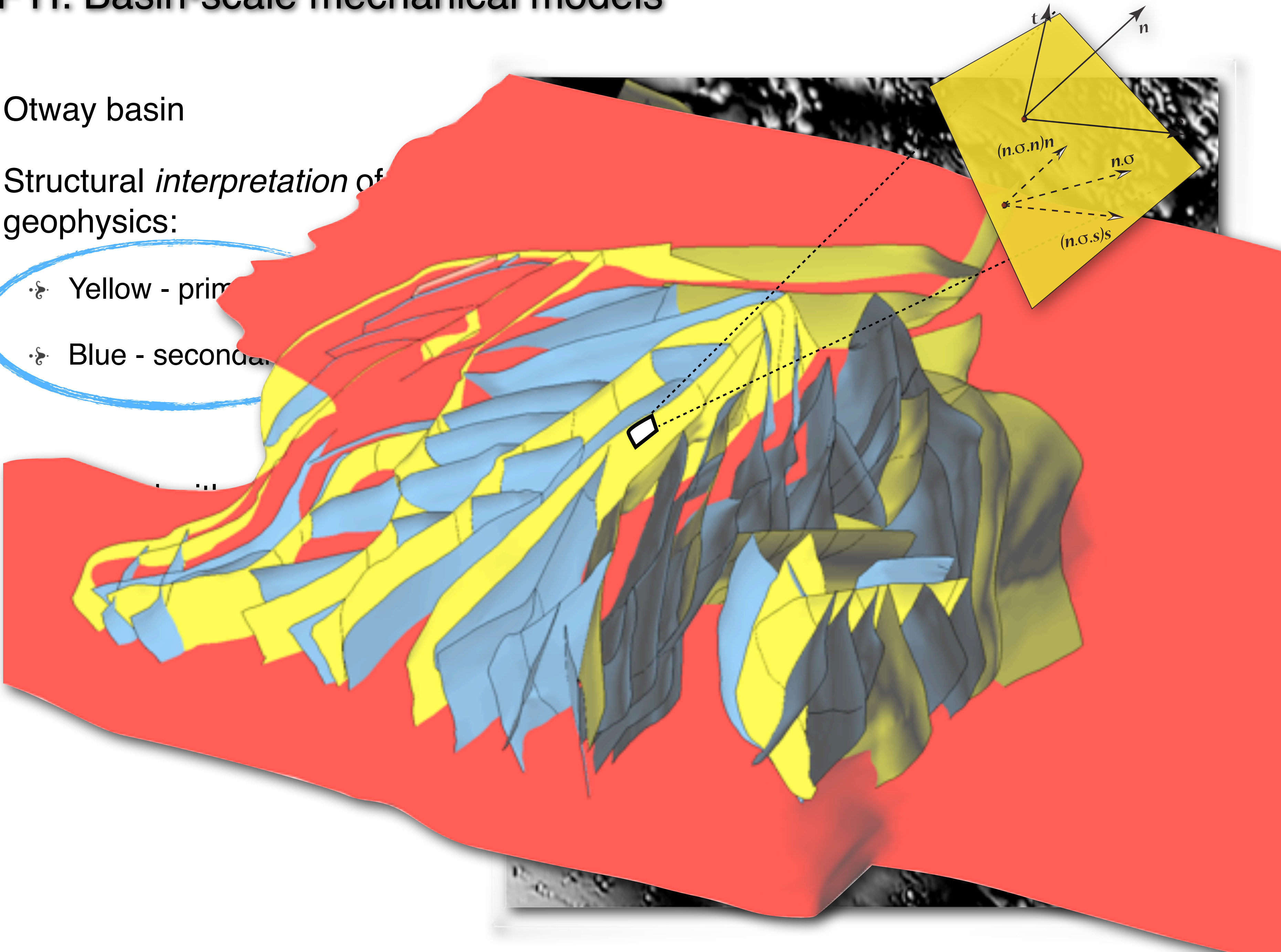
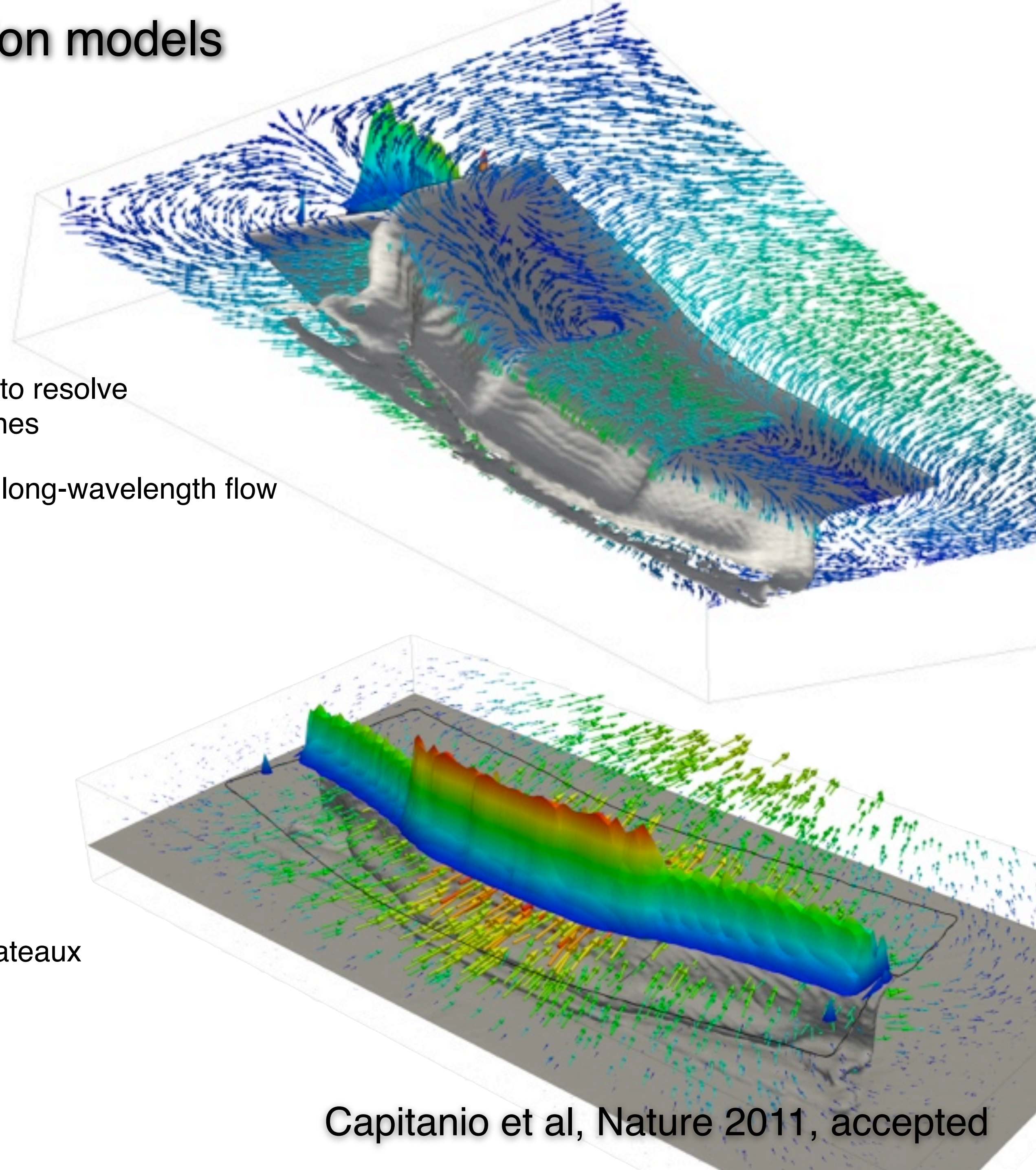


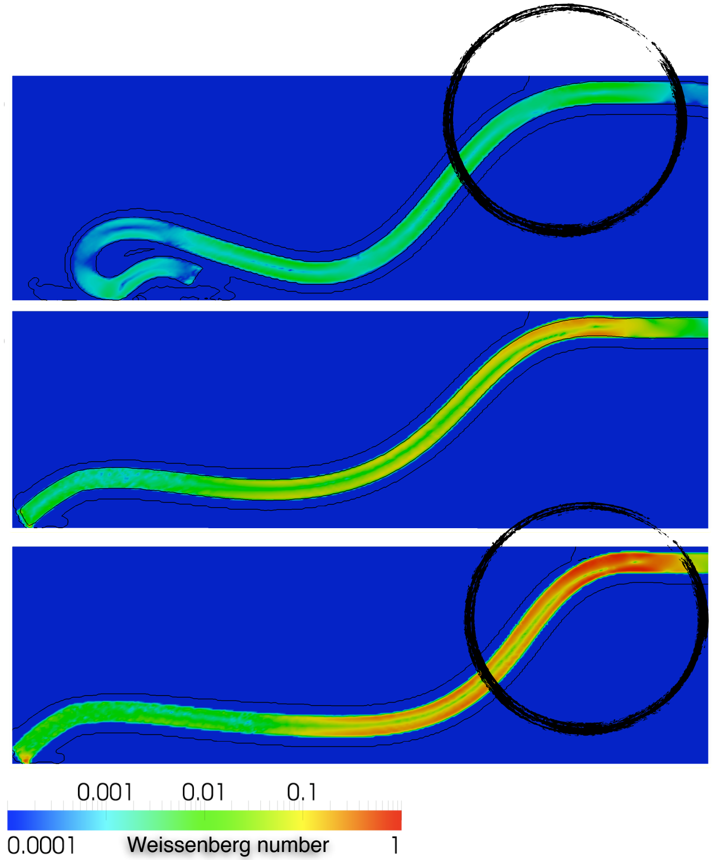
Example 3 – subduction models

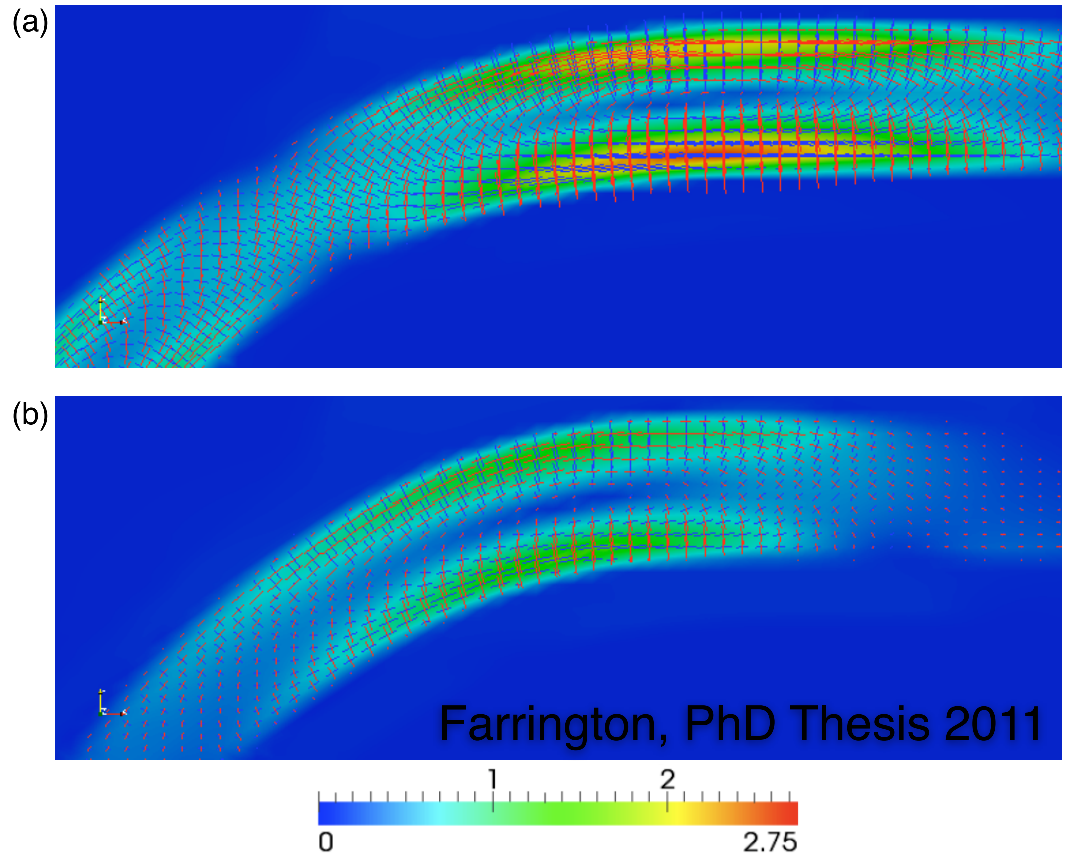
- Previously the domain of analogue models
- Mantle flow plus viscoelastic-plastic slab
- High resolution required in 3D to resolve rheological layering, failure zones
- Large scale models to resolve long-wavelength flow
- Fully dynamic calculations:
  - Topography
  - Velocity
  - Anisotropy
  - Stress in the slab
  - Coupling of over-riding plate
  - Interaction with plumes & plateaux
    - Slab tearing
    - Mantle geochemistry



Capitanio et al, Nature 2011, accepted

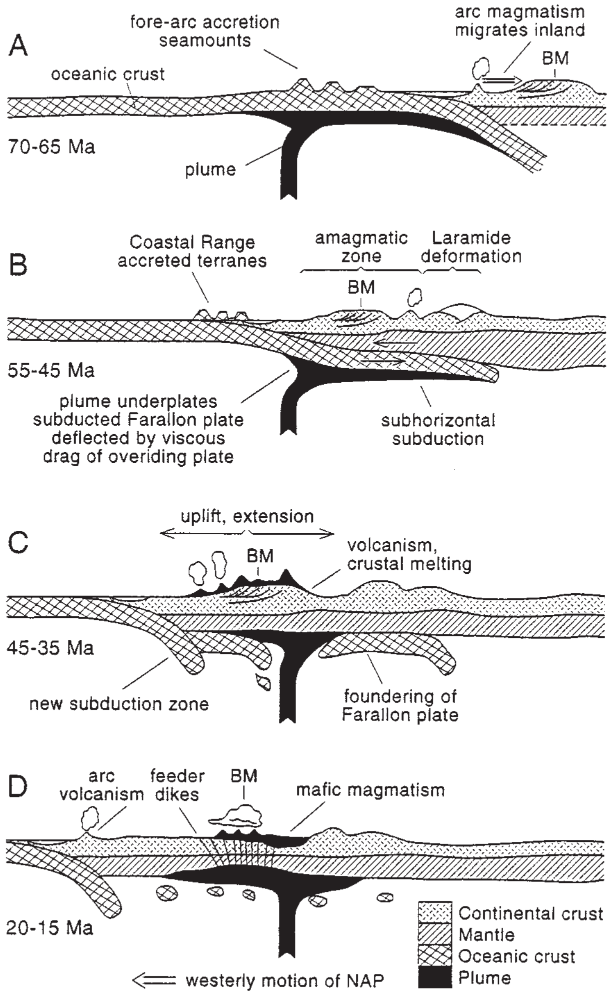
Elastic stresses v. Viscous stresses



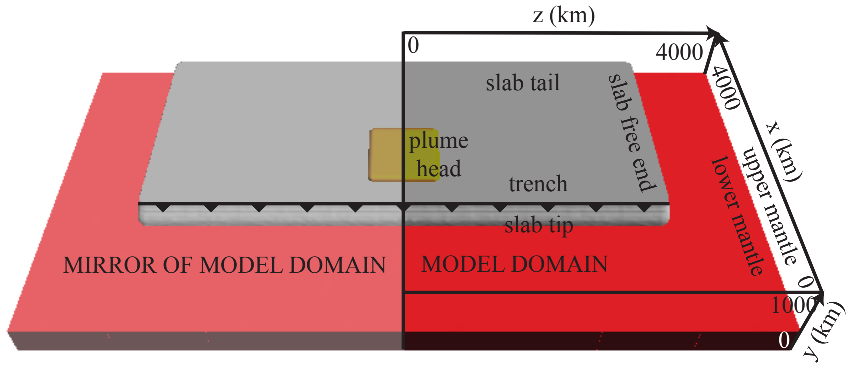


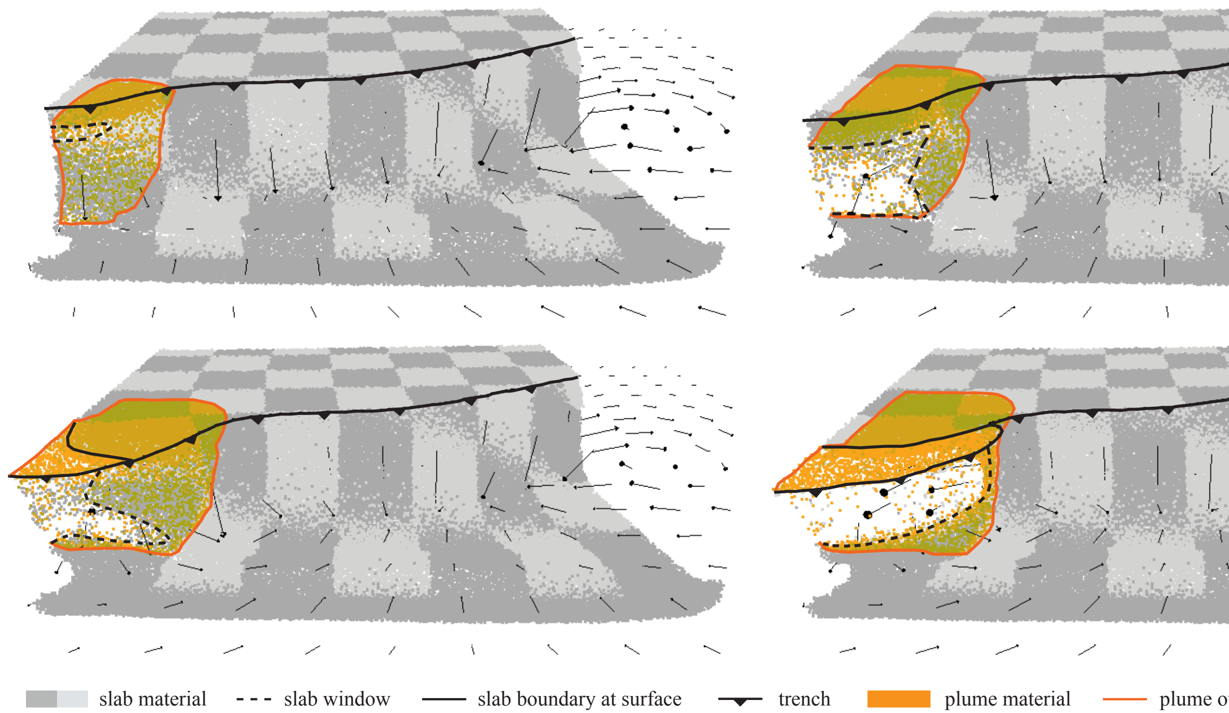
The normalised deviatoric stress invariant and stress orientation within the core showing extension (red) and compression (blue) within the steady state time step for a relaxation time of (a) 21 Kyr and (b) 2.1 Myr. The eigenvectors are plotted using the same scale for both (a) and (b).

When plumes and slabs collide



Murphy et al, Geology, 1998



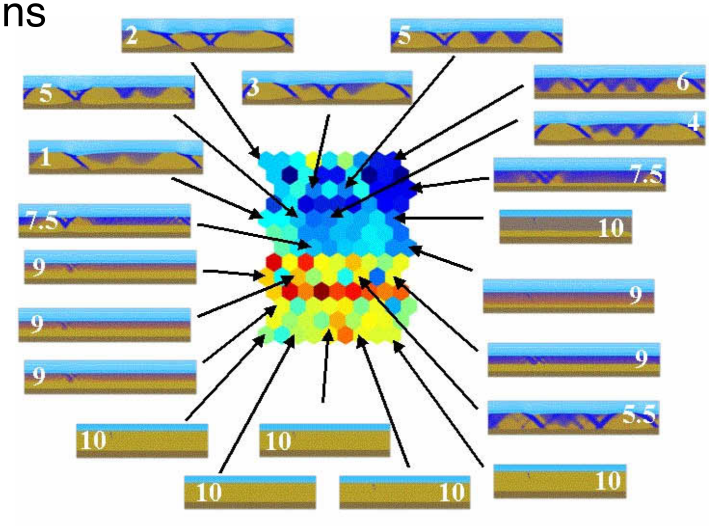


Transfer of a plume from lower to upper plate — slab break-off and re-initiation of subduction or local slab window ?

Where next ?

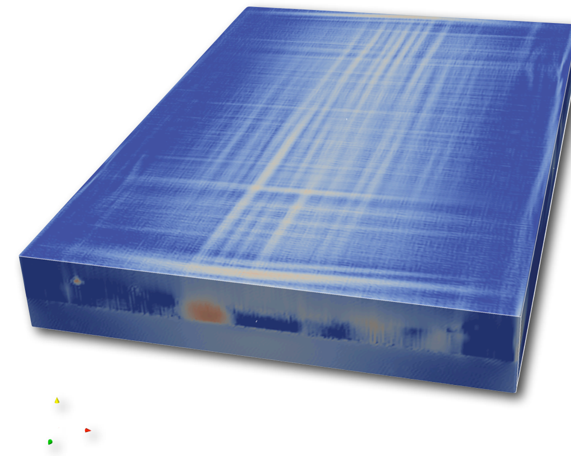
There are two distinct aspects to “intuitive” modelling

- **Forward modelling capability**
  - Natural mapping of common geological processes into the internal representation of the numerical methods
  - Capacity to ingest potentially complicated structural models
  - Capacity to evolve structure through large deformations
  - Outputs of models match observables



- **Driven exploration of parameter space**
  - Including the potential for surprise / horror
  - Potential for model libraries / data mining
  - Constraints from both quantitative fit and “experience / gut feeling”

Conclusion



Always need to use numerical models that match the problem in hand

- Choose the models to best answer the science question (not choosing the science which your codes can do)
- Good match between physics and numerics
- You must know/learn the capabilities and limitations of your code

Simple problems in modelling continental dynamics remain unsolved and are worth studying first — this is particularly true in 3D: emergence of patterns and planforms

Application to understanding specific problems is also possible, but should be designed carefully and with realistic expectations.

Ways to explore distinctive behaviours implied by simple models are helpful in improving understanding.

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Shear Banding

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- Subduction dynamics and the origin of Andean orogeny and Bolivian Orocline. F. A. Capitanio, C. Faccenna, S. Zlotnik and D.R. Stegman, Nature, in press 2011
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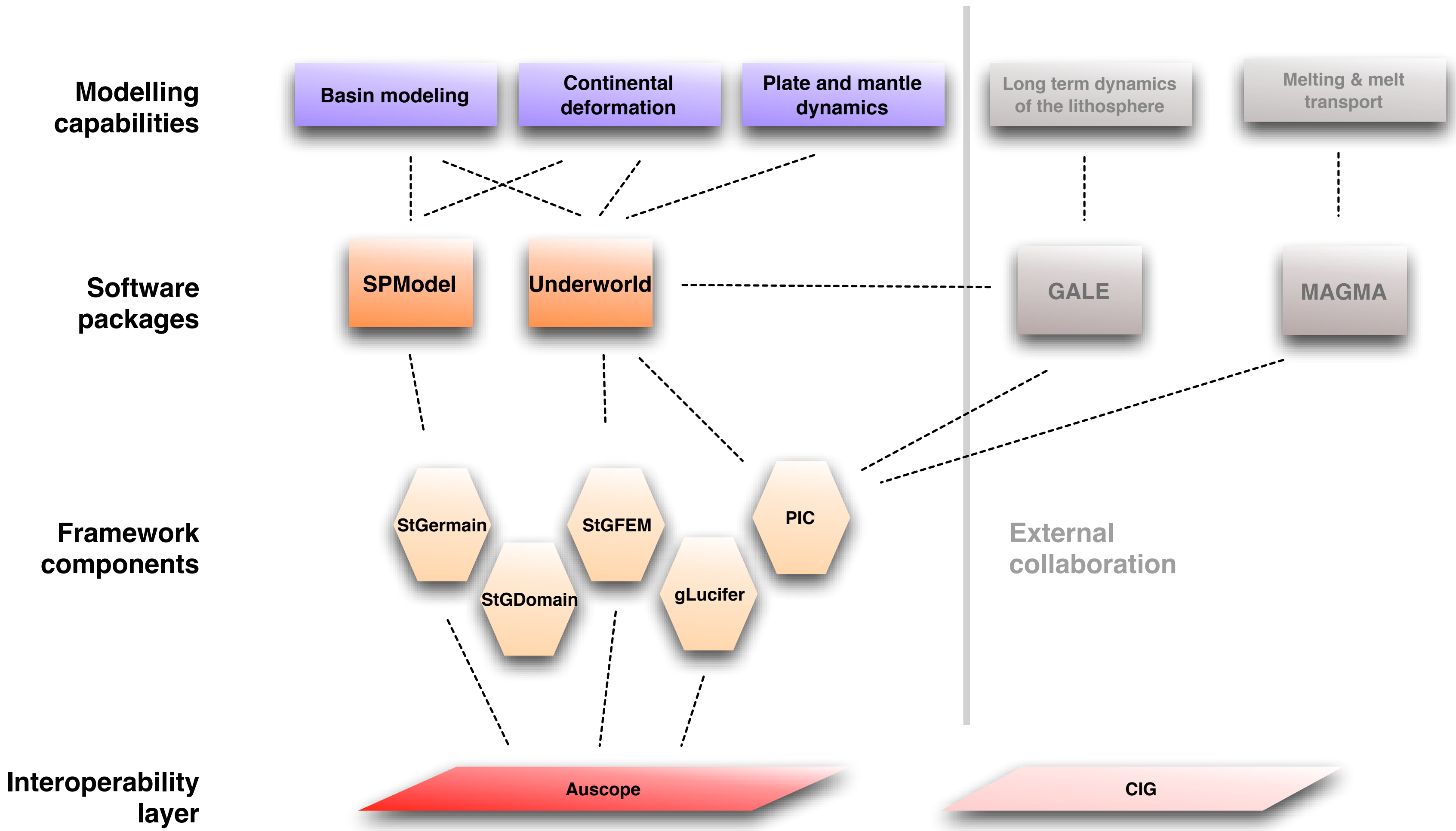
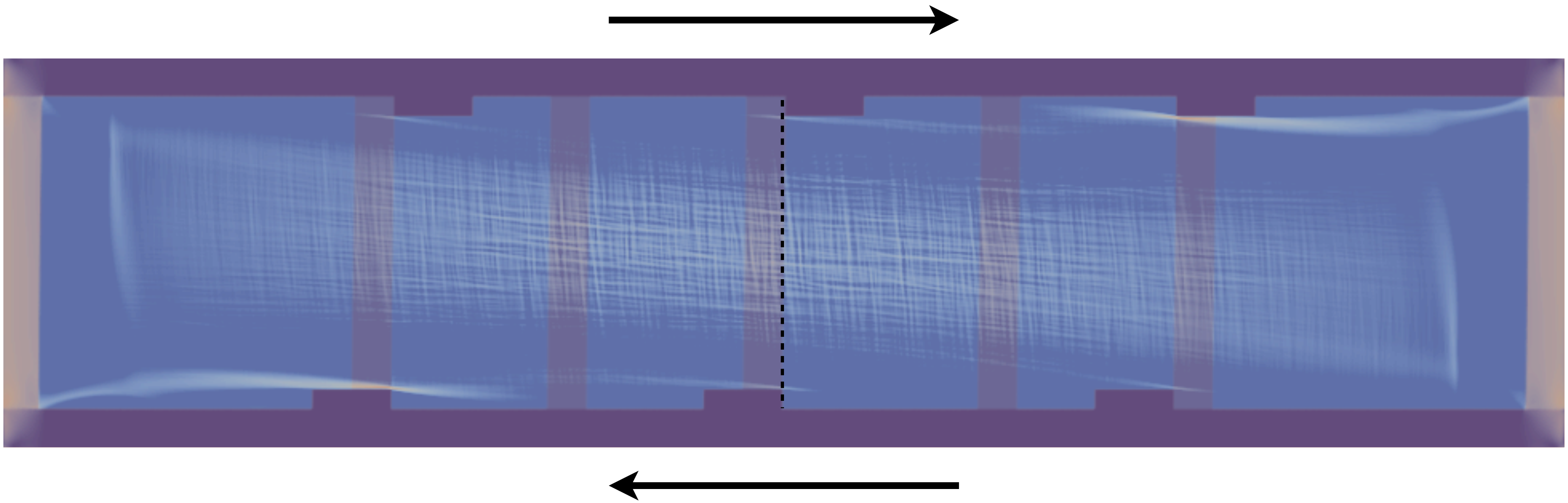
Overview of software packages



Shear banding in 2D shear



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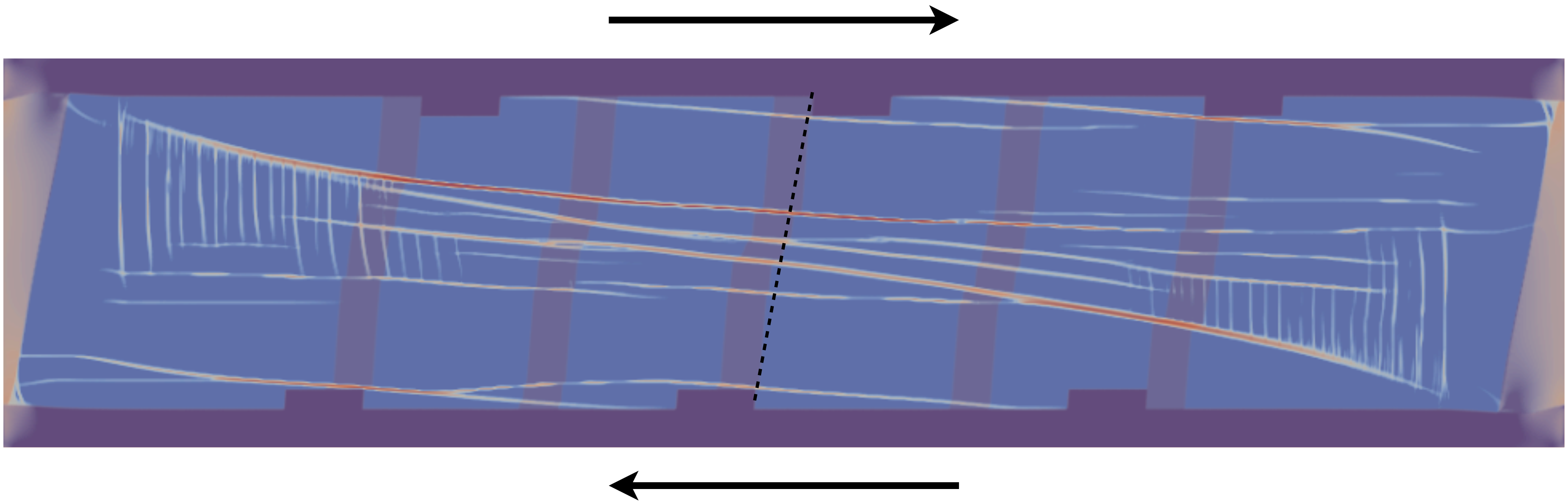
Shear banding in 2D shear



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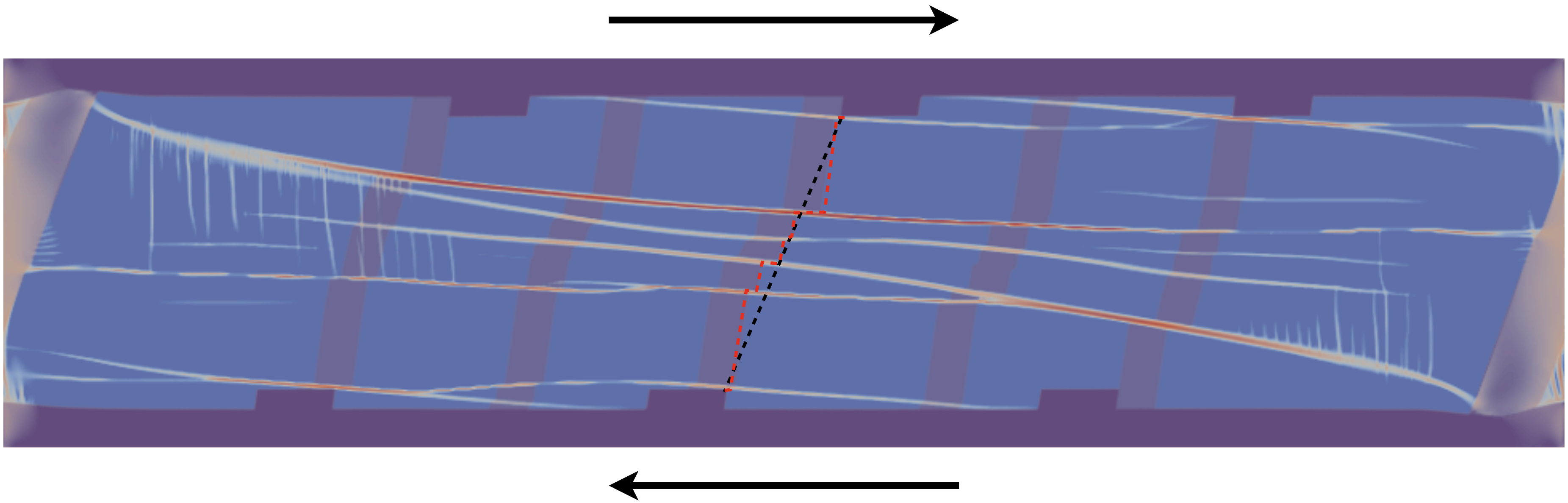

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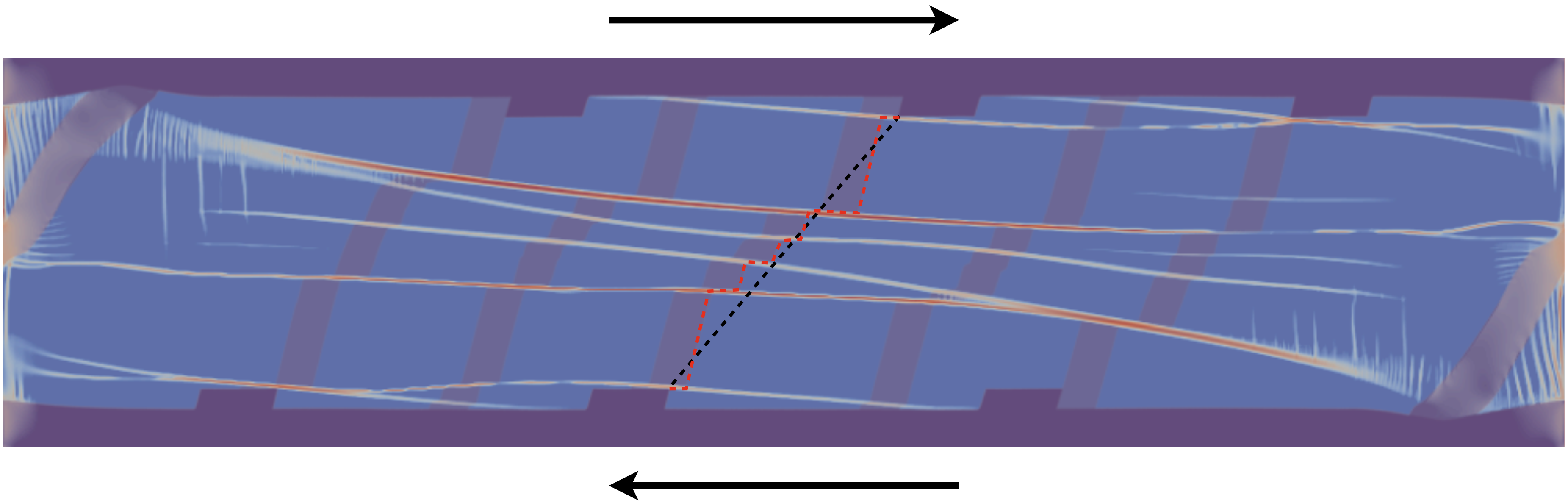

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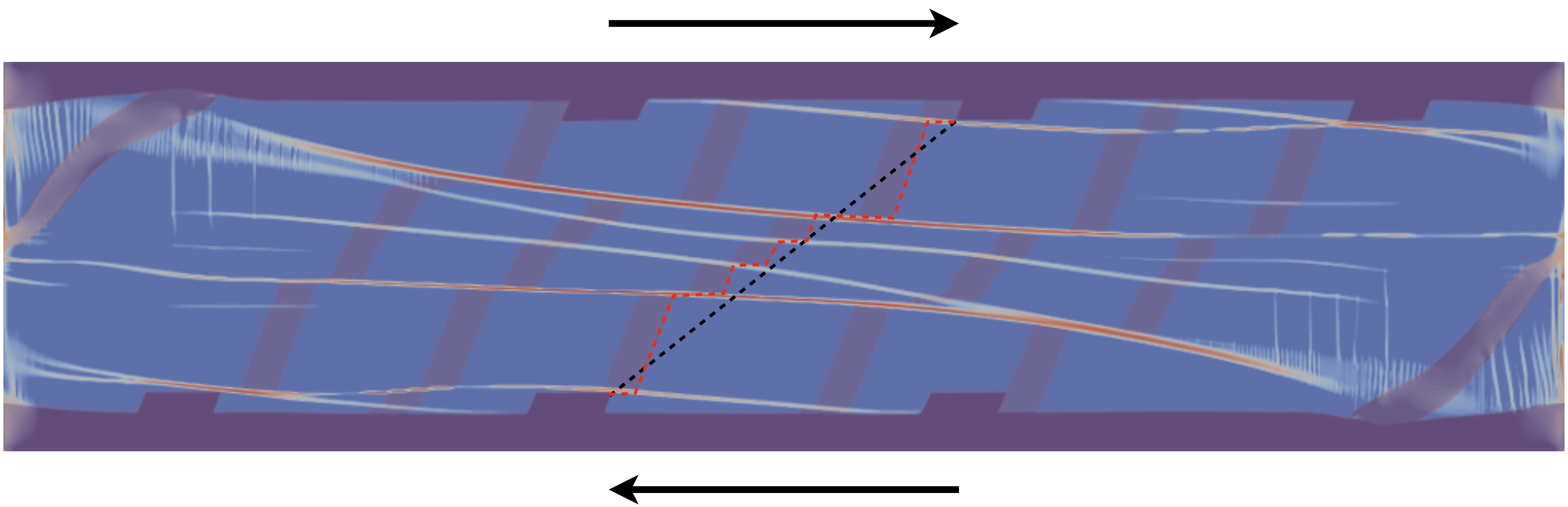
Shear banding in 2D shear



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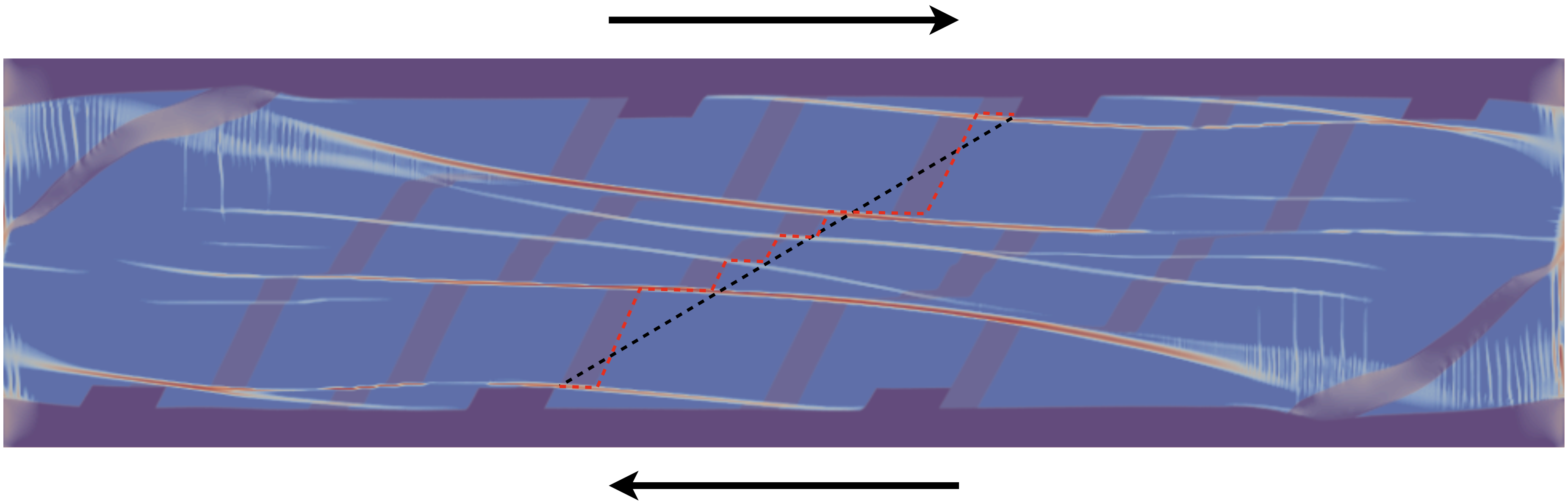
Shear banding in 2D shear



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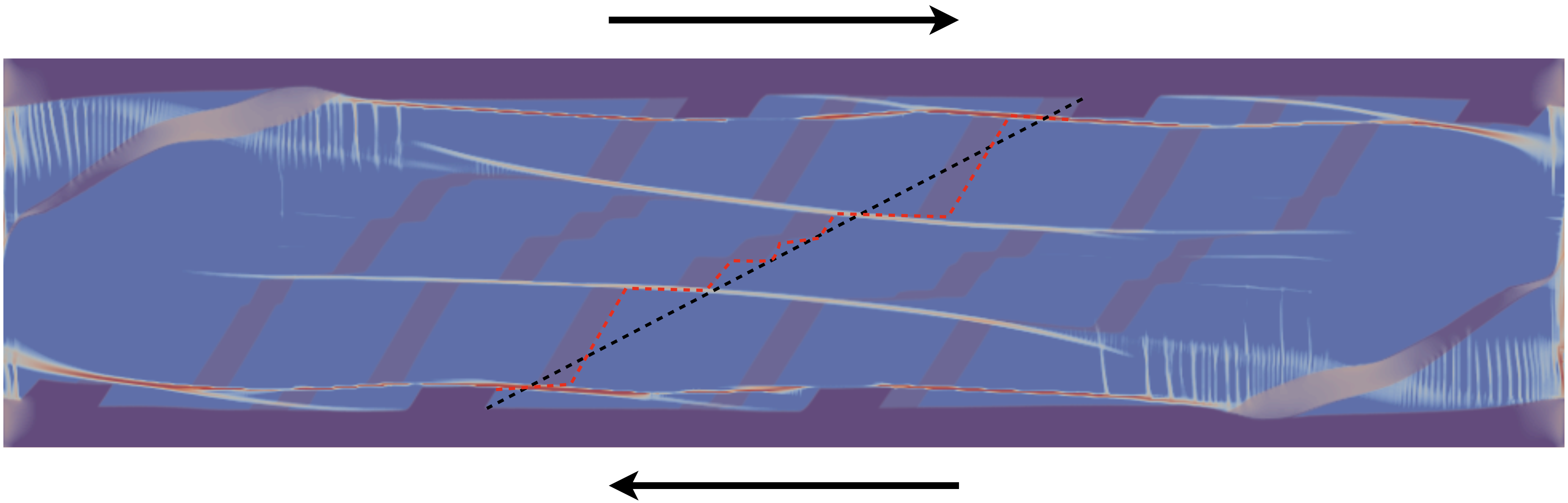

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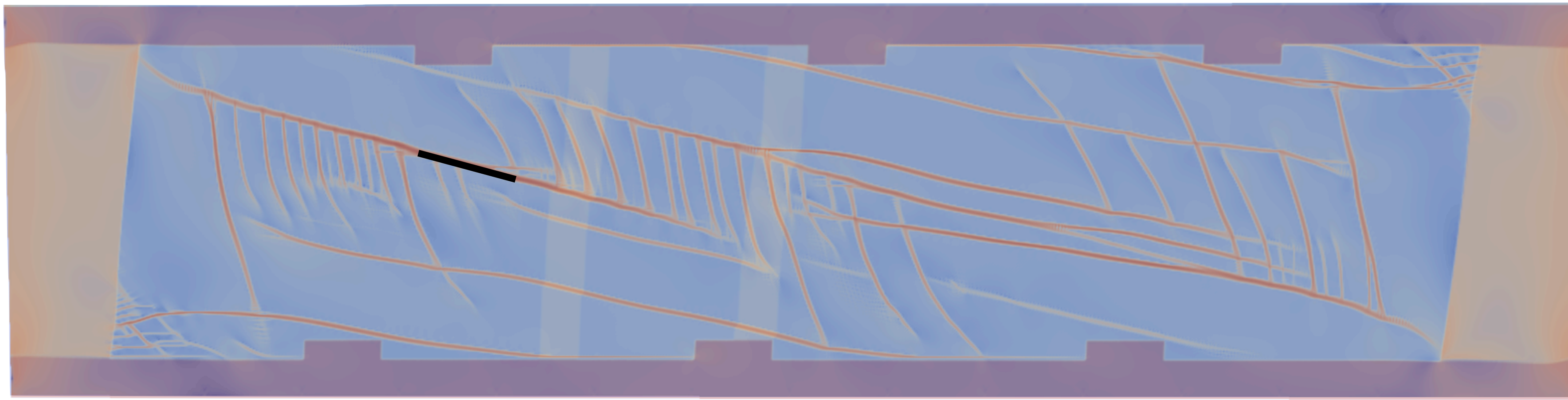
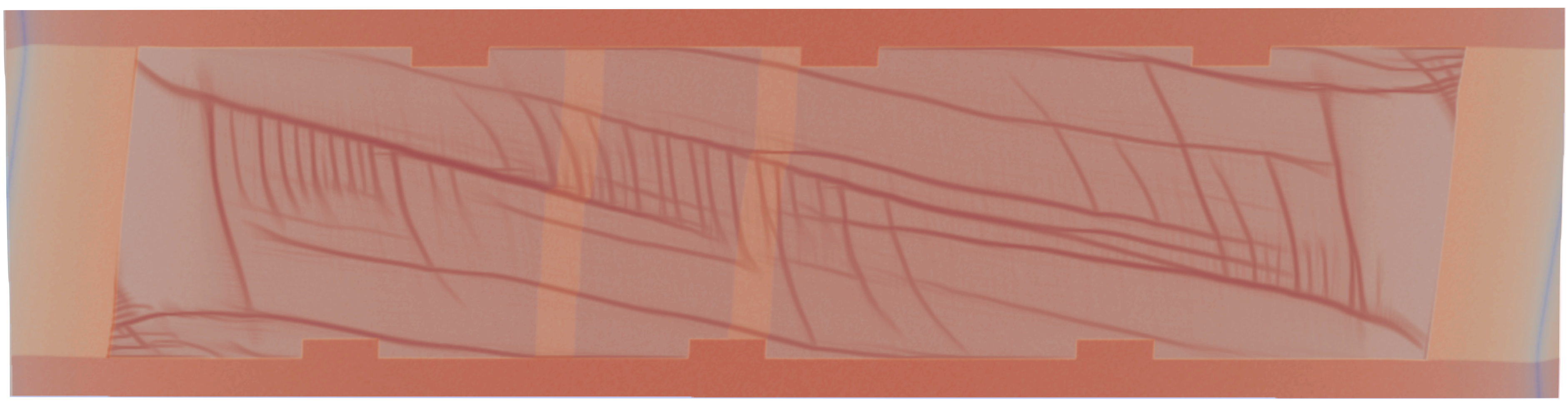
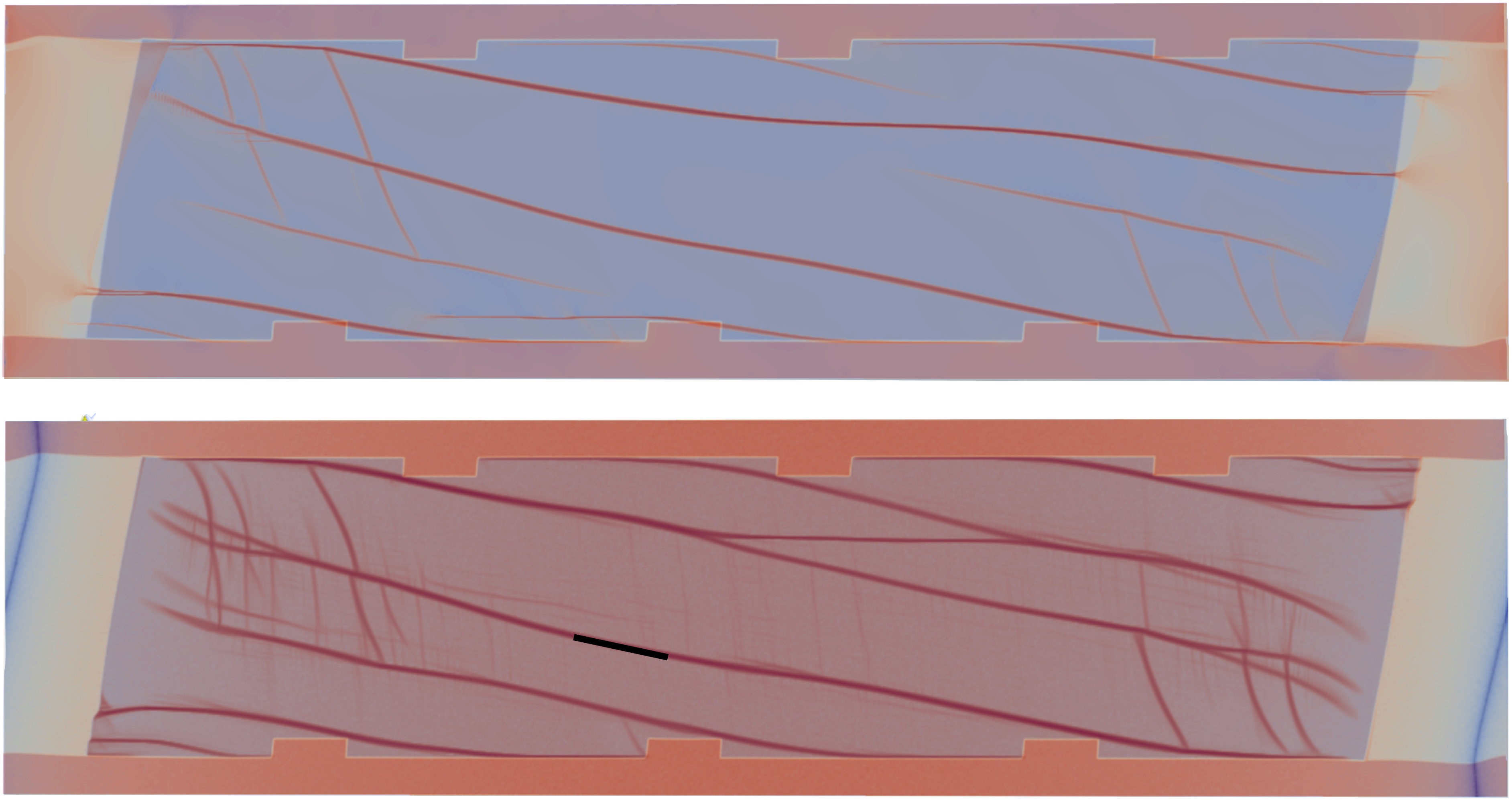
Strain-rate and Plastic strain — initial





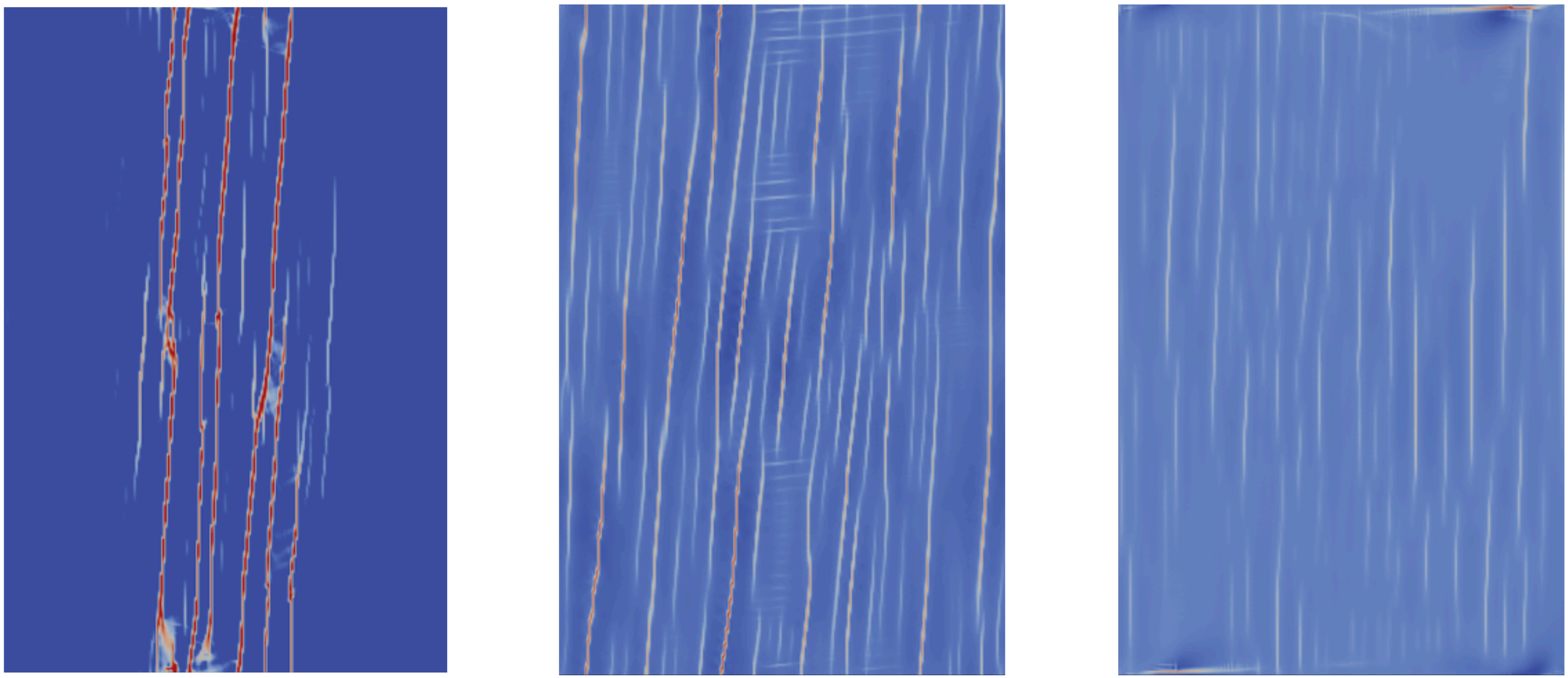
Elasticity 10^4; viscosity 10^2; C_1 50, C_2 40; $t = 0.1$; friction 0.6

Strain-rate and Plastic strain — mature



Elasticity 10^4; viscosity 10^2; C_1 50, C_2 40; $t = 0.33$; friction 0.6

Influence of strength of lower layer — strength increases with depth



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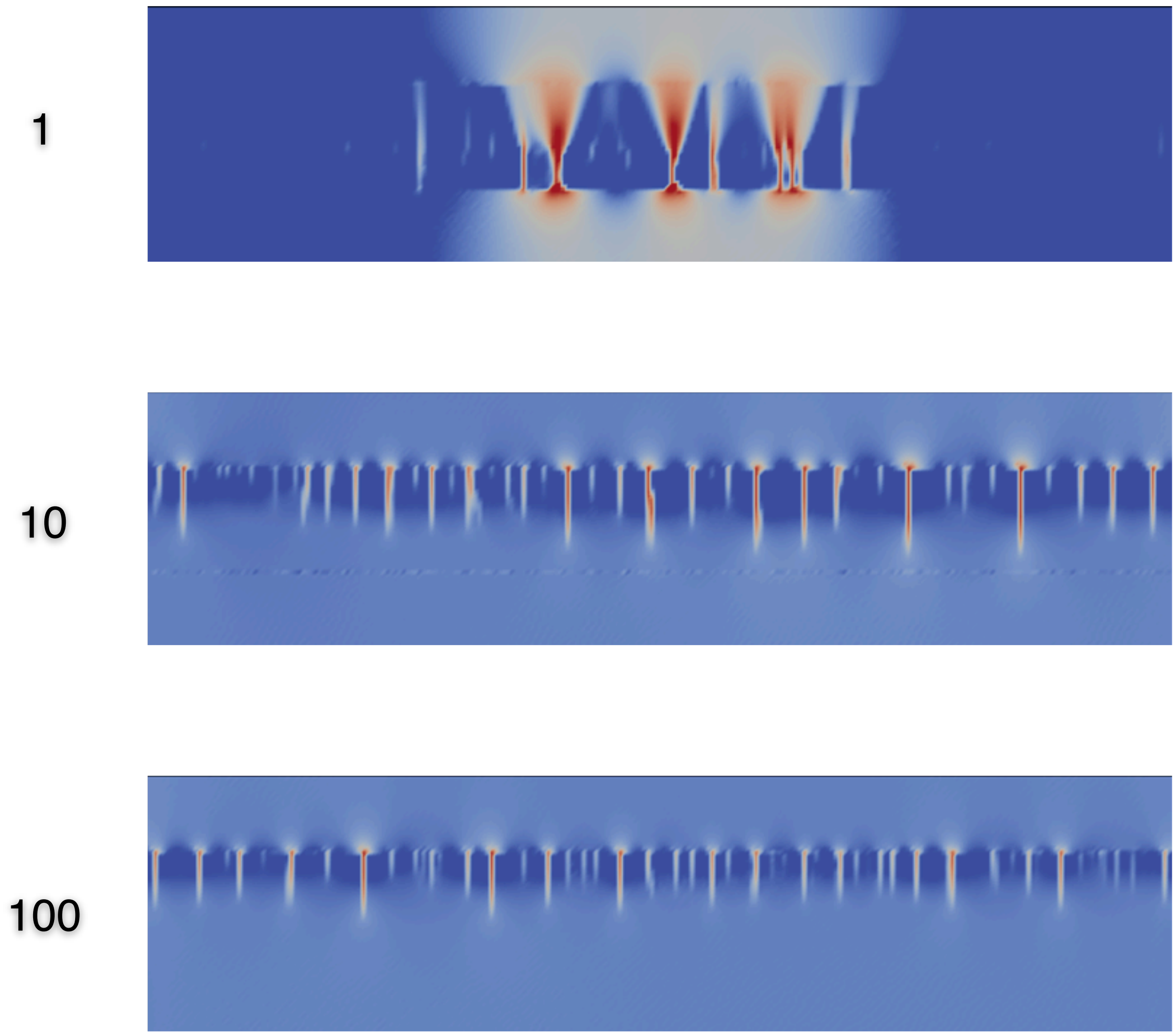
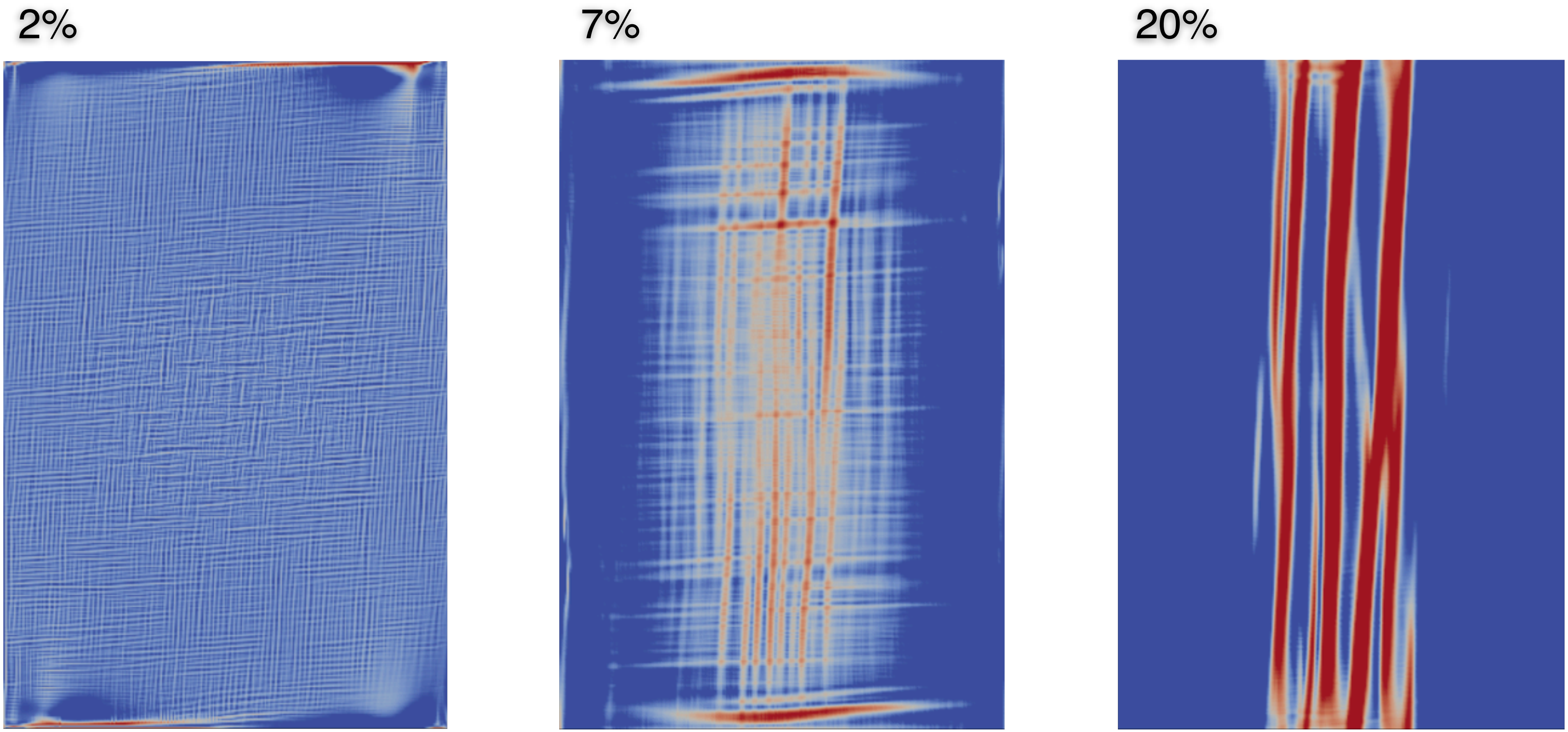
Strain-rate invariant

Influence of strength of lower layer — strength increases with depth

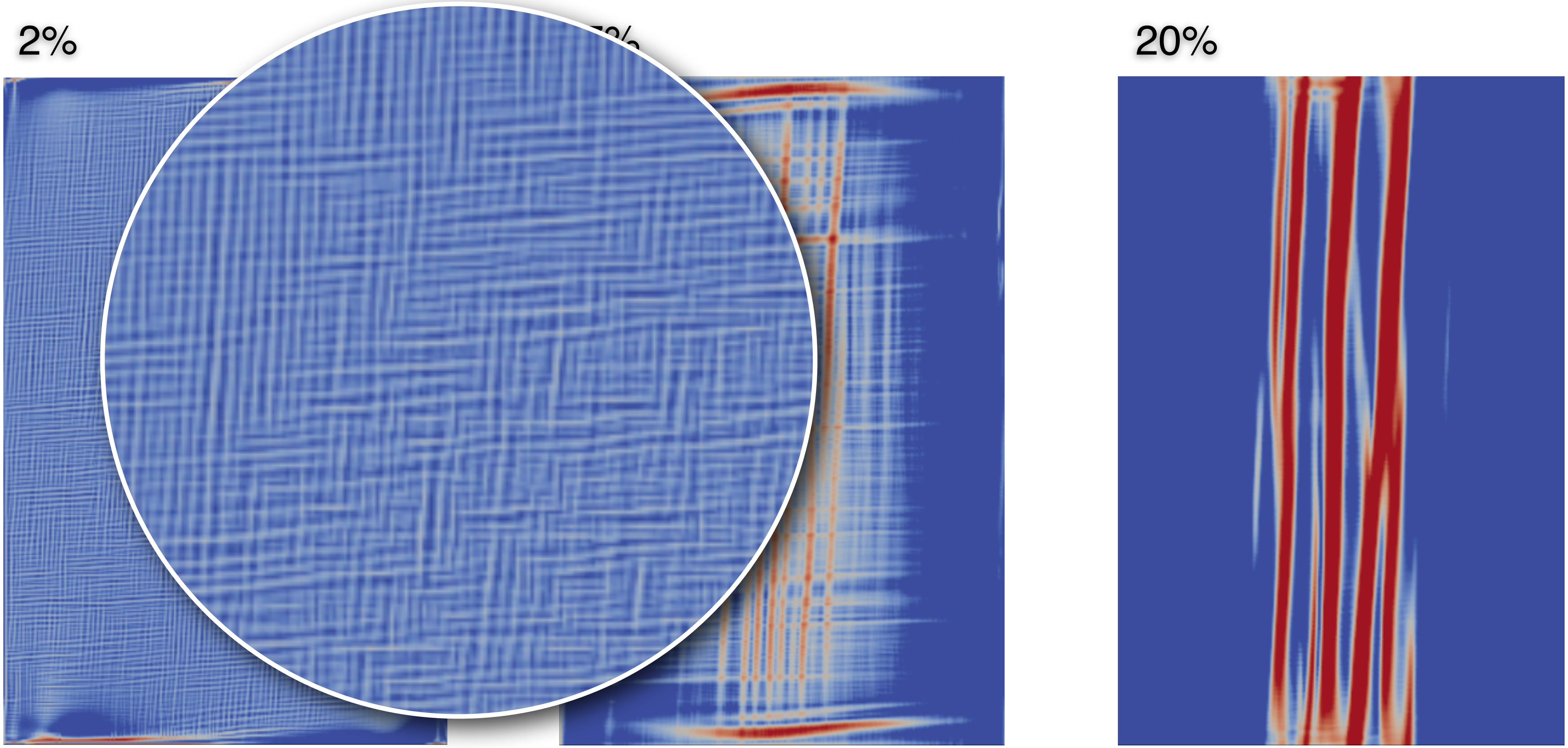


Development of shear bands — weak substrate / depth



Slices through the strain-rate invariant at upper depth in the viscoplastic layer

Development of shear bands — weak substrate / depth



Slices through the strain-rate invariant at upper depth in the viscoplastic layer