Introduction to DynEarthSol2D/3D and How to make Coulomb angle-oriented shear bands

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Outline

- DynEarthSol2D/3D
  - Key algorithmic components of DynEarthSol2D.
  - Validation and verification by benchmarks.
  - Challenges with 3D extension:
    - parallelization
    - meshing/remeshing.
- Strain localization: How to get shear bands oriented at the Coulomb angle.

Collaborators

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Motivations: Desirable Features

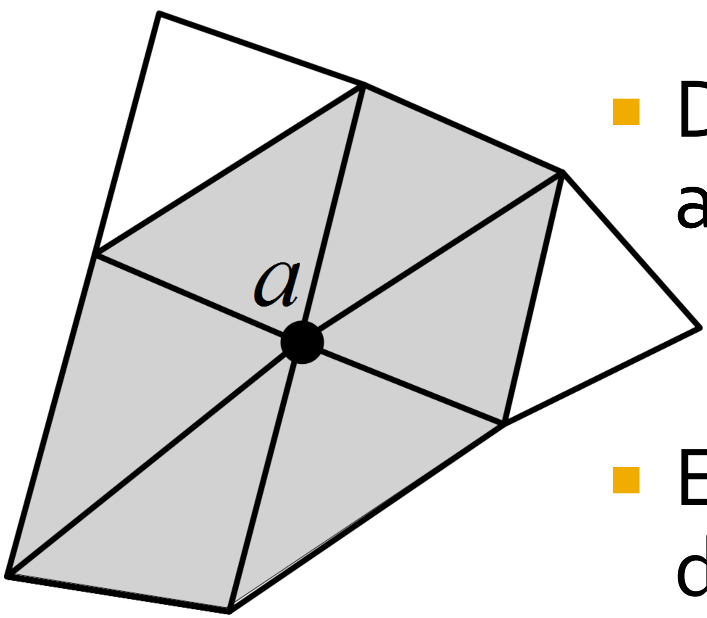
- Fast Lagrangian Analysis of Continua (FLAC)
  - Based on algorithms proposed by Cundall (1989).
  - A long list of successful applications.
  - Many variants out there.
  - FYI, one version being maintained as an open source: https://bitbucket.org/tan2/flac
    - OpenMP-parallel. Shows a good scaling.

- Unstructured meshes are often desirable for a wider range of applications and computational efficiency.

Key Components of DynEarthSol2D

- **Dyn**amic **Earth Sol**ver for 2D.
- Principle of virtual power

$$0 = \int_\Omega \delta\boldsymbol{v} \left(\rho \frac{\partial \boldsymbol{v}}{\partial t} \right) d\Omega - \int_\Omega \nabla(\delta\boldsymbol{v}) : \boldsymbol{\sigma} d\Omega - \int_\Omega \delta\boldsymbol{v} \rho \boldsymbol{g} d\Omega$$



- Discretized momentum equation after the standard FE procedure

$$m_a \mathbf{a}_a = \mathbf{F}_a^{int} + \mathbf{F}_a^{ext}$$

- Energy balance equation is discretized similarly.

Key Components of DynEarthSol2D

- Unstructured mesh created by
  - `triangle` (http://www.cs.cmu.edu/~quake/triangle.html) in 2D
  - `tetgen` (http://wias-berlin.de/software/tetgen/) in 3D.

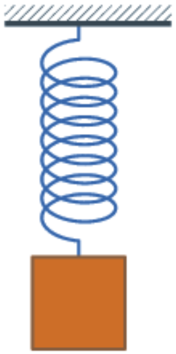
- **Lagrangian** description of motion with e***xplicit*** time integration.

$$\mathbf{v}_a^{(t+\Delta t/2)} = \mathbf{v}_a^{(t-\Delta t/2)} + \mathbf{F}_a^{(t)} \frac{\Delta t}{m_a}$$

$$\mathbf{x}_a^{(t+\Delta t)} = \mathbf{x}_a^{(t)} + \mathbf{v}_a^{(t+\Delta t/2)} \Delta t$$

Key Components of DynEarthSol2D

- ***Dynamic relaxation*** for (quasi-)static solutions
  - Local damping



$$v_a^{i,(t+\Delta t/2)} = v_a^{i,(t-\Delta t/2)} + (F_a^{i,(t)} + F_d^i)\frac{\Delta t}{m_a},$$

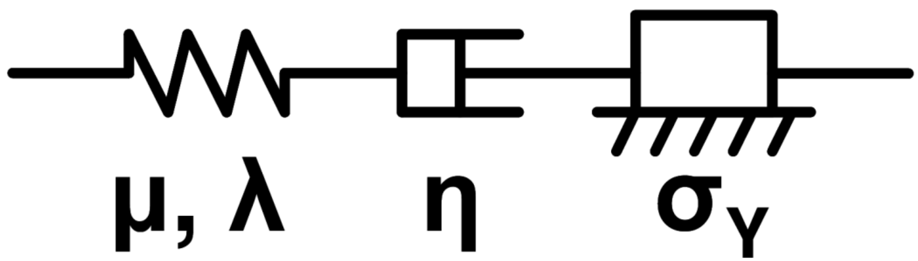
$$\text{where} \quad F_d^i = -\alpha |F_a^{i,(t)}| \text{sgn}(v_a^i), \ \text{where}\, 0 \leq \alpha < 1.$$

- ***Mass scaling*** for a large and stable Δt

$$\Delta t < \frac{\Delta x}{v_p} \qquad v_p = \sqrt{\frac{K}{m_s}} \qquad m_s \gg m_g = \int \rho \, dV$$

Key Components of DynEarthSol2D

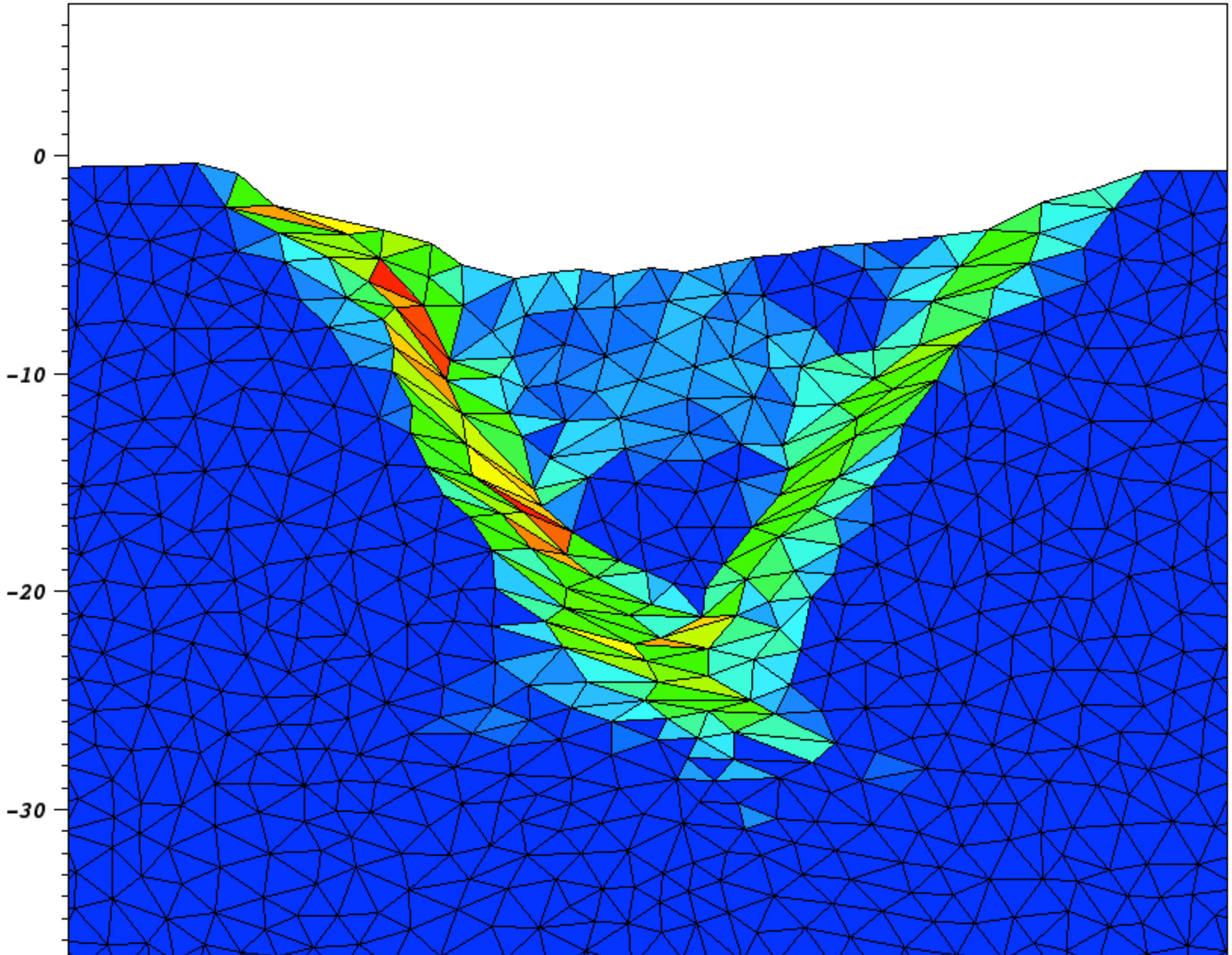
- Constitutive model: **elasto-visco-plastic**



  - $\eta \rightarrow \infty$: Mohr-Coulomb plasticity.
  - $\sigma_Y \rightarrow \infty$: Maxwell viscoelasticity.
  - $\eta = \eta(T, \sigma)$: temperature-determined brittle-ductile transition
  - $\sigma_Y = \sigma_Y(\varepsilon^*)$: strain hardening/softening

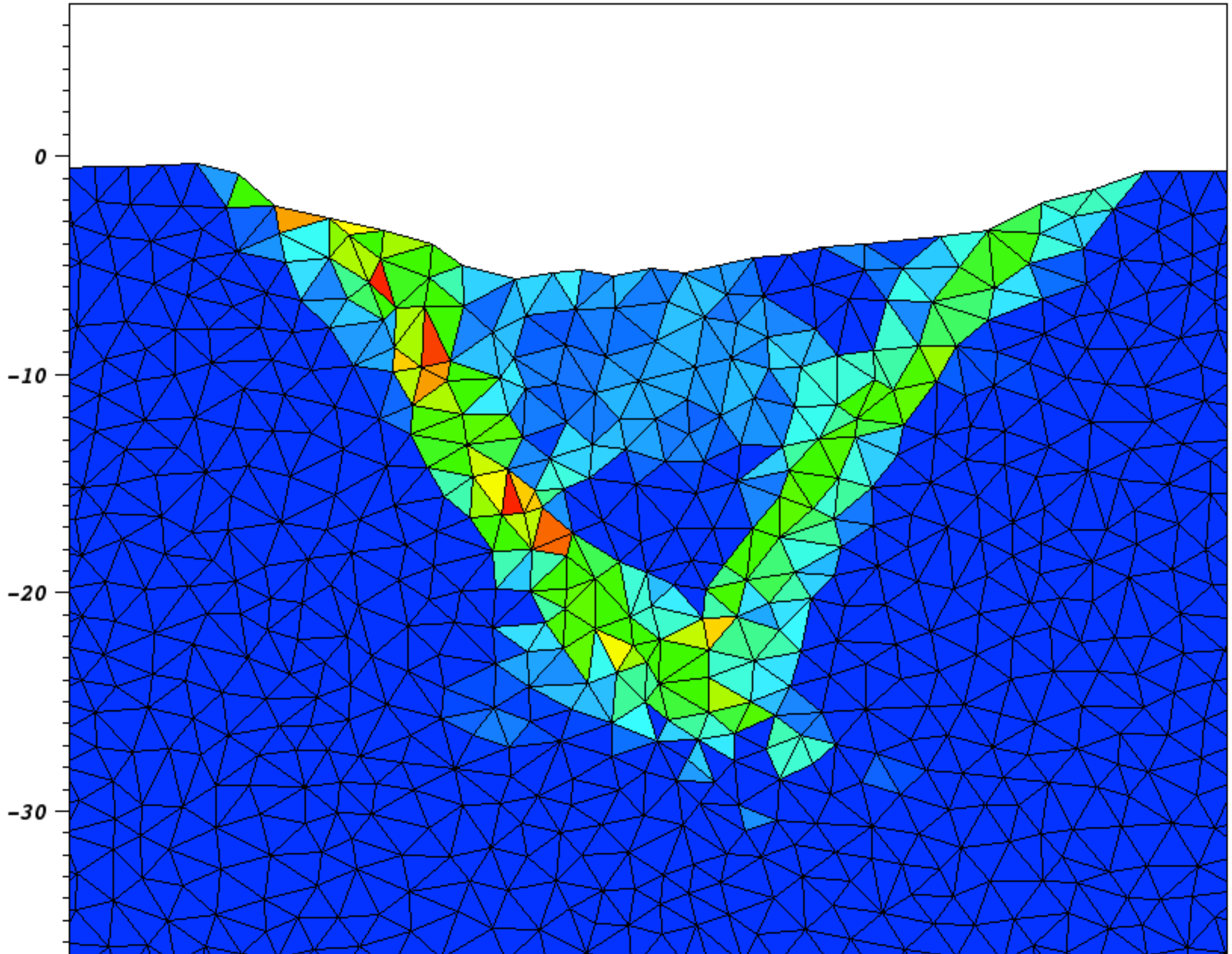
Key Components of DynEarthSol2D

- Remeshing



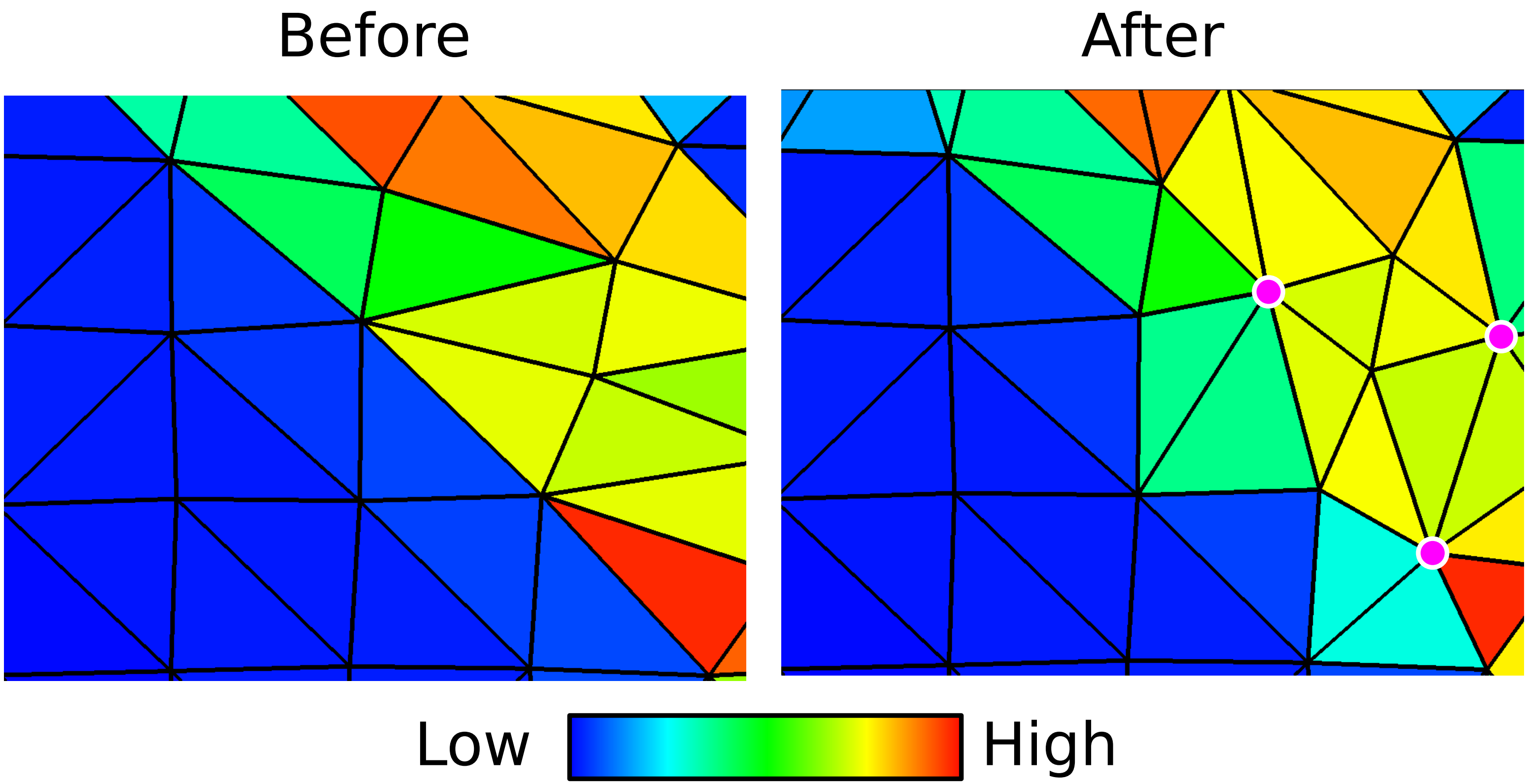
Key Components of DynEarthSol2D

- Remeshing



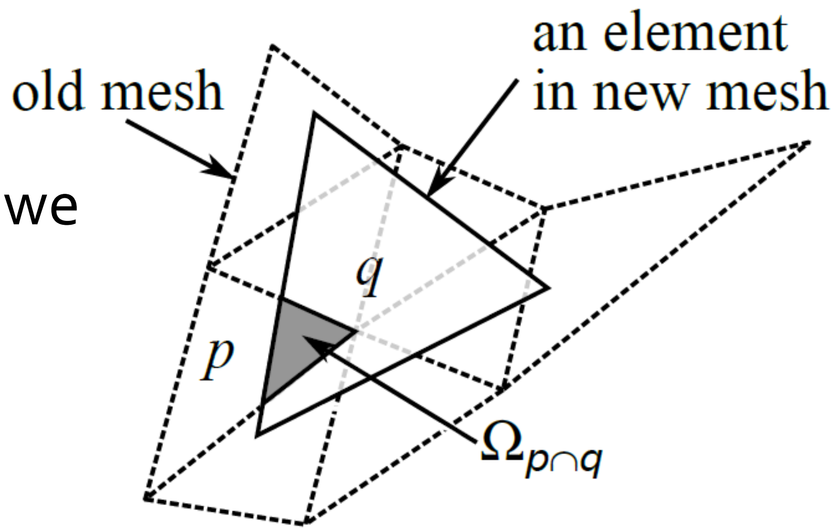
Key Components of DynEarthSol2D

- Remeshing by **edge-flipping** and **node addition/subtraction** (via *triangle* library by Shewchuk)



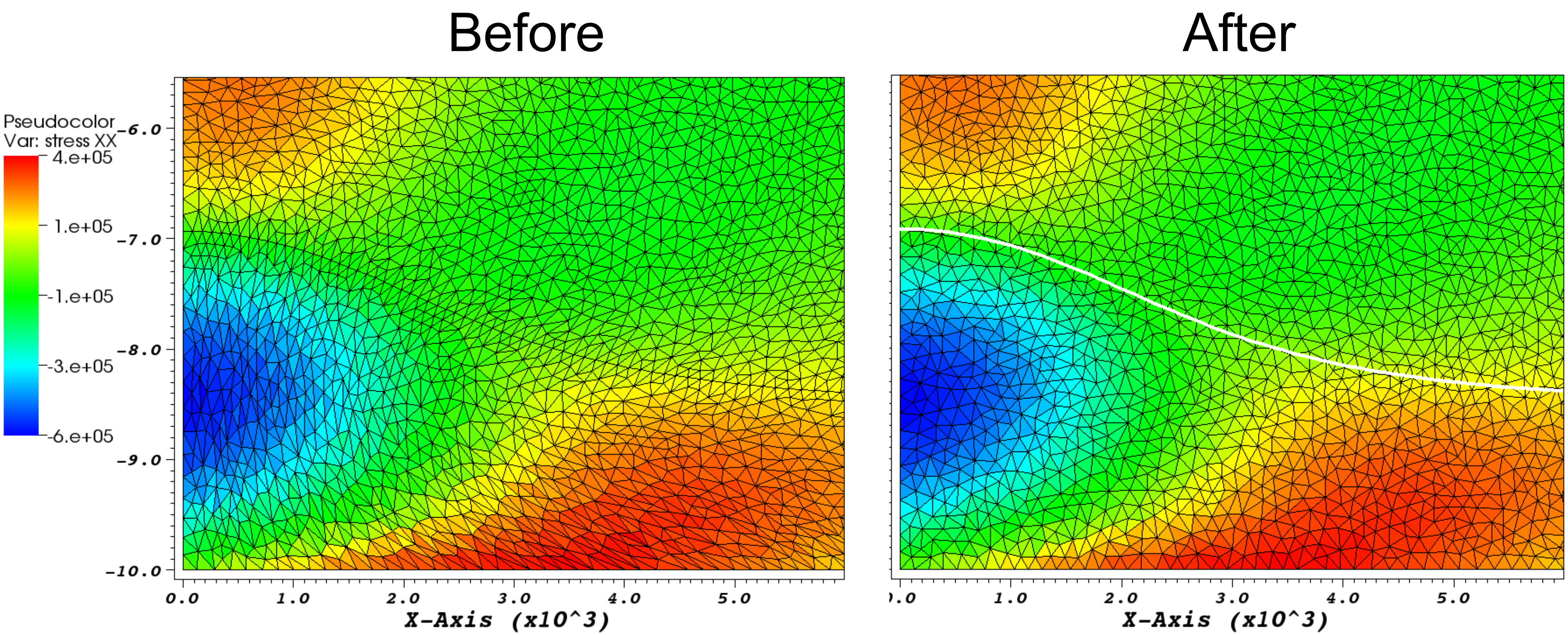
Key Components of DynEarthSol2D

- Remeshing (cont'd)
  - Fields defined on nodes are easily interpolated.
  - For quadrature-registered fields, we tried one of the conservative mappings: **Local supermesh construction** (Farrel & Maddison, CMAME, 2011) implemented in `Fluidity` library (Davies et al., G3, 2011).



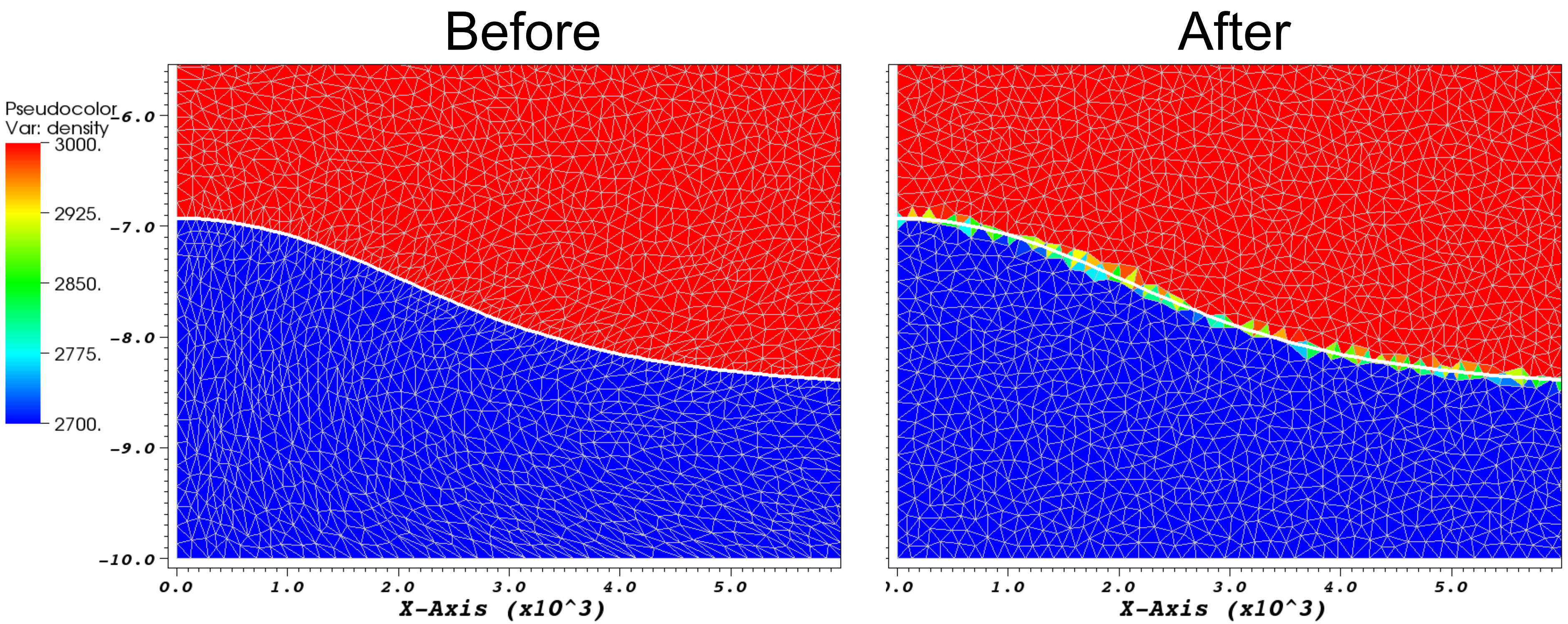
Key Components of DynEarthSol2D

- Remeshing (cont'd)
  - Mapping of smooth fields

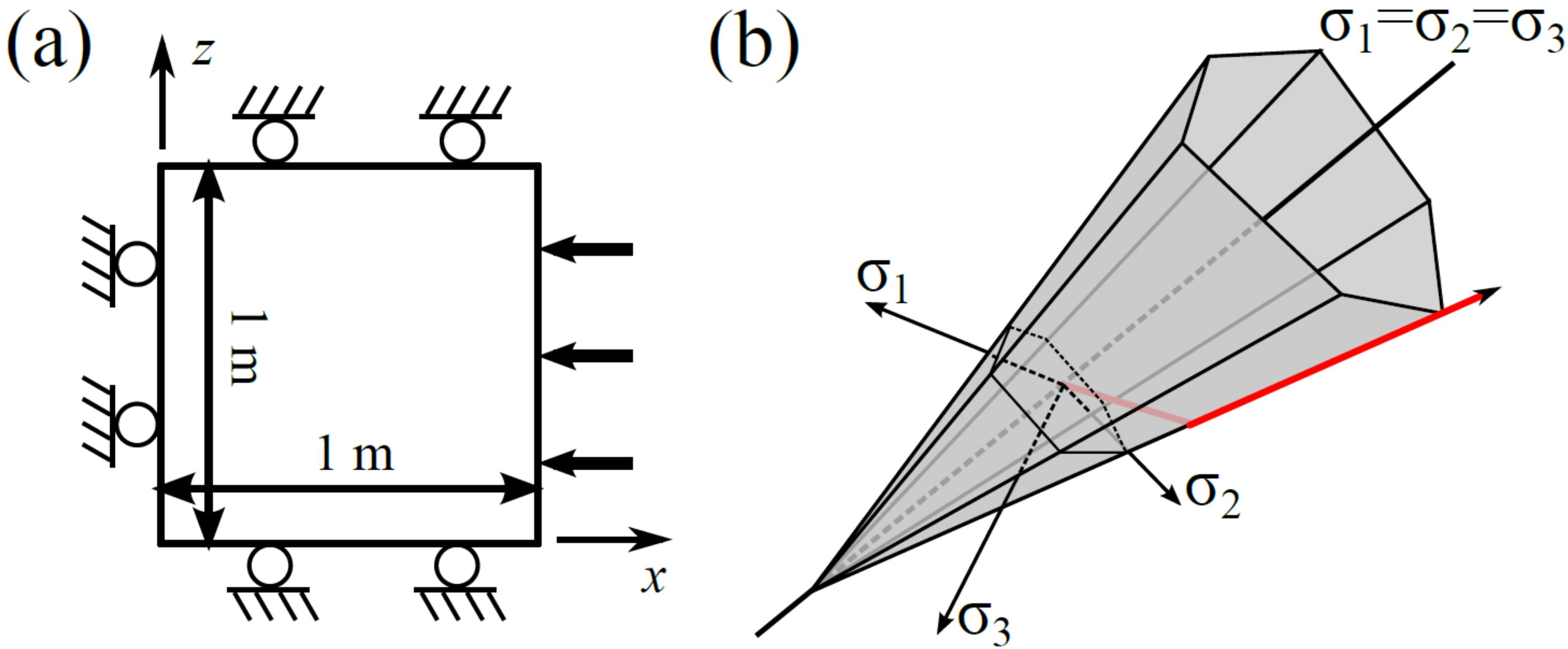


Key Components of DynEarthSol2D

- Remeshing (cont'd)
  - Mapping of sharp boundaries: **Markers** further needed.



Benchmarks: Plastic Oedometer



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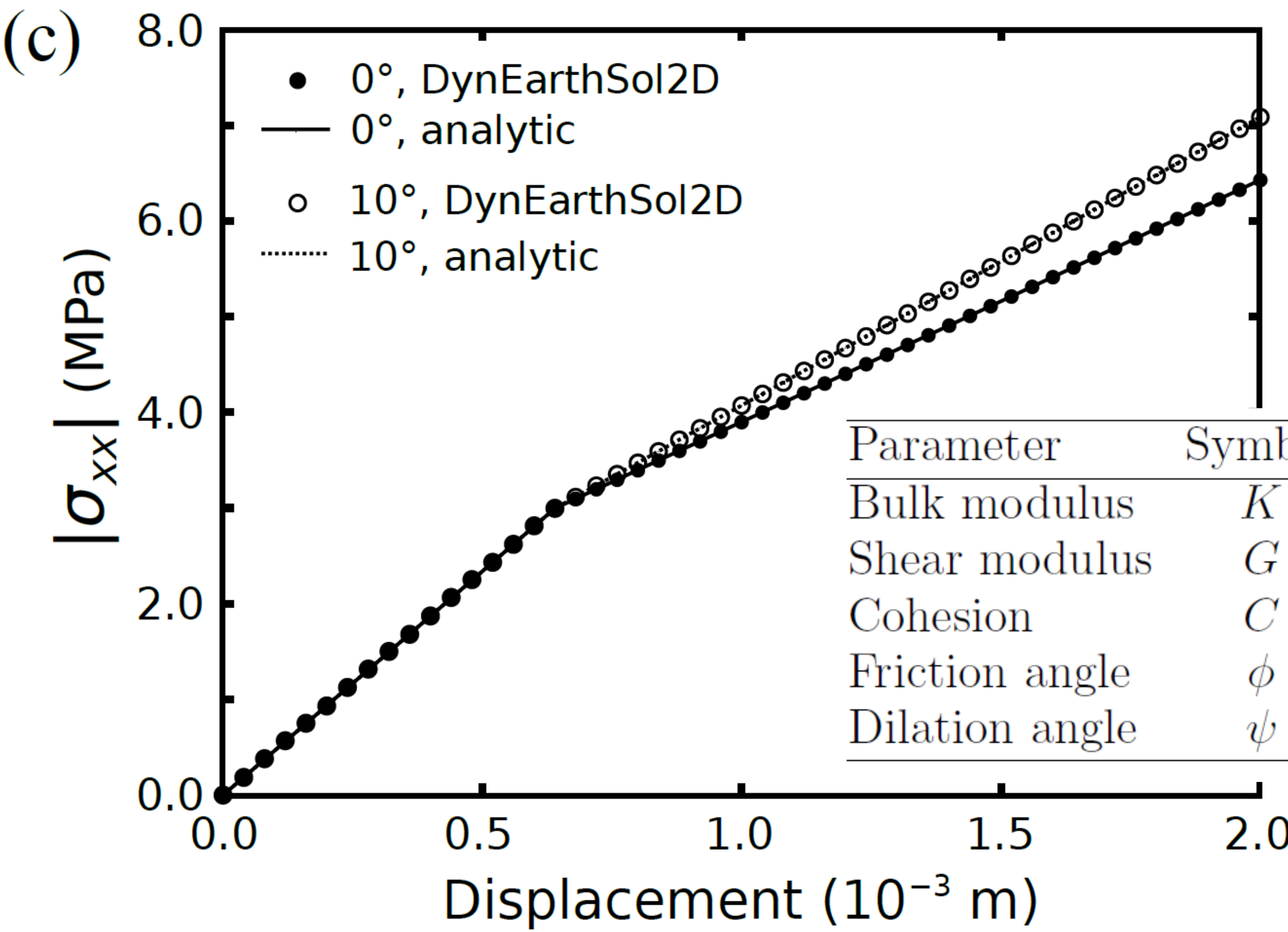
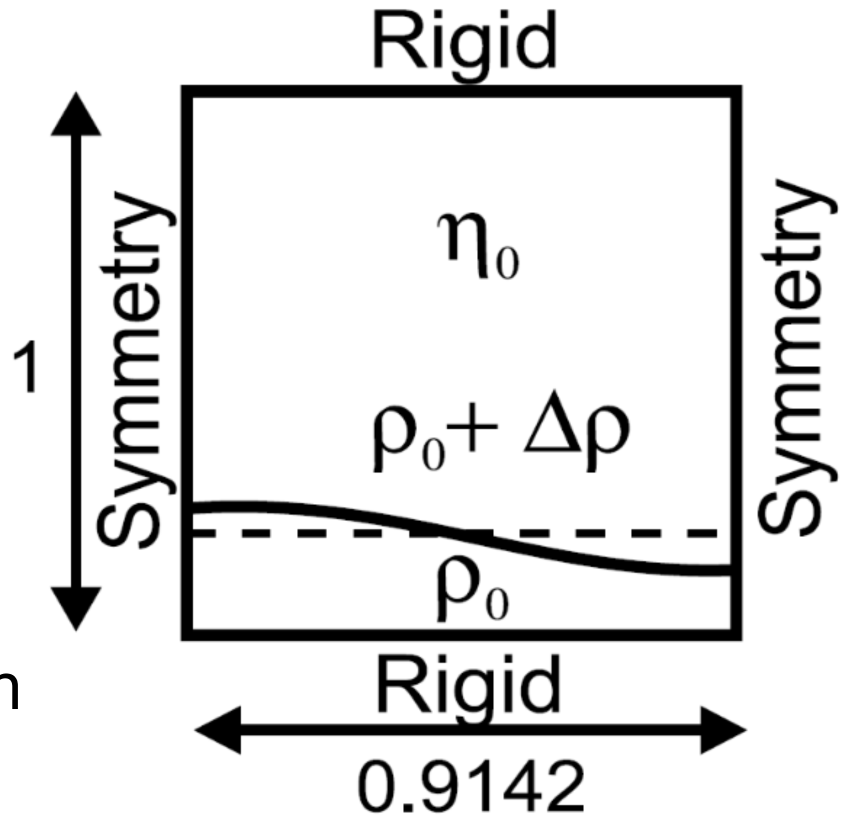


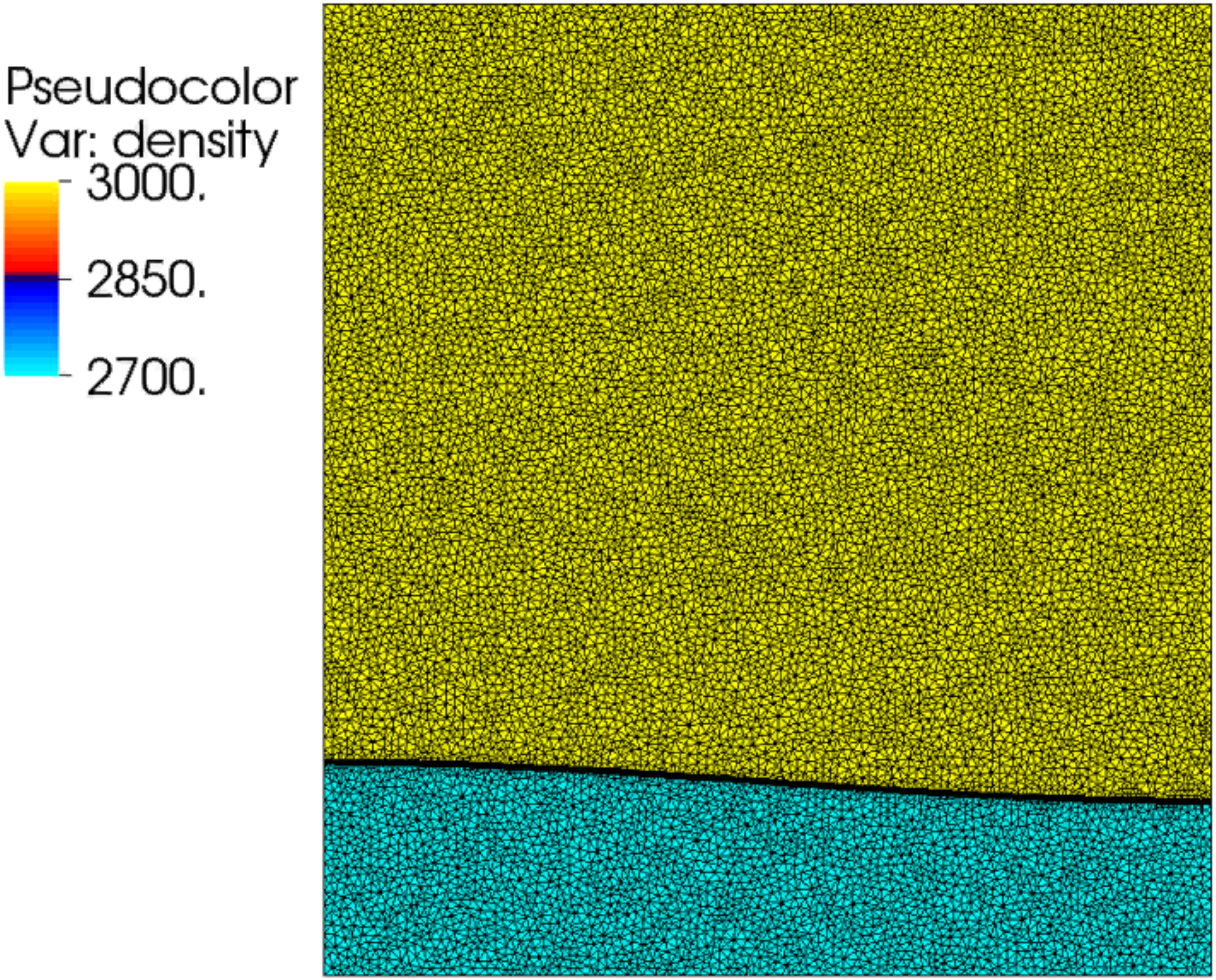
Parameter	Symbol	Value
Bulk modulus	K	200 MPa
Shear modulus	G	200 MPa
Cohesion	C	1 MPa
Friction angle	ϕ	10°
Dilation angle	ψ	0 or 10°

Benchmarks: Rayleigh-Taylor Instability

- G = 30 GPa, ν = 0.25
- g = 10 m/s^2
- η = 10^{17} Pa·s
- ρ_o = 2700,
  $\Delta\rho$ = 300 kg/m^3
- Length scale factor: 10 km
- Resolution: ~100 m

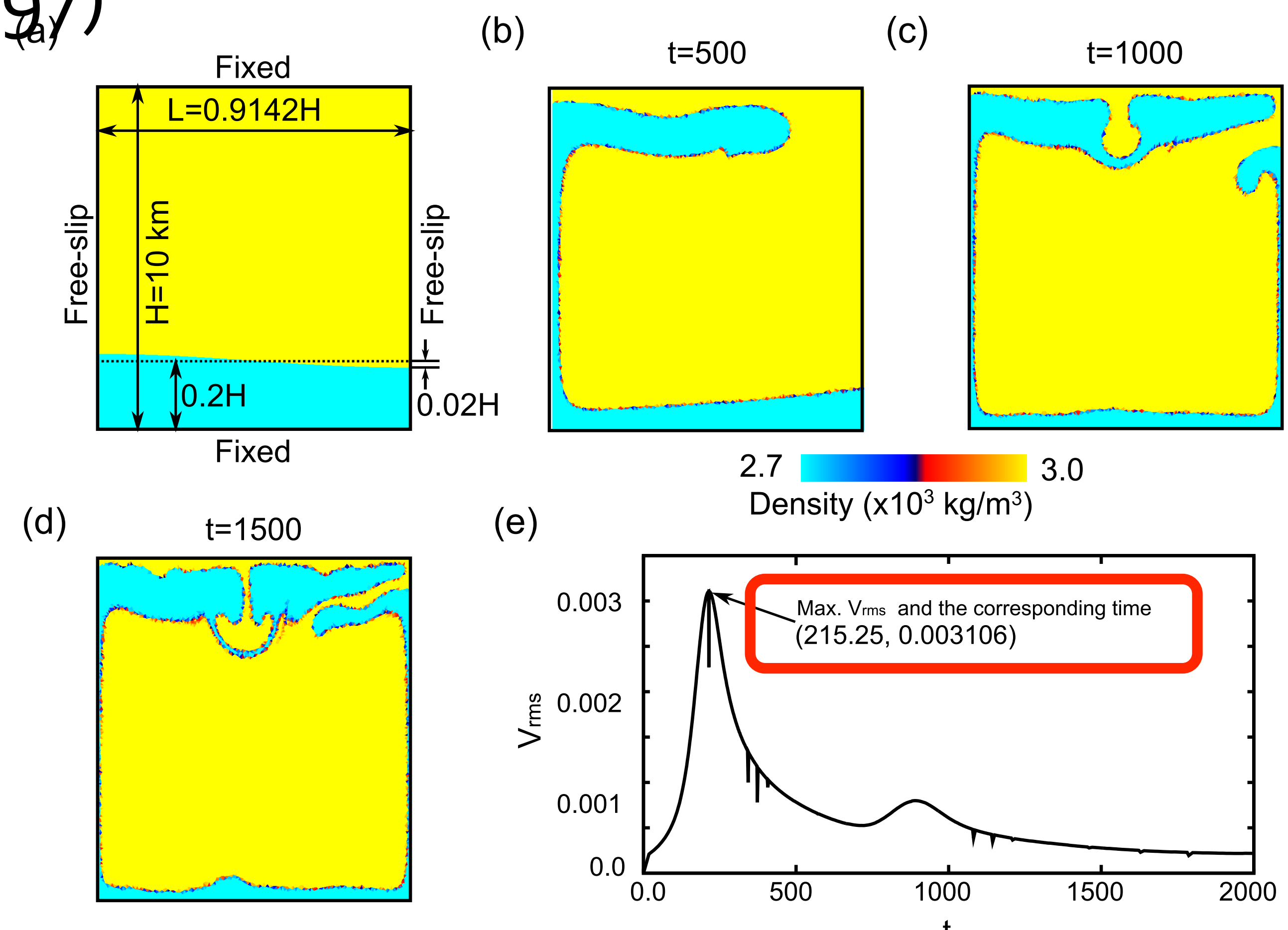


Benchmarks: Rayleigh-Taylor Instability

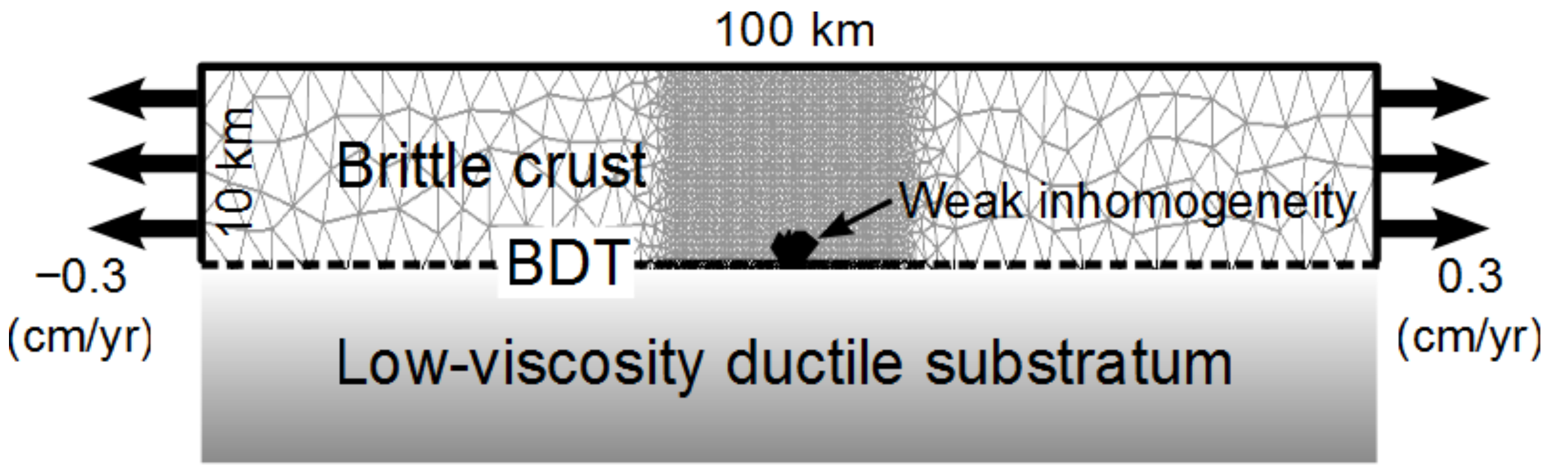


Benchmarks: Rayleigh-Taylor Instability

- 1st peak of v_{rms} is within the range reported in the benchmark study by Van Keken et al. (1997)

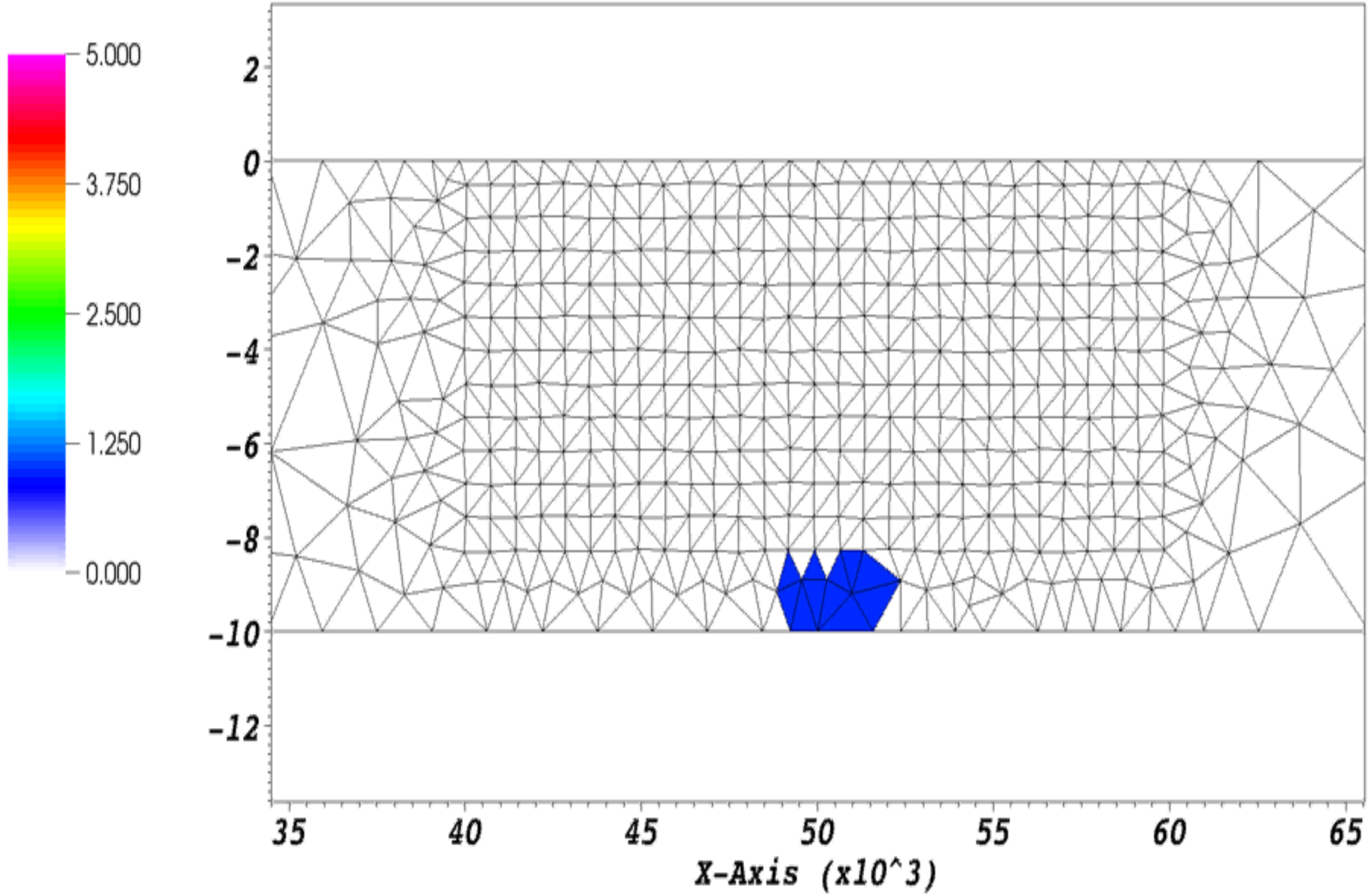


Benchmarks: Fault Evolution

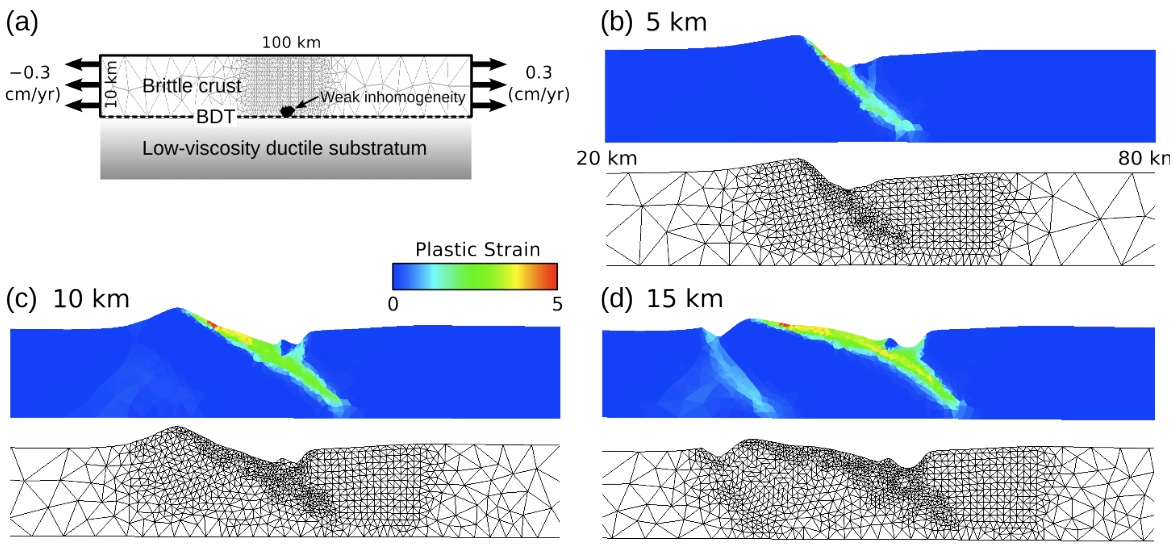


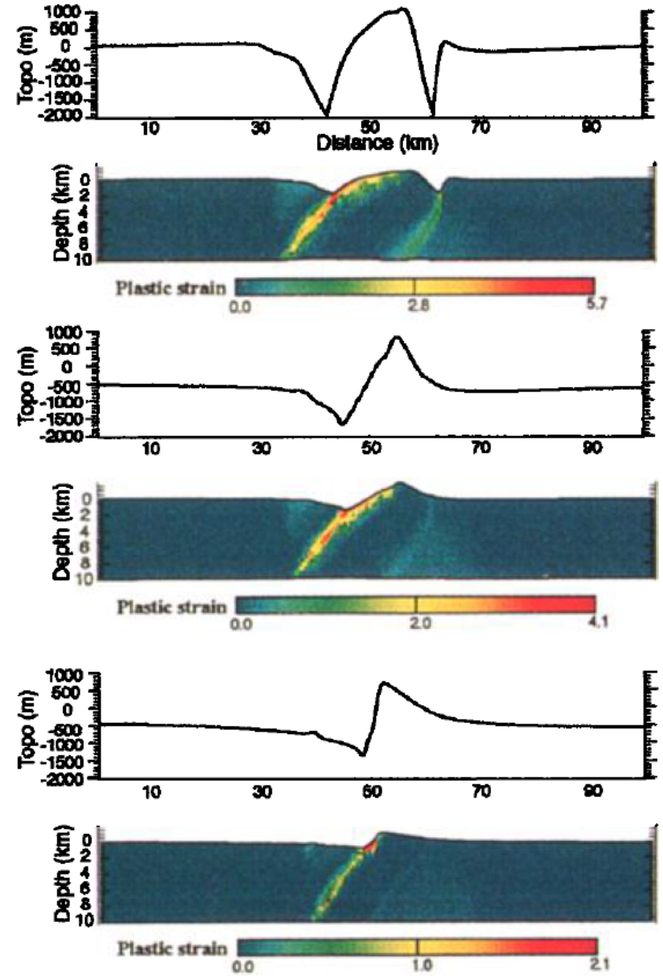
- Lamé's constants: 30 GPa.
- More-Coulomb plasticity:
  - Friction angle = 30°
  - Initial Cohesion = 20 Mpa
  - Strain softening:
    - Cohesion 20 → 4 Mpa as pl. strain increases to 5.0.

Benchmarks: Fault Evolution



Benchmarks: Fault Evolution





- Reproduced the "footwall snapping" mode.
- Contingent **dynamic mesh refinement** along shear zones.

(Lavier et al., JGR, 2000)

Challenges with 3D version

- Important operations become much slower than in 2D:
  - Remeshing with `tetgen` → Local modification.
  - Local supermesh construction → Markers only.

- Parallelization
  - For performance gain with domain decomposition,

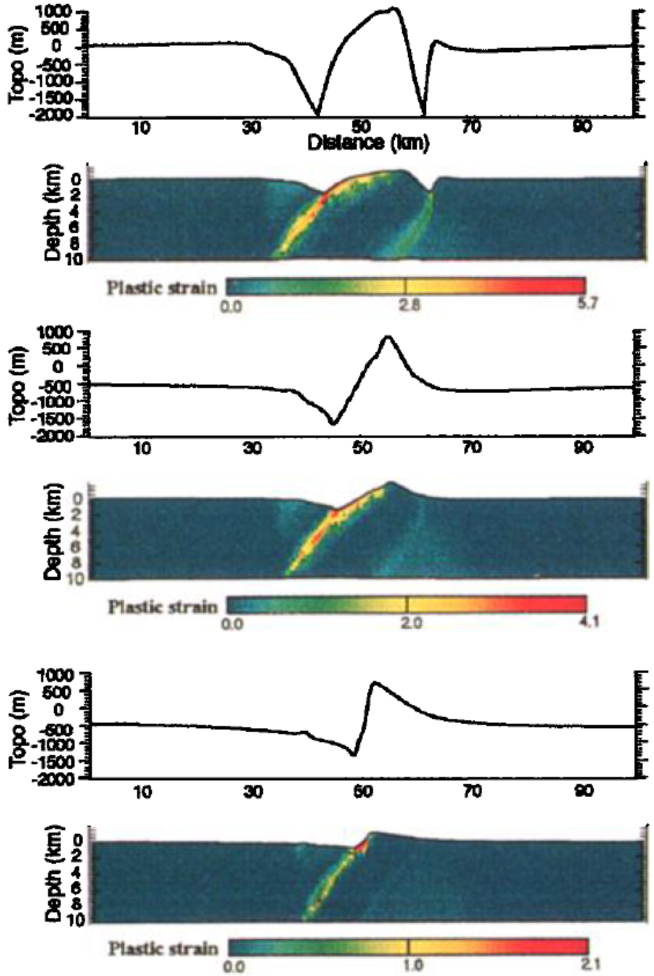
each time step >> MPI overhead. However, in DynEarthSol3D, each time step < MPI overhead even for a decent size of model.
  - Thread-level parallelism with OpenMP.
  - For massive thread generation, trying out co-processors (e.g., GPGPU and Intel Xeon Phi).

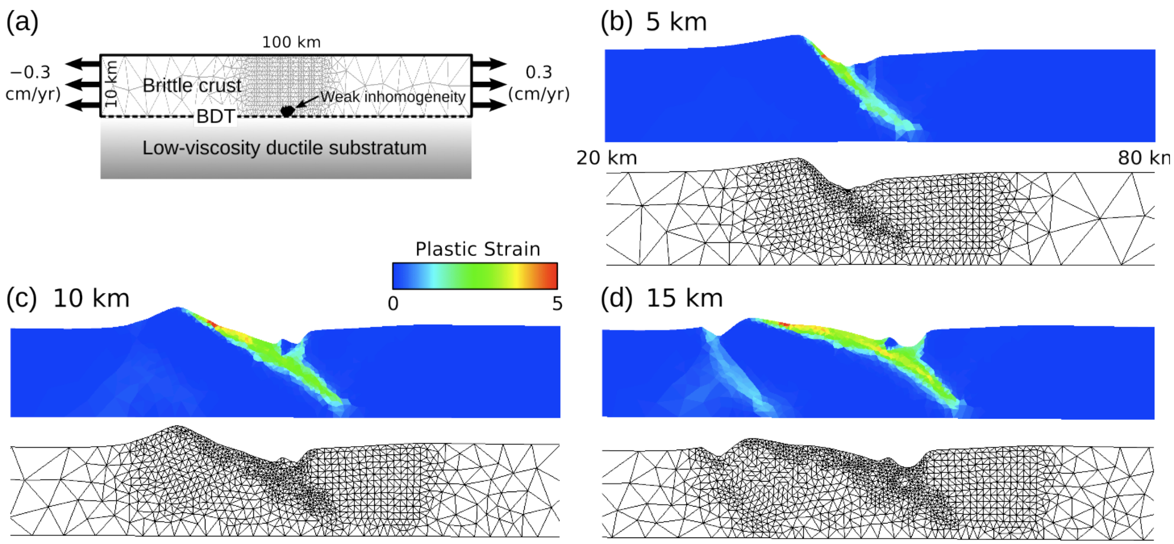
Summary

- DynEarthSol2D/3D
  - **Explicit**, **Lagrangian FE** code for **thermo-mechanical** modeling.
  - Open source:
    https://bitbucket.org/tan2/dynearthsol3d
    https://bitbucket.org/tan2/dynearthsol2d
  - **Dynamic relaxation** and **mass scaling** for (quasi-) static solutions.
  - **Unstructured**, **non-uniform mesh.**
  - **Elasto-visco-plastic** base rheology.
  - **Remeshing** for indefinite amount of deformation
    - Contingent **dynamic mesh refinement.**
  - **Benchmarked.**

Strain Localization at Coulomb Angle

- Strain localization is extremely useful for representing discontinuities like faults in continuum models.





Strain Localization at Coulomb Angle

- Sometimes, we want to predict the orientation of strain localization just as we want to predict fault orientation w.r.t. σ_1.
  - Coulomb angle

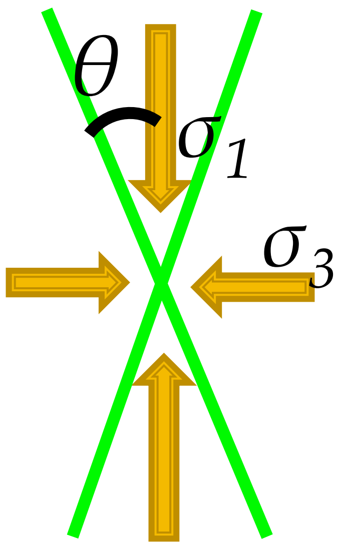
$$\theta = \frac{\pi}{4} - \frac{\phi}{2}$$

  - Roscoe angle

$$\theta = \frac{\pi}{4} - \frac{\psi}{2}$$

  - Arthur angle

$$\theta = \frac{\pi}{4} - \frac{\phi + \psi}{4}$$



Strain Localization at Coulomb Angle

- Meaning of dilation angle

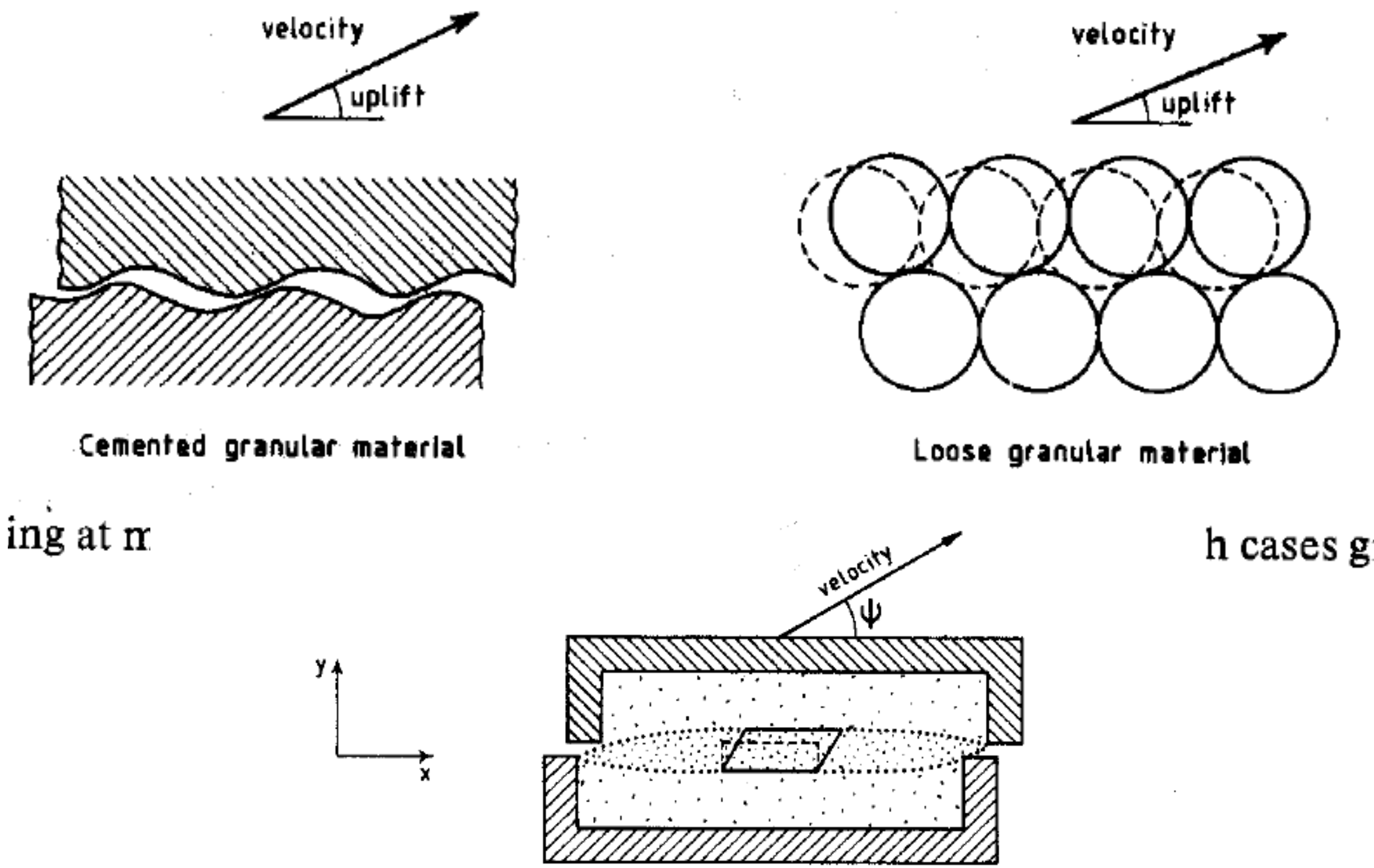
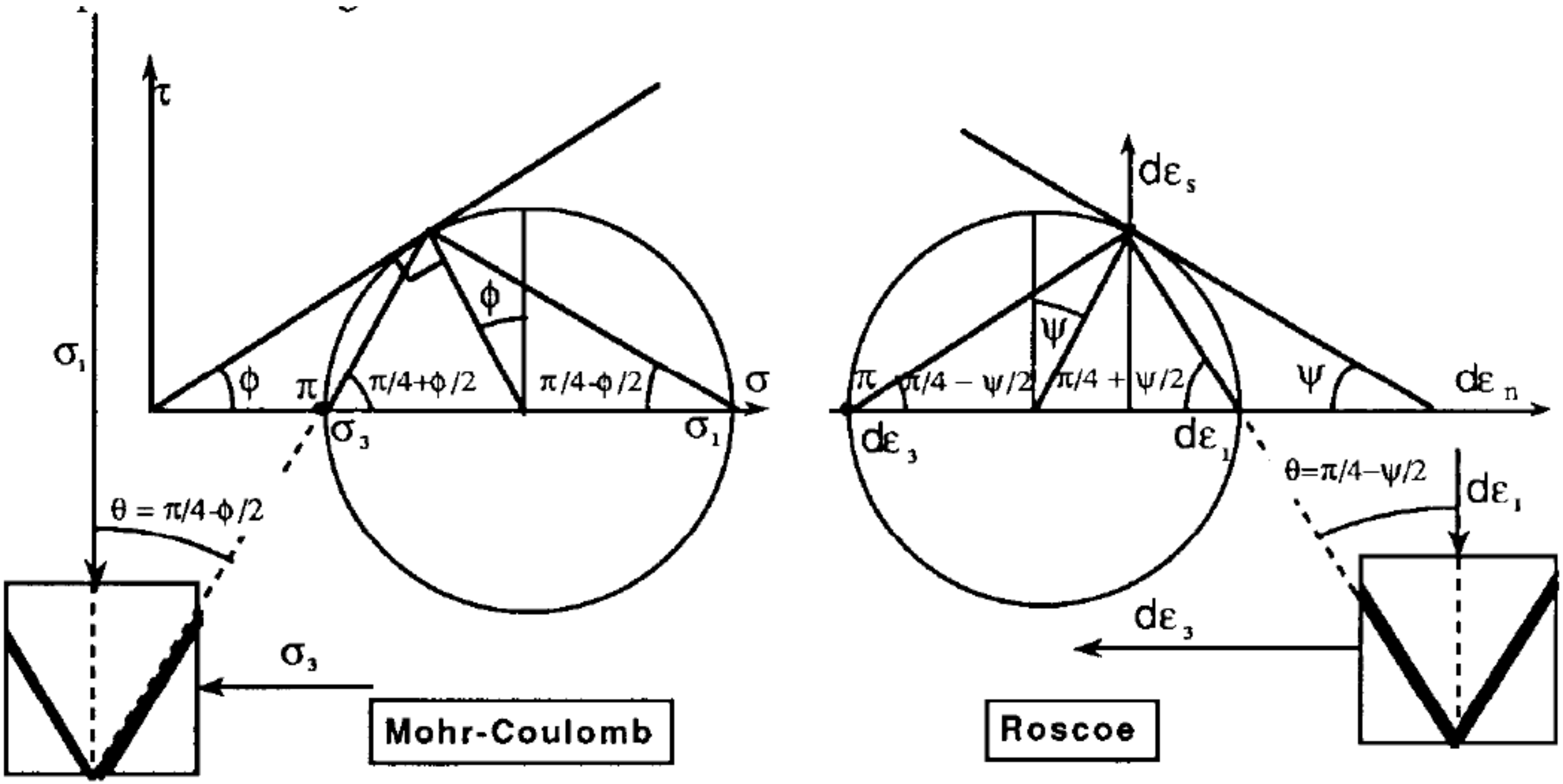


Fig. 4.2 The model predicts an uplift angle ψ for shear bands.

(Vermeer and de Borst, Heron, 1984)

Strain Localization at Coulomb Angle

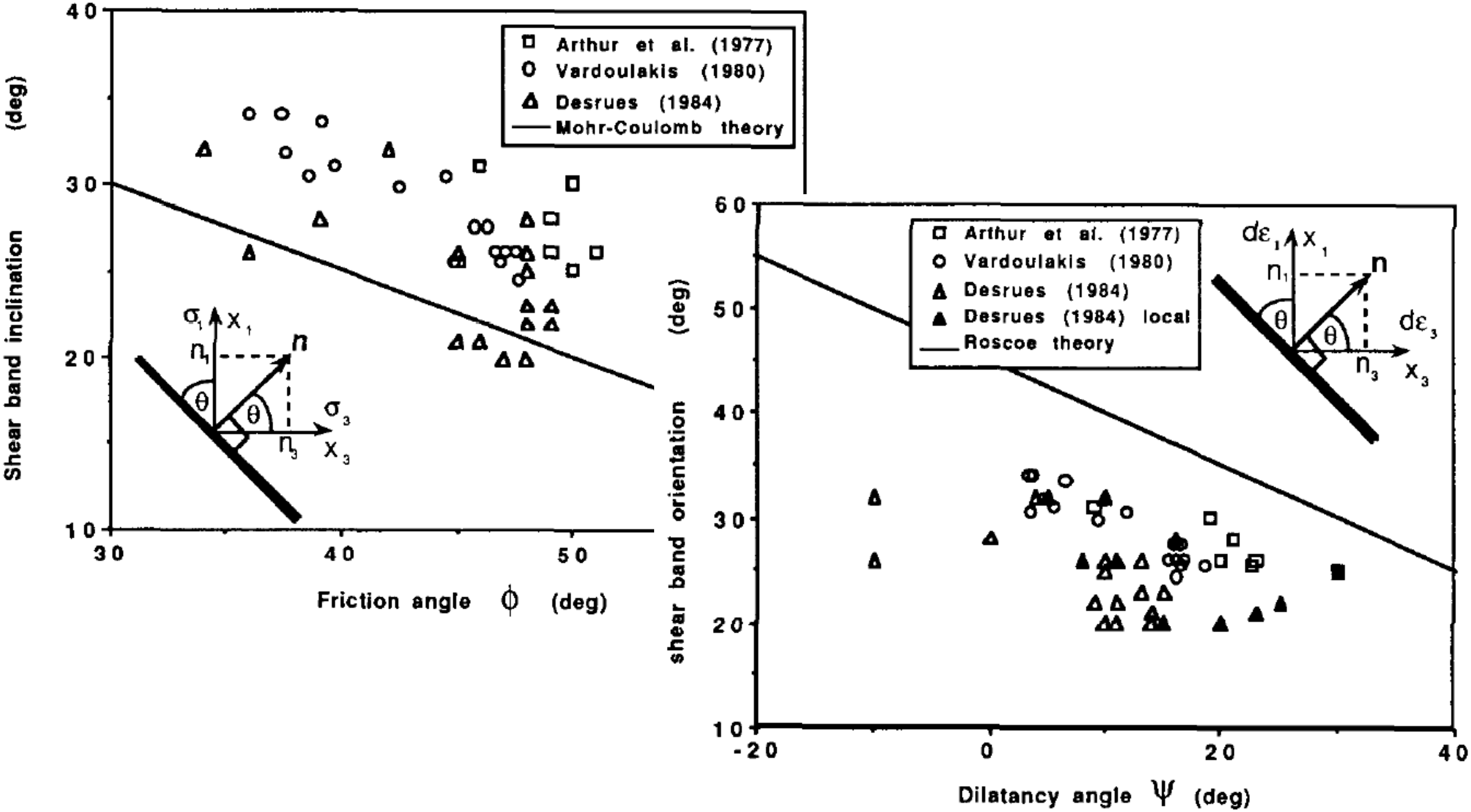
- Geometric derivation



(Bardet, Computers and Geotechnics, 1990)

Strain Localization at Coulomb Angle

- Comparison with experiments



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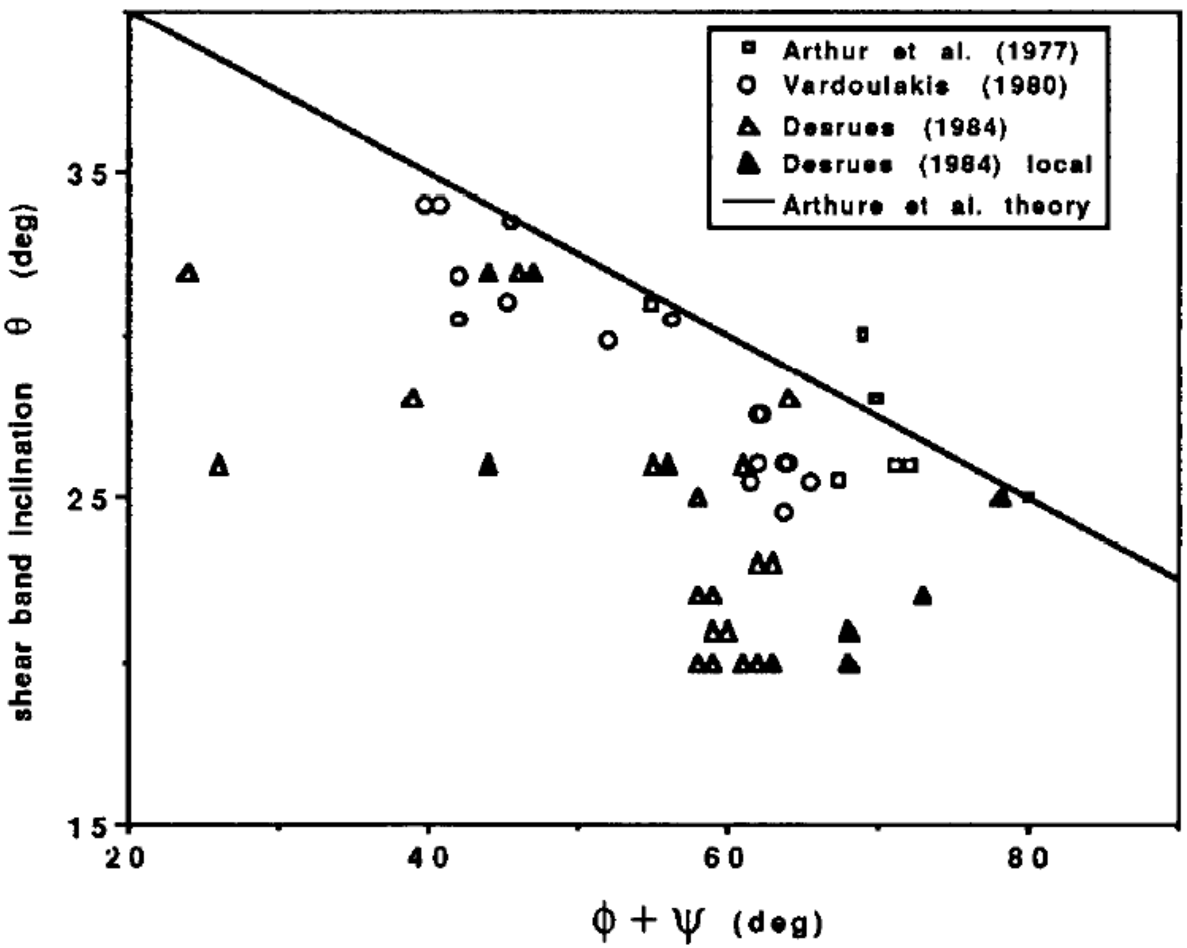
Strain Localization at Coulomb Angle

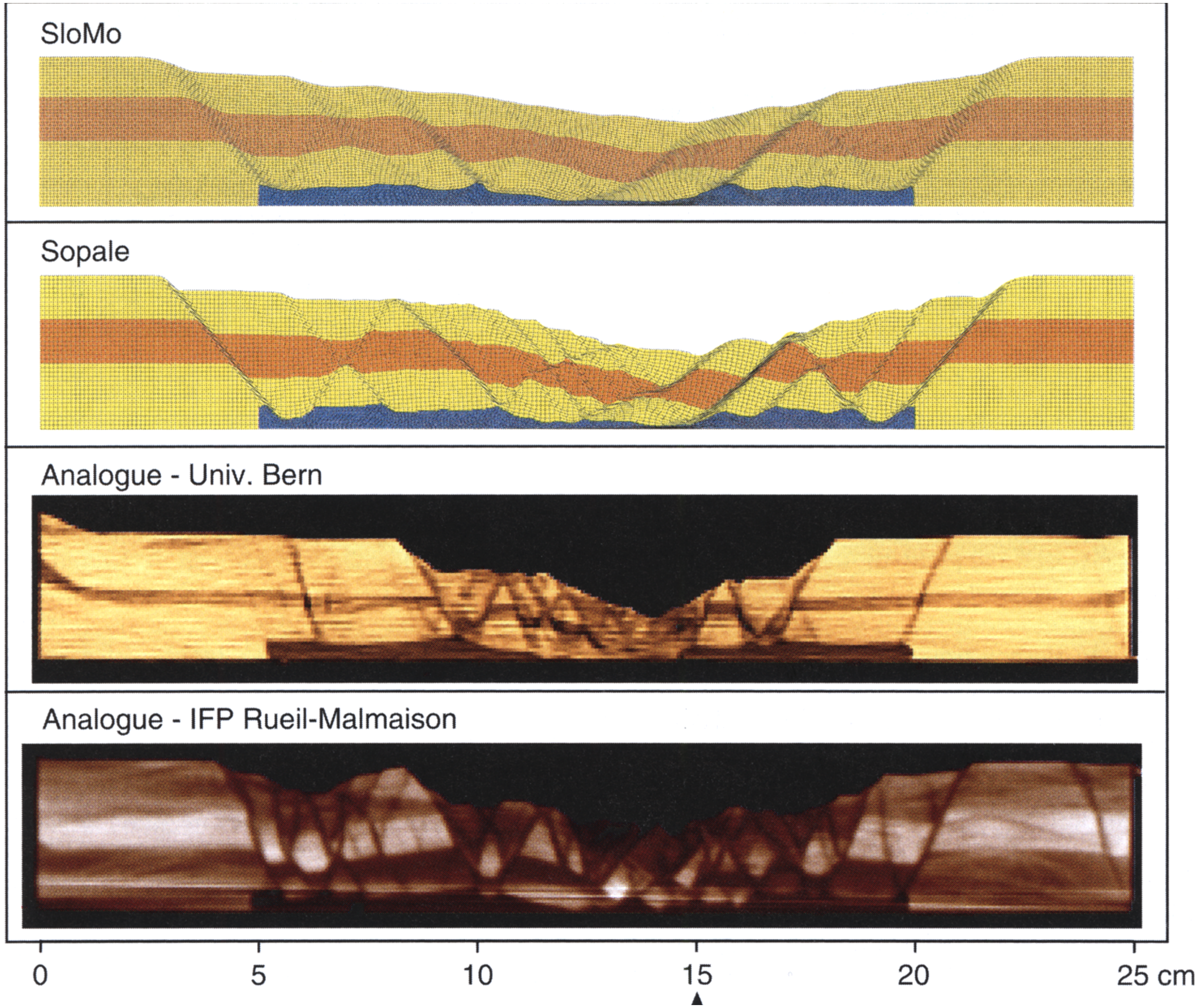
- Comparison with experiments



(Bardet, Computers and Geotechnics, 1990)

Strain Localization at Coulomb Angle

- Numerical and analogue models



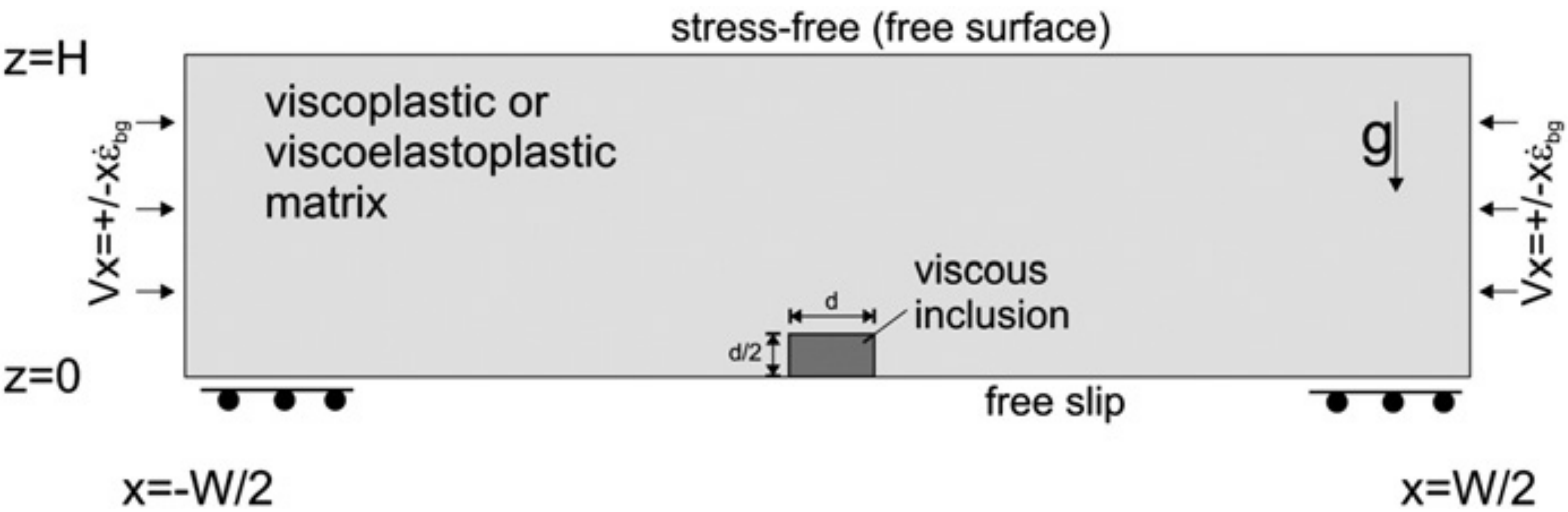
Numerical Models

Analogue Models

(Buiter et al., 2006)

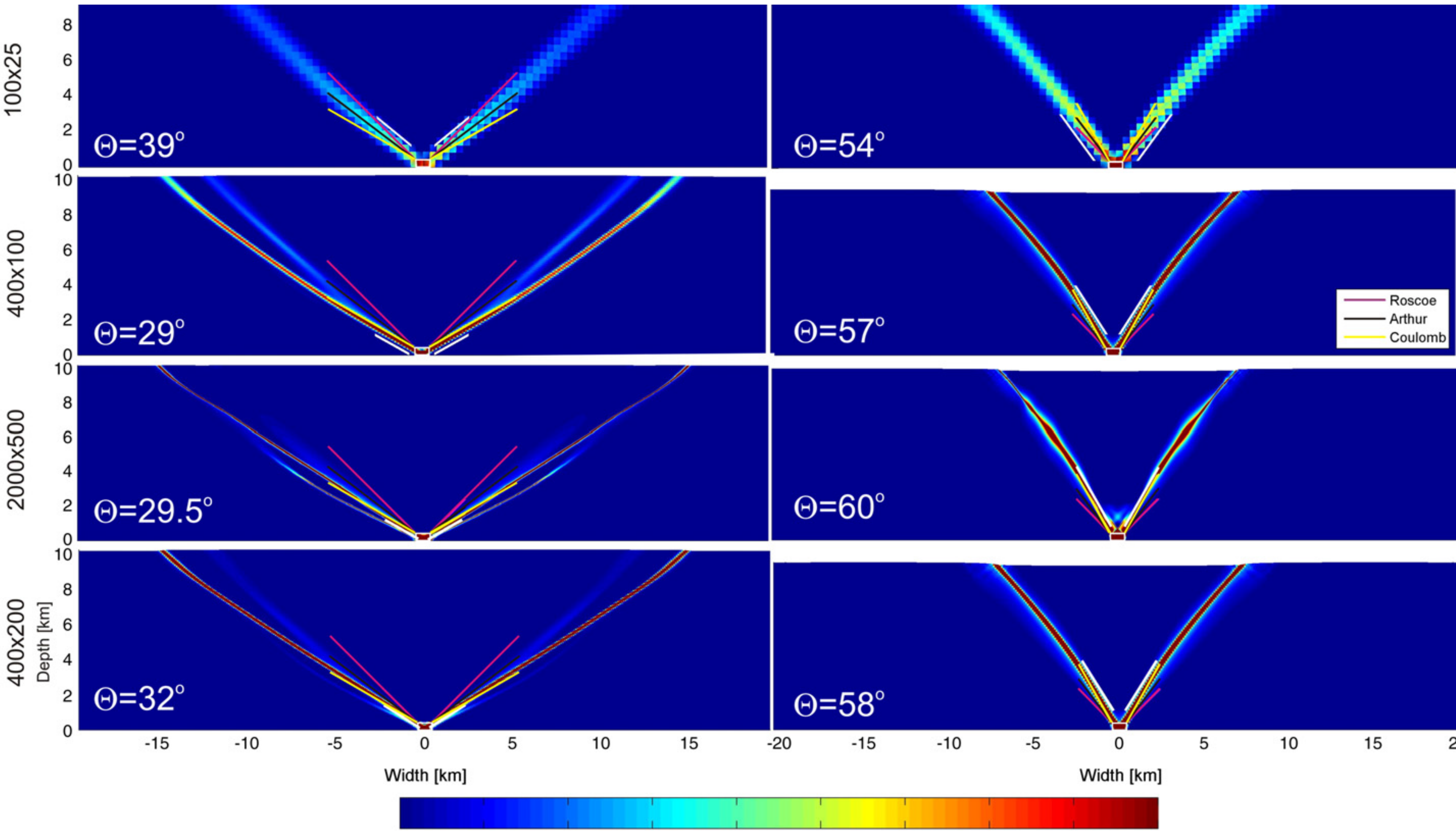
Strain Localization at Coulomb Angle

- Numerical models compared with simple theories (Kaus, 2010).



(Kaus, Tectonophysics, 2010)

Strain Localization at Coulomb Angle



(Kaus, Tectonophysics, 2010)

Strain Localization at Coulomb Angle

- We have shear band orientations from theory, experiments and numerical models.
  - theory ≠ experiments : maybe ok (blame theory!)
  - numerical models ≠ experiments: maybe ok, too.

- What about theory ≠ numerical models?
  - e.g.: shear band from the Mohr-Coulomb plasticity ≠ the Coulomb angle
  - Problematic considering models are based on the theory.
  - This type of discrepancy is often termed "mesh dependence".
  - Maybe not a critical issue but certainly inconvenient for some type of analysis.

Strain Localization at Coulomb Angle

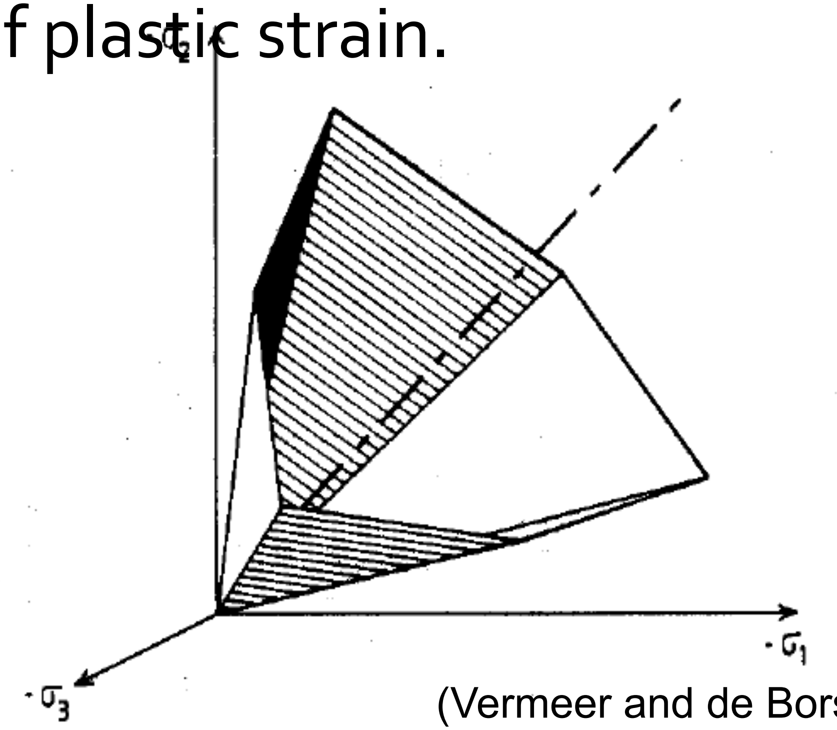
- As a solution, Kaus (2010) suggested that the key to achieving the Coulomb angle is to resolve inhomogeneity (weak "seed") with sufficiently many elements.
- Often the size of seed and the mesh resolution needs to be independent of each other.
- Still need to understand why models show discrepancy from simple theoretical predictions.

Strain Localization at Coulomb Angle

- Strain localization theory: Mohr-Coulomb yield function

$$f(\sigma_1, \sigma_3, \alpha) = (\sigma_1 - \sigma_3) - \sin\phi(\alpha)\left(\sigma_1 + \sigma_3 + \frac{C(\alpha)}{\tan\phi(\alpha)}\right) = 0.$$

  - α: Internal variable, a metric (typically, second invariant) of plastic strain.



(Vermeer and de Borst, Heron, 1984)

Strain Localization at Coulomb Angle

- Strain localization theory: Hardening modulus

$$H = \frac{\partial f}{\partial \alpha} = \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial \alpha} + \frac{\partial f}{\partial C}\frac{\partial C}{\partial \alpha}$$

  - $H > 0$: strain hardening, $H < 0$: strain weakening/ softening.

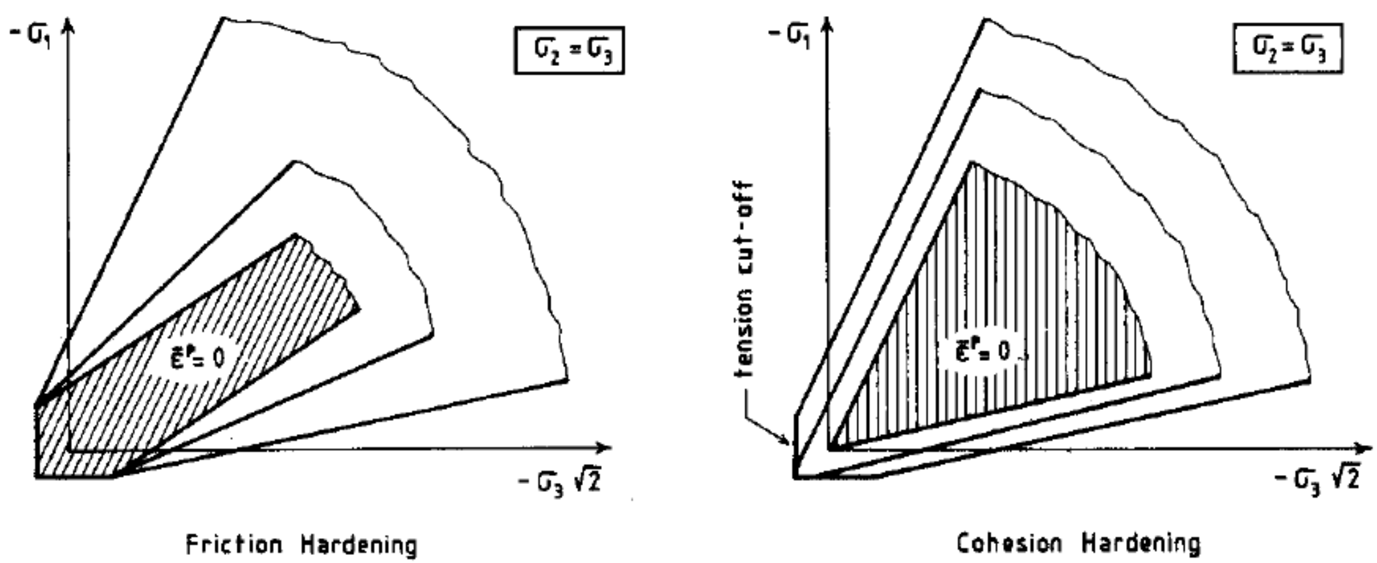


Fig. 6.4 Largely different modes of expansion for the elastic range.
(Vermeer and de Borst, Heron, 1984)

Strain Localization at Coulomb Angle

- Strain localization theory: Conditions on stress/strain
  - normal traction must be continuous across the shear band boundaries.
  - Don't allow band-parallel strain.

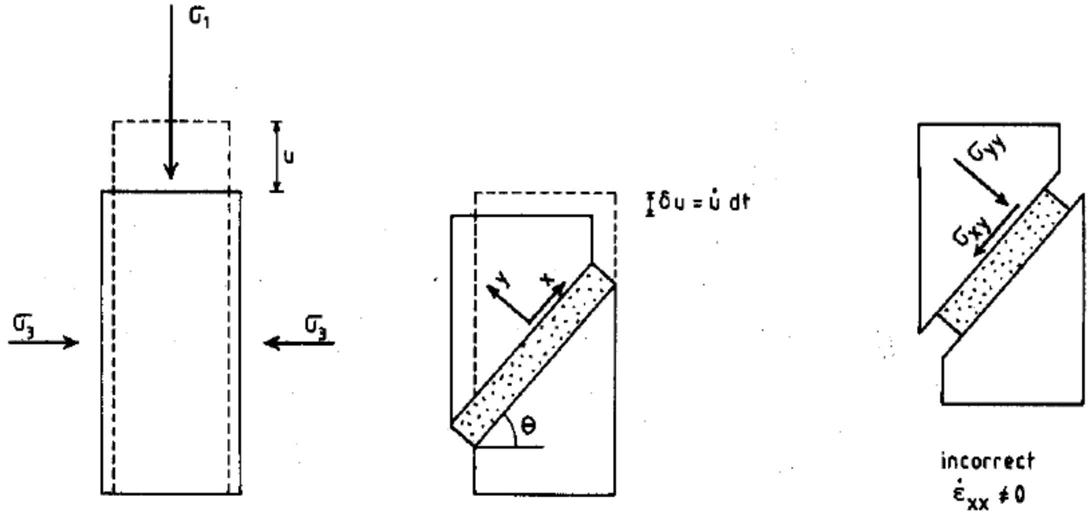


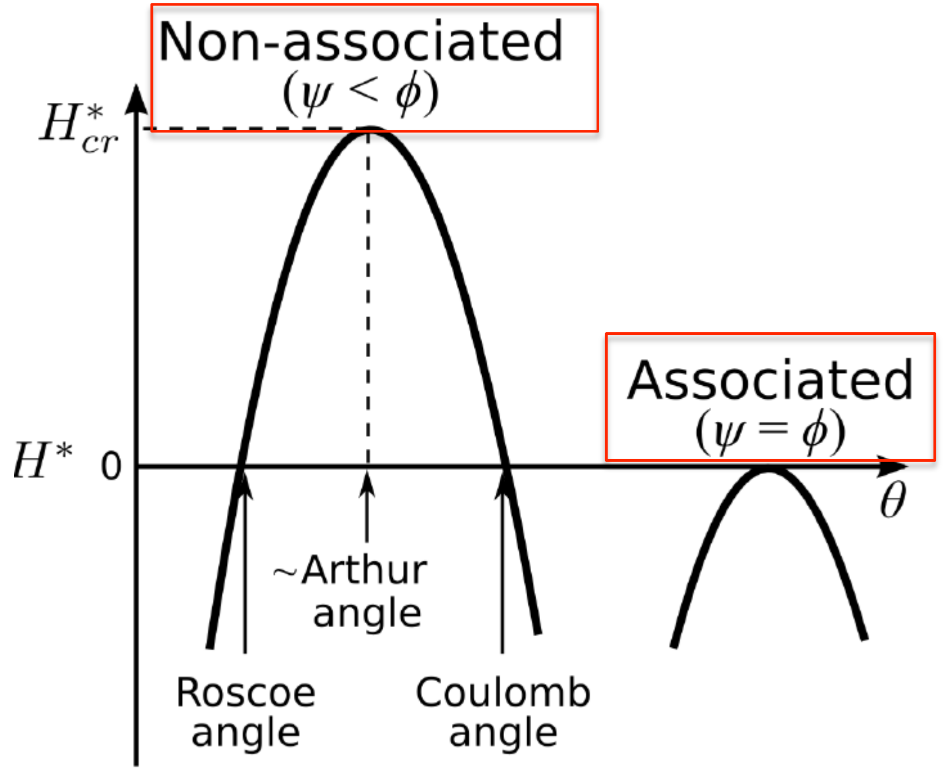
Fig. 8.3 a. Uniform deformation up to current state
b. Further deformation localized in a shear band
c. Incorrect mechanism.

(Vermeer and de Borst, Heron, 1984)

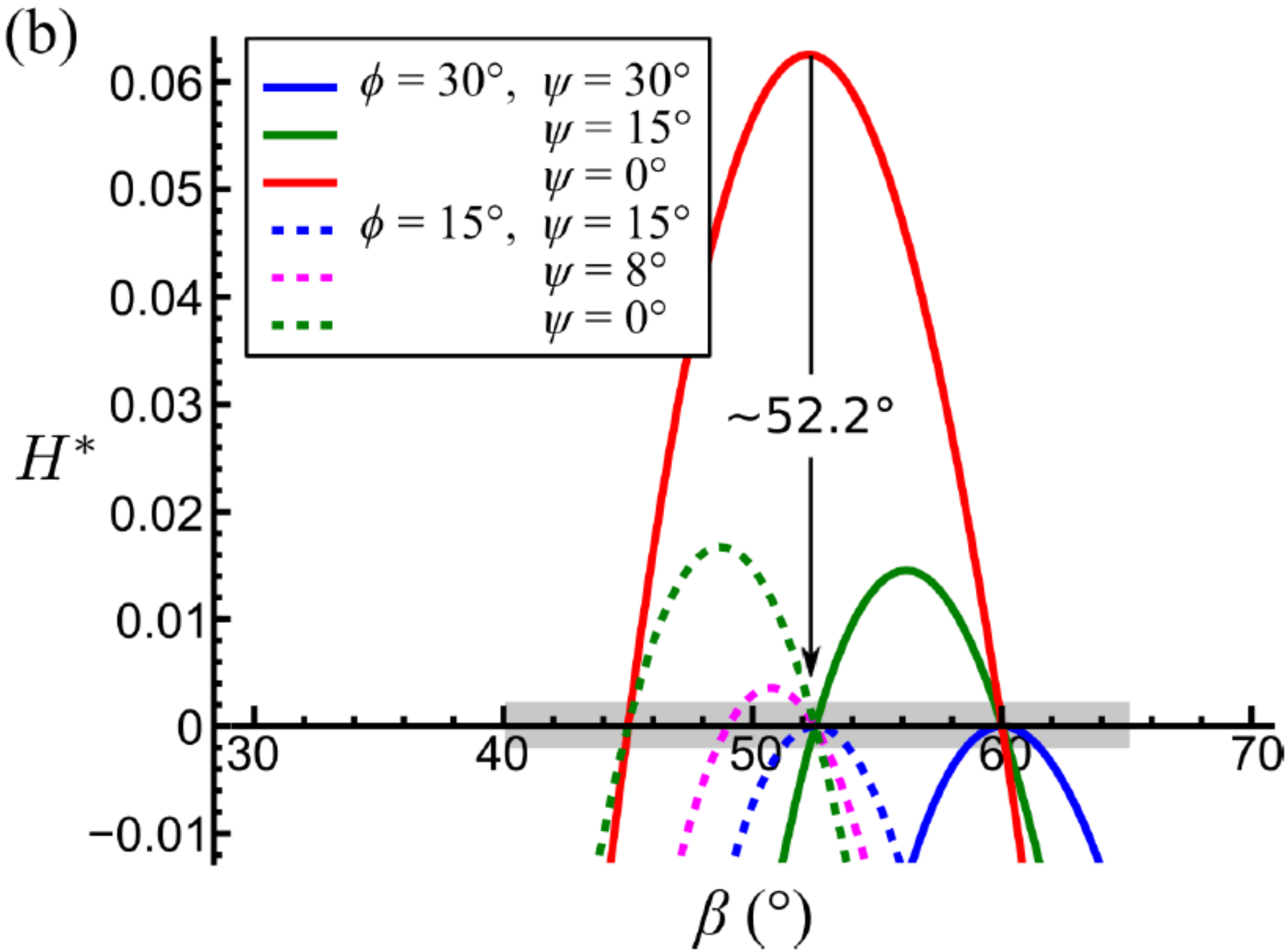
Strain Localization at Coulomb Angle

- From these conditions, we get a relationship between H^* and ϑ:

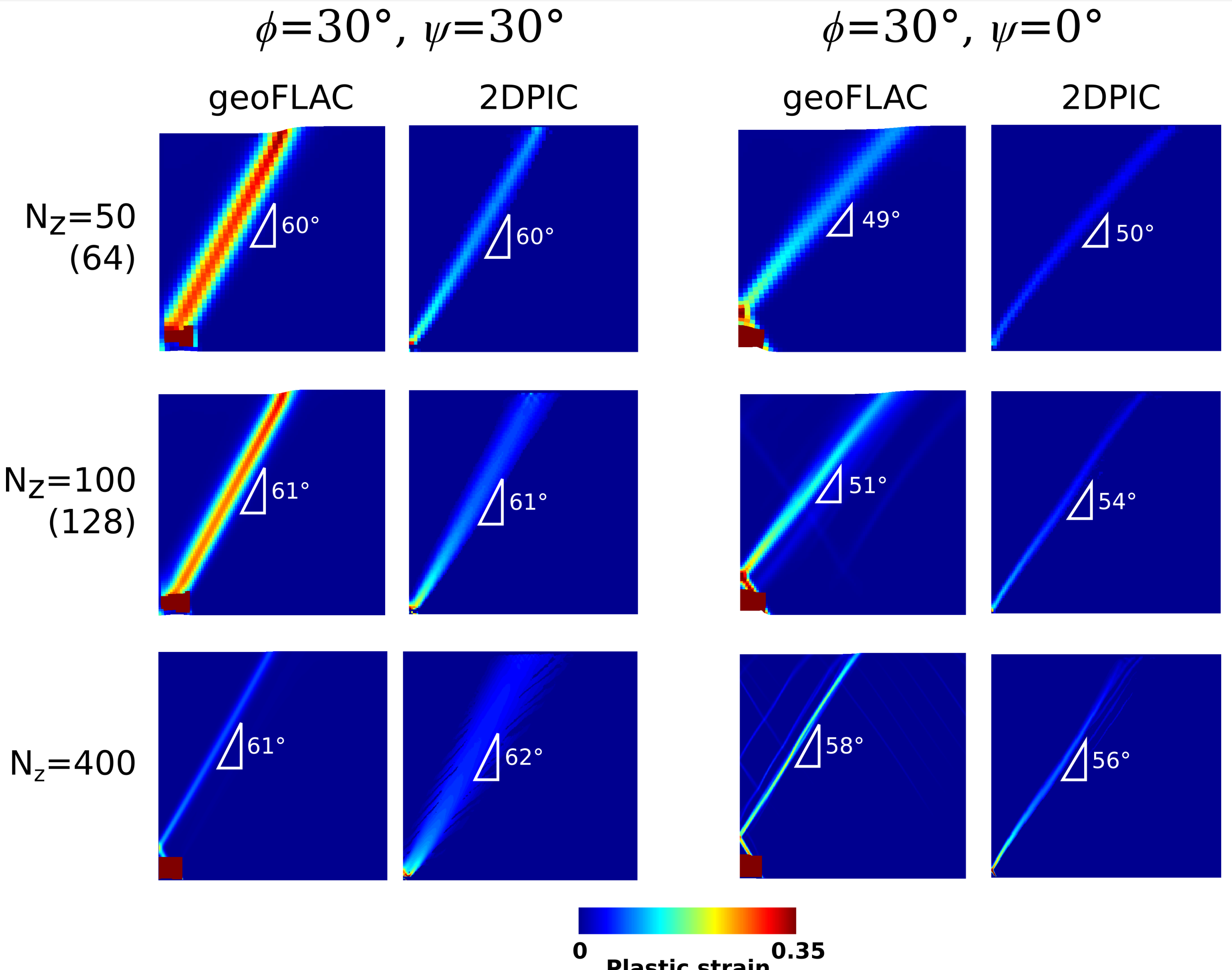
$$H^* = \frac{H}{2G} = \frac{(\sin\psi - \sin\phi)^2 - (2\cos 2\theta - \sin\psi - \sin\phi)^2}{8(1-\nu)\sqrt{(1+\sin^2\psi)(1+\sin^2\phi)}}$$



Strain Localization at Coulomb Angle



Strain Localization at Coulomb Angle



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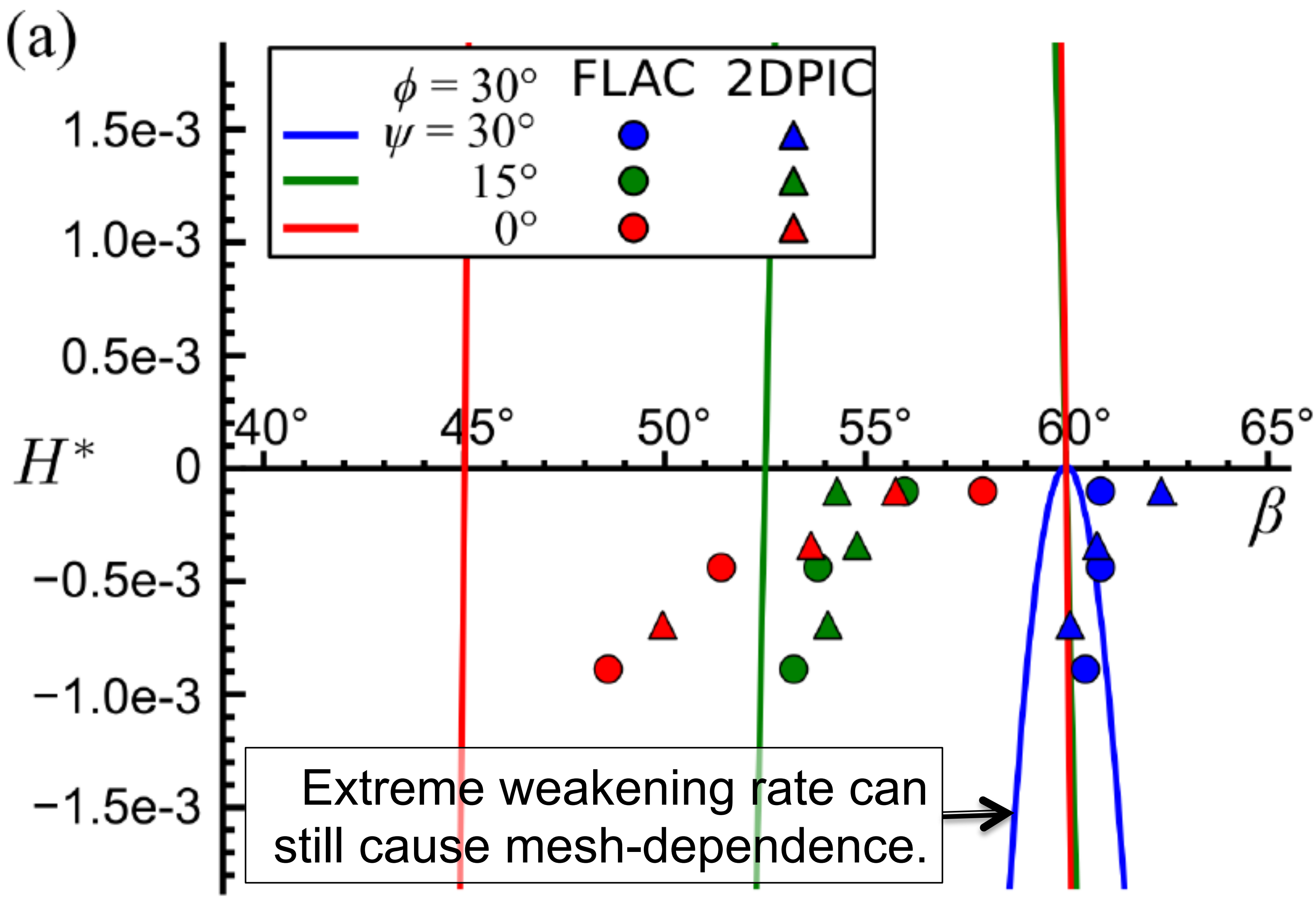
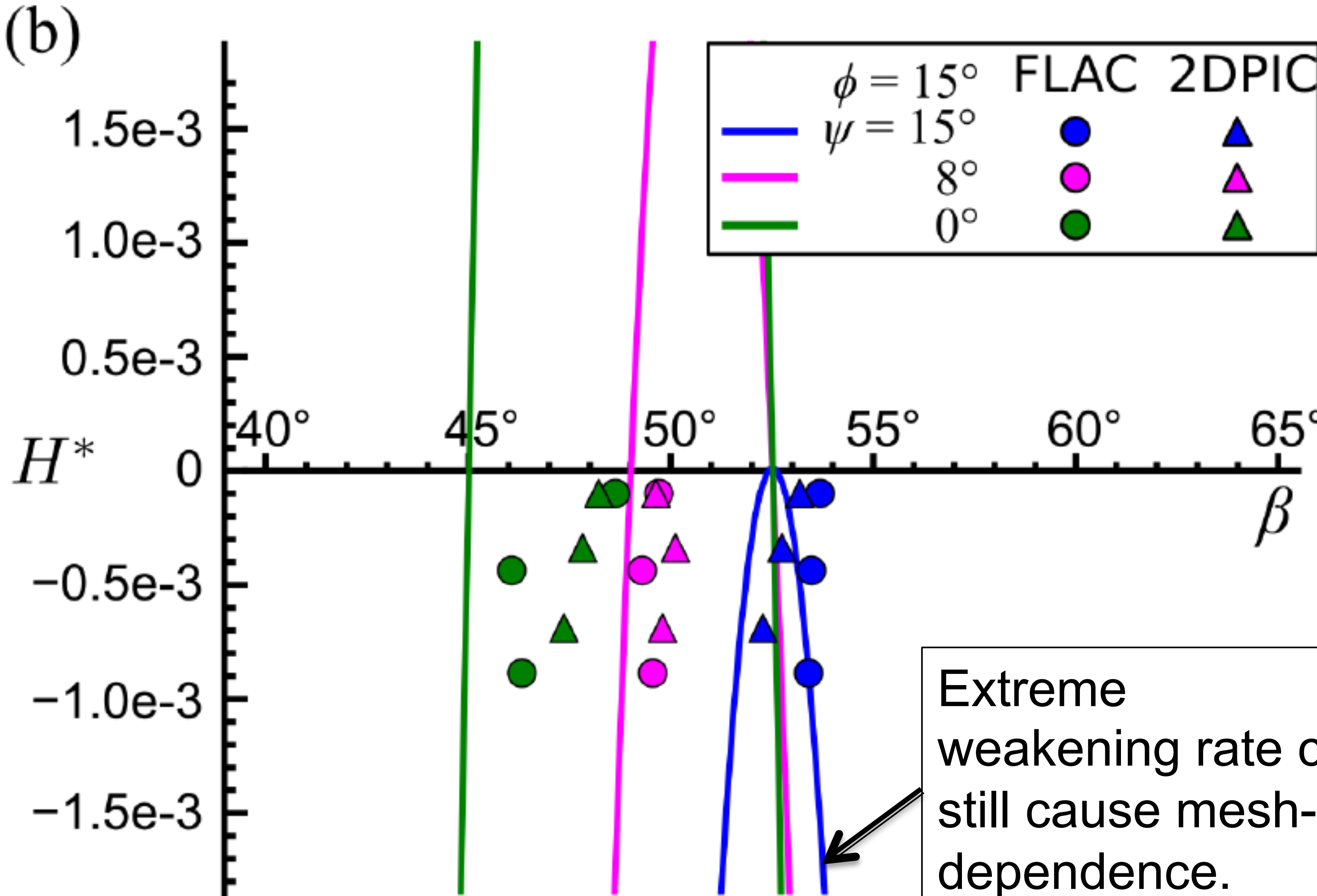


Strain Localization at Coulomb Angle



Extreme weakening rate can still cause mesh-dependence.

Strain Localization at Coulomb Angle

- In summary, the combination of **associated flow rule** and **modest *H*** is a sufficient condition for Coulomb angle-oriented shear bands.
  - Seems insensitive to mesh resolution and inhomogeneity resolution.

- Caveat: A constant dilation angle means non-stopping expansion of shear band
  - Need to decrease gradually.
  - Might correspond to the process of asperity abrasion.

Strain Localization at Coulomb Angle

- Dilation angle reduction also necessary for modeling long-term evolution.