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

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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.
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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](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

- **Dynamic Earth Solver for 2D.**

- Principle of virtual power

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

- Discretized momentum equation after the standard FE procedure

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

- Energy balance equation is discretized similarly.
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 explicit time integration.

\[
\begin{align*}
\mathbf{v}_a(t+\Delta t/2) &= \mathbf{v}_a(t-\Delta t/2) + \mathbf{F}_a(t) \frac{\Delta t}{m_a} \\
\mathbf{x}_a(t+\Delta t) &= \mathbf{x}_a(t) + \mathbf{v}_a(t+\Delta t/2) \Delta t
\end{align*}
\]
Key Components of DynEarthSol2D

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

\[
v_{a_i}^{i,(t+\Delta t/2)} = v_{a_i}^{i,(t-\Delta t/2)} + (F_{a_i}^{i,(t)} + F_d^i) \frac{\Delta t}{m_a},
\]

where \( F_d^i = -\alpha |F_{a_i}^{i,(t)}| \text{sgn}(v_{a_i}^{i}) \), where \( 0 \leq \alpha < 1 \).

- **Mass scaling** for a large and stable \( \Delta t \)

\[
\Delta t < \frac{\Delta x}{v_p} \quad v_p = \sqrt{\frac{K}{m_s}} \quad m_s \gg m_g = \int \rho \, dV
\]
Key Components of DynEarthSol2D

- Constitutive model: elastovisco-plastic

  \[ \sigma_Y \rightarrow \infty: \text{Maxwell viscoelasticity.} \]
  \[ \eta \rightarrow \infty: \text{Mohr-Coulomb plasticity.} \]
  \[ \eta = \eta(T, \sigma): \text{temperature-determined brittle-ductile transition} \]
  \[ \sigma_Y = \sigma_Y(\varepsilon^*): \text{strain hardening/softening} \]
Key Components of DynEarthSol2D

- Remeshing
Key Components of DynEarthSol2D

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

Before

After
Key Components of DynEarthSol2D

- Remeshing (cont’d)
  - Mapping of sharp boundaries: **Markers** further needed.
Benchmarks: Plastic Oedometer

(a)

(b)

\sigma_1 = \sigma_2 = \sigma_3

\sigma_1

\sigma_2

\sigma_3
Benchmarks: Plastic Oedometer

Parameter | Symbol | Value
---|---|---
Bulk modulus | $K$ | 200 MPa
Shear modulus | $G$ | 200 MPa
Cohesion | $C$ | 1 MPa
Friction angle | $\phi$ | 10°
Dilation angle | $\psi$ | 0 or 10°
• $G = 30 \text{ GPa}$, $\nu = 0.25$
• $g = 10 \text{ m/s}^2$
• $\eta = 10^{17} \text{ Pa}\cdot\text{s}$
• $\rho_0 = 2700$, $\Delta\rho = 300 \text{ kg/m}^3$
• Length scale factor: 10 km
• Resolution: $\sim 100 \text{ m}$
Benchmarks: Rayleigh-Taylor Instability

Pseudocolor
Var: density
- 3000.
- 2850.
- 2700.
1\textsuperscript{st} peak of $v_{rms}$ is within the range reported in the benchmark study by Van Keeken et al. (1997)
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
• 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 $\rightarrow$ Local modification.
  - Local supermesh construction $\rightarrow$ Markers only.

- Parallelization
  - For performance gain with domain decomposition, each time step $\gg$ 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/dynearthsol3d) [https://bitbucket.org/tan2/dynearthsol2d](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 is extremely useful for representing discontinuities like faults in continuum models.
Sometimes, we want to predict the orientation of strain localization just as we want to predict fault orientation w.r.t. $\sigma_1$.

- **Coulomb angle**
  \[ \theta = \frac{\pi}{4} - \frac{\phi}{2} \]

- **Roscoe angle**
  \[ \theta = \frac{\pi}{4} - \frac{\psi}{2} \]

- **Arthur angle**
  \[ \theta = \frac{\pi}{4} - \frac{\phi + \psi}{4} \]
Meaning of dilation angle

Fig. 4.2 The model predicts an uplift angle $\psi$ 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

(Bardet, Computers and Geotechnics, 1990)
Strain Localization at Coulomb Angle

- Comparison with experiments

(Bardet, Computers and Geotechnics, 1990)
Strain Localization at Coulomb Angle

- Numerical and analogue models

(Buiter et al., 2006)
Numerical models compared with simple theories (Kaus, 2010).
Strain Localization at Coulomb Angle

(Kaus, Tectonophysics, 2010)
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.
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

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

- \( \alpha \): 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.

\[ \varepsilon^* = 0 \]

![Friction Hardening](image1)

![Cohesion Hardening](image2)

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)
From these conditions, we get a relationship between $H^*$ and $\theta$:

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

- **Non-associated** ($\psi < \phi$)
- **Associated** ($\psi = \phi$)
Strain Localization at Coulomb Angle

(b)

$H^*$

$\phi = 30^\circ$, $\psi = 30^\circ$
$\psi = 15^\circ$
$\psi = 0^\circ$
$\phi = 15^\circ$, $\psi = 15^\circ$
$\psi = 8^\circ$
$\psi = 0^\circ$

$\sim 52.2^\circ$

$\beta (^\circ)$
Strain Localization at Coulomb Angle

$\phi=30^\circ, \psi=30^\circ$

$\phi=30^\circ, \psi=0^\circ$

geoFLAC  2DPIC  geoFLAC  2DPIC

$N_z=50$ (64)

$N_z=100$ (128)

$N_z=400$

Plastic strain

0  0.35
Extreme weakening rate can still cause mesh-dependence.
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.
Dilation angle reduction also necessary for modeling long-term evolution.