SNAC: a tutorial

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What is SNAC?

- StGermaiN Analysis of Continua
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- **StGermain Analysis of Continua**
- 3-D Version of FLAC
What is SNAC?

• StGermain Analysis of Continua
• 3-D Version of FLAC
• Essentially,
  ○ dynamic,
  ○ explicit, and
  ○ Lagrangian
  ○ finite element code with
  ○ linear tetrahedral elements.
Governing Equations

- Principle of virtual power in **dynamic** form

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

- Heat energy balance.
Discrete Equations

• Local equilibrium on a node
  \[ \mathbf{a}^{tn+\Delta t} = \frac{1}{M} (\mathbf{F}_{int}^{tn} + \mathbf{F}_{ext}^{tn}) \]

• Forward Euler (explicit)
  \[ M\dot{\mathbf{v}} = \mathbf{F}_{int} + \mathbf{F}_{ext} = \mathbf{F}_{res} \]
  \[ \mathbf{v}(t + \Delta t) = \mathbf{v}(t) + \Delta t \frac{\mathbf{F}_{res}}{M} \]

• Updated Lagrangian
  \[ \mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \mathbf{v}(t) \]

• No matrix assembly.
Then, why called "finite difference" code?

Algebraic approximation to partial derivatives. No shape functions.

\[
\int_{\Omega} f_{,i} \, dV = \int_{\partial \Omega} f n_i \, d\Gamma, \quad (1)
\]

\[
f_{,i} = \frac{1}{V} \int_{\partial \Omega} f n_i \, d\Gamma, \quad (2)
\]

\[
f_{,i} = \frac{1}{V} \sum_{l=1}^{4} \bar{f}^l n_i^l A^l = \frac{1}{V} \sum_{l=1}^{4} \frac{1}{3} \sum_{m=1, \neq l}^{4} f^m n_i^l A^l
\]

\[
= \frac{1}{3V} \sum_{m=1}^{4} f^m \sum_{l=1, \neq m}^{4} n_i^l A^l
\]

\[
= -\frac{1}{3V} \sum_{m=1}^{4} f^m n_i^m A^m, \quad (3)
\]
Features

- **3-D, MPI-parallel, domain decomposition.** All supported by StGermain. Decent performance known up to 4K cores.
- **Force damping** for static/steady state equilibrium.
- **Remeshing** for large deformation (∵ Lagrangian).
- Conditionally stable (∵ explicit) but large time step allowed through **Mass scaling**.
- **Mixed discretization** for incompressibility and symmetric response.
- Easy to implement **non-linear rheologies**: No need for consistent tangential stiffness.
- **Verified** through benchmarking.
Benefits from StGermain

StGermain Software framework for scientific applications. Provides sustainable, collaborative computational development environments. Written in C. (https://csd.vpac.org/twiki/bin/view/Stgermain)

• Benefits
  ○ Input file in XML format: Logical organization of parameter.
  ○ Modular: Can try things without compiling the whole code and by changing input files only.
    • Various BC including user-defined functions.
    • Switching between rheologies.
  ○ Generation of structured mesh.
  ○ Optimized domain decomposition.
Mixed Discretization

• Structured **hexahedral** mesh $\rightarrow$ two sets of linear **tetrahedra**.

• $\epsilon_{ij} = \theta \delta_{ij} + e_{ij}$, where $\theta = \epsilon_{ii}/3$.

• $\theta$ of each tet is replaced with $\bar{\theta} \equiv \frac{1}{N_{tet}} \sum_{n=1}^{N_{tet}} \theta_n$.

• Two equivalent overlays are required for symmetric response.
Mixed Discretization

<How bad it can be without M.D.: 2-D Example>
Mixed Discretization

<How bad it can be without M.D.: 2-D Example>
Mixed Discretization

<Results from the Lucky mesh>

<Results from the Bad mesh>
Elasto-Visco-Plastic Rheology

- \( \eta = \eta(T, \sigma, \dot{\epsilon}) \): Effective viscosity approach for creep.
- \( \eta \to \infty \): Mohr-Coulomb plasticity.
- \( \sigma_Y \to \infty \): Maxwell viscoelasticity.
- Brittle and plastic(creeping) regimes do not need to be pre-determined.
Remeshing

<Field interpolation>

Blue: Deformed, Red: Remeshed

5.00 kyr

<Superconvergent Patch Recovery>
SNAC and GALE

<table>
<thead>
<tr>
<th></th>
<th>GALE</th>
<th>SNAC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Basis</strong></td>
<td>FEM solving momentum balance (quasi-)statically</td>
<td></td>
</tr>
<tr>
<td><strong>Time marching</strong></td>
<td>Implicit</td>
<td>Explicit</td>
</tr>
<tr>
<td><strong>Meshing</strong></td>
<td>Structured (no need for complex mesh)</td>
<td>Structured (more flexibility desired)</td>
</tr>
<tr>
<td><strong>Specific Technique</strong></td>
<td>PIC/ALE</td>
<td>Remeshing</td>
</tr>
<tr>
<td><strong>Rheology</strong></td>
<td>Viscoplastic</td>
<td><strong>Elasto</strong>-visco-plastic</td>
</tr>
</tbody>
</table>
### SNAC and GALE

<table>
<thead>
<tr>
<th>Feature</th>
<th>GALE</th>
<th>SNAC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Large deformation</td>
<td>Yes, by accumulating small strain.</td>
<td></td>
</tr>
<tr>
<td>Prediction of structural evolution</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Free surface</td>
<td>Yes with &quot;air&quot; layer</td>
<td>Yes by free surface</td>
</tr>
<tr>
<td>Tracking interface</td>
<td>Yes</td>
<td>suffers numerical diffusion</td>
</tr>
<tr>
<td>Multi-physics</td>
<td>Diking, erosion</td>
<td>Thermal stress, simple erosion</td>
</tr>
</tbody>
</table>
Challenges

- **Optimization** for improved performance
  - Parallel performance is fine, but the overall efficiency needs improvements.

- More sophisticated **multi-physics**
  - e.g., melting and melt migration, fully coupled thermomechanics.

- More realistic **rheology**
  - Rate-dependent plasticity, damage models, various creep mechanisms.

- **Mesh- and resolution-dependence** of localization
  - Embedding weak/strong discontinuity is one solution.

- Reducing **remeshing-induced diffusion**: Particles?
To help and be helped...

send emails to

cig-long@geodynamics.org
or
echoi@ldeo.columbia.edu

with explicit titles. Please post

• questions,
• bug reports,
• feature requests,
• other suggestions,
• etc.
Preparation

- How to get it: SNAC, libxml2, mpi, GNU Scientific Library.
- How to build it: ./configure.sh; make. Consider optimization option: --options=optimised.
How to run it

- Environment setup
- command line
- Basics of XML input file
  - simulation control
  - plugins: what are available, how to load one.
  - material properties
  - IC/BCs
Post-processing
Advanced topics

- How to extend the capabilities: Modifying