Computational Modeling Issues in Mesoscale Solid Mechanics

A. Needleman, Brown University, Providence RI
What is mesoscale solid mechanics?

A description of mechanical behavior between an atomistic description and an unstructured continuum.

- Direct description of mesoscale deformation and failure processes.
  - Material and mechanism dependent.
    - Discrete dislocation plasticity.
    - Discrete grain description of granular media.
    - Microvoid modeling of ductile fracture.
    - Asperity/lubrication modeling of friction.

- Addition of structure to a phenomenological continuum model.
  - Size dependent metal plasticity.
  - Cohesive modeling of fracture.
  - Characterization of friction.
Why mesoscale scale solid mechanics?

- Critical deformation and fracture processes cannot be adequately described using a conventional continuum formulation.

- A direct description of the mesoscale deformation and/or fracture process is (in principle) predictive but presents enormous computational challenges.

  - Length scale issues.
  - Time scale issues.

- A phenomenological description has parameters with a less direct connection to the physics (and thus is generally harder to relate to experimental measurements) but is typically more flexible and computationally much more tractable.
A Top Down View

Examples – phenomenological mesoscale formulations for (i) size dependent metal plasticity; (ii) fracture; and (iii) frictional sliding.

- Some relevant features of the conventional continuum approach.
- Some limitations of the conventional continuum approach.
- Representative mesoscale phenomenological formulations.
  - Characteristics of the formulation.
  - Computational modeling issues.
    - Computation plays a key role because of the complexity of the formulations.
    - Mesoscale constitutive relations do not generally introduce severe time scale computational limitations.
Conventional Continuum Plasticity

- Small deformations – geometry changes neglected:
  \[ \dot{\varepsilon}_{ij} = \frac{1}{2} (\dot{u}_{i,j} + \dot{u}_{j,i}) \]

- Quasi-static:
  \[ \dot{\sigma}_{ij,j} = 0 \quad \dot{\sigma}_{ij} = \dot{\sigma}_{ji} \]

- Constitutive characterization (metal plasticity):
  \[ \dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p \quad \dot{\varepsilon}_{ij}^p = \Lambda \frac{\partial \phi}{\partial \sigma_{ij}} = \dot{\varepsilon}_{e} \sigma_{ij} \quad \dot{\varepsilon}_{e} = \dot{\varepsilon}_{e}(Y, z_I) \]
  \[ \dot{\sigma}_{ij} = L_{ijkl}\dot{\varepsilon}_{ij}^e \]

- Predictions are size independent.
Metal Plasticity – Size Dependence

- Conventional continuum plasticity theory predicts a size independent response.

- For crystalline metals, there is a considerable body of experimental evidence that this size independence breaks down at length scales of the order of tens of microns and smaller.

- Indentation size effect, Swadener et al. (2002); metal-matrix composites, Seleznev et al. (1998).
Metal Plasticity – Size Dependence

Tension vs. torsion, Fleck et al. (1994).

Size effects emerge from:

- Plastic strain gradients.
- Constraint on plastic flow that occurs even when an overall homogeneous response is possible.
- Source limited plasticity.
Size Dependent Plasticity Theories

- Many formulations which attempt to account for size effects that arise from plastic strain gradients.
  - Requires a material parameter with the dimension of length.
  - Different theories give rise to a different boundary value problem formulation, different boundary conditions and a different interpretation of the length scale parameter(s).

Examples.

- Size dependent hardening, Acharya and Bassani (2000), Bassani (2001); Fleck and Hutchinson (2003)
- Free energy and hardening; Gurtin (2002).
Acharya-Bassani like (Qualitative)

\[ \varepsilon_{ij}^p = \dot{\varepsilon}_p \delta_{ij} \quad \alpha_{ij} = e_{jkl} \varepsilon_{i,l,k}^p \quad \alpha^2 = \frac{3}{2} \alpha_{ij} \alpha_{ij} \]

Equilibrium:

\[ \sigma_{ij,j} = 0 \quad \sigma_{ij} = \sigma_{ji} \]

\[ \sigma_e - Y = 0 \]

where \( \sigma_e \) is the effective stress and

\[ \dot{Y} = H(\varepsilon_e, \ell \alpha) \dot{\varepsilon}_e \]

Boundary conditions – prescribe either \( t_i = \sigma_{ij} n_j \) or \( u_i \)

- Material length enters the expression for the hardening.
- No additional boundary conditions.
FH-I or MSG like (Qualitative)

Equilibrium:

$$\sigma_{ji,j} - \tau_{kji,kj} = 0 \quad \sigma_{ij} \neq \sigma_{ji}$$

Boundary conditions – prescribe either

$$t_i \quad \text{or} \quad u_i \quad \text{and} \quad r_i \quad \text{or} \quad u_{i,j} n_j$$

$$t_i = n_k \left( \sigma_{ki} - \tau_{kji,j} \right) + n_k n_j \tau_{kji} (D_p n_p) - D_j (n_k \tau_{kji})$$

with $D_j$ the surface derivative and $r_i = \tau_{ijk} n_j n_k$.

Constitutive:

$$Y = Y_0 \sqrt{\epsilon_e + \ell \eta} \quad \eta_{ijk} = u_{k,ij} \quad \eta = \sqrt{2 \eta_{ijk} \eta_{ijk}}$$

$$\tau_{ijm} = \ell_e \Lambda_{ijk} n_j n_k$$
FH-III or Gurtin like (Qualitative)

Equilibrium:

\[ \sigma_{ij,j} = 0 \quad \sigma_e - Y - \xi_{i,i} = 0 \]

Boundary conditions – prescribe either

\[ t_i = \sigma_{ij} n_j \quad \text{or} \quad u_i \quad \text{and} \quad q = \xi_i n_i \quad \text{or} \quad \epsilon_e \]

Constitutive:

\[ \dot{\epsilon}_{ij}^p = \dot{E}_{e} p_{ij} \quad \alpha_i = \epsilon_{e,i} \quad \Psi = \frac{1}{2} L_{ijkl} \epsilon_{ij}^e \epsilon_{kl}^e + \frac{1}{2} \ell_G^2 Y_0 \alpha_i \alpha_i \]

\[ \sigma_{ij} = L_{ijkl} \epsilon_{kl}^e \quad \dot{Y} = H(E_e, \alpha_i) \dot{E}_e \quad E_e = \sqrt{\epsilon_e^2 + \ell_{FH}^2 \alpha_i \alpha_i} \]

\[ \xi_i = \ell_G^2 Y_0 \alpha_i \quad \text{or} \quad \dot{\xi}_i = A_{ij} \dot{\alpha}_j + B_i \dot{\epsilon}_e \]
Finite Element Implementation

• Acharya-Bassani like.
  - $\varepsilon_{ij}^p$ known at integration points.
  - Extrapolate $\varepsilon_{ij}^p$ to nodes and smooth (average over elements connected to that node).
  - Use element shape functions to compute $\alpha_{ij} = \varepsilon_{ij}^p$ at integration points.
  - Compute $\alpha$ and $H(\varepsilon_e, \ell\alpha)$.

• FH-I, MSG like
  - Higher order shape functions or incompatible elements needed because of the strain gradients ($u_{k,ij}$).

• FH-III, Gurtin like.
  - $\varepsilon_e$ enters as a nodal variable leading to a mixed formulation.
Predictions of Size Dependence


Different frameworks can give very similar results.
Size Dependent Plasticity

- Acharya-Bassani like
  - Standard boundary value problem framework retained.
  - Boundary layer size effects absent.
- FH-I or MSG like
  - Predictions can be sensitive to the elastic length scale.
  - Higher order stresses and higher order boundary conditions.
- FH-III or Gurtin like
  - The additional boundary conditions interpretable.
  - Relative roles of the energetic and dissipative hardening.

Imposed plastic strain gradient size dependent hardening.
Source limited plasticity.
Interpretation and evaluation of the length parameter.
Conventional Fracture Mechanics

- Pre-existing dominant crack (or simple system of dominant cracks).
  - Distributed cracking in complex microstructures difficult or impossible to analyze.
  - Crack nucleation cannot be analyzed.

- Known crack path.
  - Crack branching and fragmentation difficult or impossible to analyze.

- Based on square root or HRR singular crack tip fields.
  - Fast crack growth (faster than an elastic wave speed) difficult or impossible to analyze.
Single vs. Multiple Cracking

Which mode of cracking has the greatest energy dissipation, i.e. the largest apparent toughness?

In Shaw et al. (1996), the single crack was found to have the greatest energy dissipation.
Fracture in a Complex Microstructure

Lamellar TiAl, Arata et al. (2001)
Cohesive Surface Framework

- The location of one or more cohesive surfaces is specified.
- Two constitutive relations – a bulk constitutive relation and a cohesive constitutive relation.
- A characteristic length is introduced.
- No crack tip singularity; no initial crack needed.
- Fracture, if it occurs, is a natural outcome of the imposed loading.
Finite Element Implementation

- Principle of virtual work

$$\int_V \sigma_{ij} \delta \varepsilon_{ij} dV + \int_{S_{coh}} T_i \delta \Delta_i dS = \int_{S_{ext}} T_i \delta u_i dS - \int_V f_i \delta u_i dV$$

- Ordinary finite elements for the volume integral.

- With $\dot{T}_i = K_{ij} \dot{\Delta}_j$, the cohesive contribution to the tangent stiffness is

$$\int_{S_{coh}} \dot{T}_i \delta \Delta_i dS = \int_{S_{coh}} K_{ij} \dot{\Delta}_i \delta \dot{\Delta}_j dS = \int_{S_{coh}} K_{ij} (\dot{u}_i^+ - \dot{u}_i^-)(\delta \dot{u}_j^+ - \delta \dot{u}_j^-) dS$$

which results in an additional contribution to the global stiffness matrix.

- Calculate the contributions from the volume and surface elements and assemble the global stiffness matrix.
Fracture in a Complex Microstructure

Arata et al. (2001)
Branching and Fragmentation

Dynamic crack growth.

Miller et al. (2001)
Cohesive Fracture Modeling Issues

- Identification of cohesive surfaces.
  - Possible when failure occurs along pre-defined weak planes.
  - Problematic for solids that are homogeneous on the scale being modeled.
    - Initially elastic cohesive surfaces affect elastic stiffness.
    - Initially rigid cohesive surfaces can have numerical stability issues.

- Atomistically computed cohesive strength values are too large to give useful predictions.

Van der Ven and Ceder (2003).
Sensitivity to Cohesive Strength

Conventional plasticity, interface crack growth, Tvergaard and Hutchinson (1996).

Crack growth is essentially precluded for cohesive strengths more than \( \approx 4 - 5\sigma_Y \).
The classical Amontons-Coulomb description of friction states that $T_t = \mu_s T_n$ or $T_t = \mu_d T_n$.

An jump in $T_n$ implies a jump in $T_t$ – not seen experimentally (Prakash-Clifton, 1993).

For sliding along interfaces between elastic solids there are instabilities leading to ill-posedness, Adams (1995).

Inherent mesh dependence.

An experimentally based rate and state dependent friction law (Prakash-Clifton, 1993) regularizes the problem and converged numerical solutions can then be achieved (Cochard and Rice, 2000).

Other regularizations are possible.
Rate and State Friction

\[ |T_s| = \mu(\theta_0, \Delta \dot{u}_{\text{slip}}) (\theta_1 + \theta_2) \quad \mu(\theta_0, \Delta \dot{u}_{\text{slip}}) = g(\theta_0) \left( \frac{\Delta \dot{u}_{\text{slip}}}{V_0} + 1 \right)^{1/m} \]

\[ g(\theta_0) = \frac{\mu_d + (\mu_s - \mu_d) \exp \left[ - \left( \frac{L_0/\theta_0}{V_1} \right)^p \right]}{\left[ \frac{L_0/\theta_0}{V_0} + 1 \right]^{1/m}} \]

\[ \dot{\theta}_0 = B \left( 1 - \frac{\theta_0 \Delta \dot{u}_{\text{slip}}}{L_0} \right) \]

\[ \dot{\theta}_1 = -\frac{1}{L_1} [\theta_1 - CT_n] \Delta \dot{u}_{\text{slip}} \quad \dot{\theta}_2 = -\frac{1}{L_2} [\theta_2 - DT_n] \Delta \dot{u}_{\text{slip}} \]

- **Principle of virtual work**

\[ \int_V \sigma_{ij} \delta \epsilon_{ij} dV + \int_{S_{\text{frict}}} T_i \delta \Delta_i dS = \int_{S_{\text{ext}}} T_i \delta u_i dS - \int_V f_i \delta u_i dV \]

- **Location of the sliding interfaces generally known.**

- **Integration of a stiff constitutive relation.**
Rate and State Friction

(a) 

(b) 

Rate and State Friction

Coker et al. (2004)
Comments and Questions

- Conventional continuum formulations are inadequate for modeling mesoscale processes of technological significance.

- Mesoscale deformation and fracture phenomena can be modeled using phenomenological constitutive formulations.

- When is a direct physical description needed and when is a phenomenological model adequate?

- A phenomenological model can capture essential features of a range of materials and mechanisms.

- A phenomenological mesoscale constitutive relation introduces new material properties. Identification?
  - Fitting to outcome data? Independently obtained? How?

- A phenomenological approach can have enormous computational advantages over a direct physical description but can introduce its own computational challenges.