Variational Problems in Mechanics and the Link between Microstructure and Macroscopic Behavior

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Introduction

- The case for multiscale modeling in material science and computational mechanics
- How can microstructure, scaling and size effects be built into large-scale numerical calculations?
- Is brute-force raw computational power enough?
- A marriage of convenience: Mixed numerical and analytical multiscale (subgrid) models
- A case study in inelasticity: Metal plasticity
- How can multiscale methods be applied to inelastic, dissipative, hysteretic systems?
Manufacturing Processes - Extrusion

FE model (1/6 symmetry)  

Section XY  

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160.4  

10  

(Vallellano and Ortiz ´00)
Manufacturing Processes - Riveting

(Repetto, Radovitzky and Ortiz '99)

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Manufacturing Processes - Machining

(AISI 4340 Steel)

Cutting speed = 20 m/s
Cutting speed = 20 m/s
Cutting speed = 10 m/s

(Marusich and Ortiz, IJNME ´95)
Validation and Verification

• Fundamental building blocks of simulations:
  - *Finite elements* + *time stepping algorithms*
  - *Finite deformation plasticity* + *heat conduction*
  - *Brittle and ductile fracture and fragmentation*
  - *Contact mechanics, friction*

• Main sources of error and uncertainty
  - *Discretization errors (spatial + temporal)*
  - *Uncertainties in data:*
    - *Material properties*
    - *Model geometry*
    - *Loading and boundary conditions...*
  - *Empiricism of constitutive models*
Limitations of empirical models

- Conventional engineering plasticity models fail to predict earing in deep drawing
- Prediction of earing requires consideration of polycrystalline structure, texture development

Deep-drawn cup

Grain structure of polycrystalline W (Courtesy of Clyde Briant)
Limitations of empirical models

Conventional plasticity models fail to predict scaling, size effects.

Hall-Petch scaling

Lamellar structure in shocked Ta
(MA Meyers et al´95)

Dislocation pile-up at Ti grain boundary
(I. Robertson)
The case for multiscale modeling

- Empirical models fail because they do not properly account for microstructure
- The empirical approach does not provide a systematic means of eliminating uncertainty from material models
- Instead, multiscale modeling:
  - Identify relevant mechanisms at all lengthscales
  - Bridge lengthscales by:
    - Building models of effective behavior
    - Computing material parameters from first principles
- Methods:
  - Computational: Direct multiscale computing
  - Analytical: Methods of the calculus of variations
  - Mixed: Unresolved calculations + subgrid models
Metal plasticity - Multiscale modeling

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Polycrystals
- Engineering calculations

Time scale: ns, μs, ms
Length scale: nm, μm, mm
Direct multiscale computing - Outlook

ASCI computing systems roadmap

- Computing power is growing rapidly, but...
Direct multiscale computing – Bottom up

- Computing power is growing rapidly, but $10^9 << 10^{23}$

- Ta quadrupole (T. Arias ´00)

- FCC ductile fracture (Courtesy F.F. Abraham) (F.F. Abraham ´03)

- Au nanoindentation (Knap and Ortiz ´03)
Direct multiscale computing – Top down

Polycrystalline W (Courtesy of C. Briant)

Grain-boundary sliding model

Single-crystal plasticity model

(A.M. Cuitiño and R. Radovitzky ‘02)
Direct multiscale computing – Top down

Cold-rolled @ 42% polycrystalline Ta

Experimental cold-rolled texture

Pole figure

(A.M. Cuitiño and R. Radovitzky ´03)
Direct multiscale computing - Outlook

- ~ $10^9$ elements at our disposal ($10^6$ elements/processor x 1000 processors)
- ~ 1000 elements/coordinate direction
- ~ 20 elements/grain/direction (8000 elements/grain)
- ~ 50 grains/direction (125K grains)
- ~ 2.5 mm specimen for 50 µm grains
- Not enough for complex engineering simulations!
- Subgrain scales still unresolved, require modeling!
Metal plasticity - Multiscale modeling

Accessible to first-principles calculations

Lattice defects, EoS

Dislocation dynamics

Subgrain structures

Polycrystals

Engineering calculations

Accessible to direct numerical simulation

Length:
- nm
- μm
- mm

Time:
- ns
- μs

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Subgrid models – Relaxation methods

(Cu-Al-Ni, Chunhua Chu and Richard D. James)

- Use analytically-derived effective models to represent unresolved (sub-grid) phenomena
- Methods of the calculus of variations: relaxation, \( \Gamma \)-convergence, optimal scaling, homogeneization
- Model conservative system: Nonlinear elasticity
Nonlinear elasticity - Relaxation

- Nonlinear elasticity:
\[
\inf_{y \in y_0 + W^{1,\infty}_0(\Omega)} \left\{ I(y) = \int_{\Omega} W(Dy) \, dx \right\}
\]

- Functions \( W(Dy) \) of interest have multi-well structure \( \Rightarrow I(y) \) lacks weak sequential lower-semi-continuity \( \Rightarrow \) infimum not attained in general.

- Direct numerical solutions based on \( I(y) \) tend to exhibit exceedingly slow or no convergence.
Nonlinear elasticity - Relaxation

- Instead: Do numerics on the relaxed problem:

\[
\inf_{y \in y_0 + W^{1,\infty}_0(\Omega)} \left\{ s c^{-1} I(y) = \int_\Omega QW(Dy) \, dx \right\}
\]

where \( s c^{-1} I \) is the lower semi-continuous envelope of \( I \), and

\[
QW(F) = \inf_{u \in W^{1,\infty}_0(E)} \frac{1}{|E|} \int_E W(F + Du) \, dx
\]

is the quasiconvex envelope of \( W \) (independent of \( E \subset \Omega \)).
**Theorem.** Assume that $I : X \to \mathbb{R}$ is coercive. Then:

(i) $sc^- I$ is coercive and lower semicontinuous.

(ii) $sc^- I$ has a minimum point in $X$.

(iii) $\min_{y \in X} sc^- I(y) = \inf_{y \in X} I(y)$.

(iv) Every cluster point of a minimizing sequence of $I$ is a minimum point of $sc^- I$ in $X$.

(v) If, in addition, $X$ is first-countable, then every minimum point of $sc^- I$ is the limit of a minimizing sequence of $I$ in $X$. 
Example – Nematic elastomers

\[ W(F, n) = A \text{tr}(FF^T) - B \|F^n\|_2^2 \]

(Courtesy of de Simone and Dolzmann)

De Simone and Dolzmann '00
De Simone and Dolzmann '02

Blandon et al. '93

Central region of sample at moderate stretch (Courtesy of Kunder and Finkelmann)
Nonlinear elasticity - Relaxation

• Relaxed problem exhibits easy-to-compute regular solutions
• Sub-grid microstructural information is recovered locally from the solution of the relaxed problem
• But: Quasiconvex envelopes are known explicitly in very few cases
• Instead: Consider easy-to-generate special microstructures, such as sequential laminates
  - Off-line (Dolzmann ’99; Dolzmann & Walkington ’00)
  - Concurrently with the calculations (Aubry et al. ’03)
Example - Indentation of Cu-Al-Ni

(Aubry, Fago and Ortiz ´03)
Crystal plasticity - Microstructures

Dipolar dislocation walls

Labyrinth structure in fatigued copper single crystal (Jin and Winter ´84)

Nested bands in copper single crystal fatigued to saturation (Ramussen and Pedersen ´80)
Crystal plasticity - Microstructures

- Lamellar structures are universally found on the micron scale in highly-deformed crystals.
- These microstructures are responsible for the soft behavior of crystals and for size effects.

Lamellar dislocation structure in 90% cold-rolled Ta
(Hughes and Hansen ‘97)

Lamellar structure in shocked Ta
(Meyers et al ‘95)
For conservative systems, there is a clear connection between microstructure and non-attainment

Difficulties in applying program to plasticity:
- *Plasticity involves both energetics and kinetics*
- *Plasticity exhibits strong scaling and size effects*
- *No general analytical method for relaxing functionals*

Difficulties are overcome by:
- *Incremental variational formulation* (Ortiz and Repetto 99; Ortiz and Stainier 00; Mielke 00)
- *Non-local energies* (Ortiz and Repetto 99; Mielke and Müller 03)
- *Numerical relaxation* (Dolzmann 99; Dolzmann and Walkington 00; Aubry, Fago and Ortiz 03)
Crystal plasticity - BVP

Irreversible accommodation of shear deformation by crystallographic slip

Pointwise:

\[ F_p = I + \gamma s \otimes m, \quad (s, m) \in \{\text{finite set}\} \]

\[ \dot{\gamma} = \partial_\tau \psi(\tau) \]

\[ \tau = -\partial_\gamma A(Dy F_p^{-1}, \gamma) \]

\[ \inf_{y \in y_0 + W_0^{1,\infty}(\Omega)} \left\{ I(y) = \int_{\Omega} A(Dy F_p^{-1}, \gamma) \, dx \right\} \]
Crystal plasticity - BVP

- Crystal plasticity involves both energetics and kinetics
- The variational structure of the BVP is not clear from the outset...
- ...but it can be revealed by recourse to time discretization (Ortiz and Repetto ‘99, Ortiz and Stainier ‘00, Mielke ‘00)
Crystal plasticity – Variational problem

- Discretize time: $t_0, \ldots, t_n, t_{n+1}, \ldots$

- Define incremental strain energy density (Ortiz and Repetto ’99; Ortiz and Stainier ’99):
  \[ W_n(F_{n+1}) = \inf_{\text{paths}} \int_{t_n}^{t_{n+1}} \partial_F A \cdot \dot{F} \, dt \]

- Incremental variational problem:
  \[ \inf_{y_{n+1} \in y_0 + W^{1,\infty}_0(\Omega)} \left\{ I_n(y_{n+1}) = \int_\Omega W_n(Dy_{n+1}) \, dx \right\} \]

- Incremental problem is formally identical to non-linear elasticity problem!
Crystal plasticity – Non-attainment

- Example: FCC crystal deforming on \((1\bar{1}0)\)-plane

\[
F \in SO(3) \times (I + \gamma s \otimes m)
\]
(Single slip)

- \(W_n(F)\) non-convex!
Crystal plasticity - Relaxation

- Crystal plasticity has an incremental variational structure
- Incremental energy functional lacks lower semicontinuity
- Observed microstructures are a manifestation of non-attainment
- Numerical implementation: Relax incremental energy functional
- Fall-back position: Consider special microstructures, e.g., sequential laminates
Validation – Fatigued copper

• Problem (Ortiz and Repetto ’97): Find all laminates such that $F \in SO(3) \times (I + \gamma s \otimes m)$, $(s, m) \in \text{finite set}$.

(100) walls (Jin and Winter ’84)

(111) walls (Yumen ’89)

(101) walls (Wang and Mughrabi ’84)

(131) walls (Lepisto et al., 1986)
Validation – Misorientation angles

Cold rolling deformed grains

(Hughes et al. ’97)

(Aubry and Ortiz ’03)

frequency

average angle

misorientation angle

macroscopic strain
Crystal plasticity – Nonlocal extension

• Thus far the material description is local
• Local material models do not possess a characteristic length scale and cannot predict scaling relations such as the Hall-Petch effect
• In order to predict scaling relations we need to account for additional physics:
  – Dislocation core energies
  – Dislocation wall energies
• This renders the material description nonlocal...
Crystal plasticity – Nonlocal extension

Fatigued copper (Jin ’87)

Dislocation walls carry additional energy

- Nonlocal free energy:

\[ I(y, \Omega) = \int_{\Omega} \left\{ A(Dy F_p^{-1}, \gamma) + (T/b) ||\text{curl}F_p|| \right\} dx \]

- Energy density of a subset \( E \subset \Omega \):

\[ \frac{1}{|E|} \inf_{u \in W^{1,\infty}_0(E)} I_n(Fx + u, E) \rightarrow \text{depends on } E! \]
Crystal plasticity – Nonlocal extension

- Energy density depends on size, shape of domain.
- We can no longer defined a meaningful effective energy density
- Need to model entire domains at a time!
- Analytical tools:
  - Optimal scaling (Kohn and Müller ´92, ´94; Conti ´00, ´03)
  - Young measures of micro-patterns (Alberti and Müller ´99)
- Work in progress: `Grain elements’
  - Each element represents one entire grain
  - Energy of grain depends on its size, shape and exhibits optimal scaling
Crystal plasticity – Nonlocal extension

- Optimal scaling constructions for double slip, antiplane shear (Conti ’00, ’03)

\[ \tau_c \sim d^{-1/2} \]  

\[ \tau_c \sim d^{-2/3} \]  

Hall-Petch effect!
Equal Angular Channel Extrusion

- Total deformation:
  \[ A = \begin{pmatrix} 2 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

(Beyerlein, Lebensohn and Tome, LANL, 2003)
Case study - ECAE

Observed:
Equiaxed

Observed:
~20º

Observed:
~12º

Observed:
~7º

Original
1st pass
2nd pass
3rd pass

(Beyerlein, Lebensohn and Tome, LANL, 2003)
Case study - ECAE

Evolution of microstructure (sequential lamination)

(Sivakumar and Ortiz ‘03)
Case study - ECAE

Experimental texture
(Vogel et al. ´03)

Computed texture
(Sivakumar and Ortiz ´03)
Summary and conclusions

- The multiscale modeling paradigm provides a systematic means of eliminating empiricism and uncertainty from material models.
- Present computing capacity is not sufficient to integrate entire multiscale hierarchies into large-scale engineering simulations.
- There remains a need for subgrid models (as in other fields, e.g., turbulence).
- Inroads are being made in the application of calculus of variations to inelastic systems.
- Many open questions remain (regularity of minimizers, convergence of incremental approach, relaxation of non-local functionals...).