Multiscale Analysis as a (Lossless) Approximation Scheme

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Outline

• Multiscale Analysis as an approximation scheme:
  – What is (or is not) Multiscale Analysis?
  – When does it apply? To what avail?
  – How and to what does it converge?
  – What information is lost, if any?
• The time-independent and time-dependent cases
• The rate-independent case, deformation theory
• Implementation and applications:
  – Crystal plasticity
  – Initiation in energetic materials
Separation of Scales - Homogeneization

- Separation of scales:
  \[ \varepsilon = \frac{l}{L} \rightarrow 0 \]

- Seek macroscopic response \( P - \Delta \)
- Seek to eliminate microscopic scale
- Wish return option...

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Separation of Scales - Homogeneization

- Separation of scales:
  \[ \epsilon = \frac{l}{L} \rightarrow 0 \]

uniform?

same macroscopic response!

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Gamma Convergence of functionals

- Equicoercive functionals $F_\varepsilon : X \to [0, +\infty]$, e.g.:
  \[ F_\varepsilon(u) = \int_\Omega W\left(\frac{x}{\varepsilon}, Du(x)\right) \, dx \to \inf! \]

- Separation-of-scales limit: $\varepsilon \to 0$:

- $\Gamma$-limit $F_\varepsilon = F_0$ (w/loc) iff, for all $f \in X^*$ (loadings),
  \[ \inf_{u \in X} \left( F_\varepsilon(u) + \langle f, u \rangle \right) \to \inf_{u \in X} \left( F_0(u) + \langle f, u \rangle \right) \]

  minimum energies of sequence of functionals

  minimum energy of limiting functional

- Example: Homogenization limit,
  \[ W_0(\xi) = \inf_{W_{1,1}^{1,1}(P)} \left\{ \frac{1}{|P|} \int_P W\left(x, \xi + Du(x)\right) \, dx \right\} \]
Separation of Scales - Relaxation

- Separation of scales:
  \[ \epsilon = \frac{l}{L} \rightarrow 0 \]
  no deformation microstructures!

SMA
CuAlNi

Chu, C. and James, R.D., *J. Phys. IV*, 1995

same macroscopic response!

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Separation of Scales - Relaxation

- Coercive functional \( F : X \to [0, +\infty] \), e.g.:
  \[
  F(u) = \int_{\Omega} W(\nabla u(x)) \, dx \to \inf!
  \]
- \( F_0 \) is the relaxation of \( F \) iff:
  - \( F_0 \) stable w.r.t. affine deformations (w/ sc),
  - For all applied loadings \( f \in X^* \),
    \[
    \inf_{u \in X} \left( F(u) + \langle f, u \rangle \right) \to \inf_{u \in X} \left( F_0(u) + \langle f, u \rangle \right)
    \]
      minimum energy of original functional
      minimum energy of relaxed functional
- Example: Quasiconvex envelope
  \[
  W_0(\xi) = \inf_{W_0^{1,p}(E)} \frac{1}{|E|} \int_{E} W(\xi + \nabla u(x)) \, dx
  \]
Separation of Scales - Relaxation

- Quasiconvex envelop:
  \[ W_0(F') = \inf_{v \in W_0^{1,p}(E)} \frac{1}{|E|} \int_E W(F + \nabla v) \, dx \]

- Microstructure construction, optimality (hard)
- List of problems whose relaxation is known explicitly is small but growing...

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Relaxation as ‘optimal’ multiscale scheme

- The relaxed problem is well-posed, exhibits no microstructure, can be approximated by, e.g., finite elements
- The relaxed and unrelaxed problems deliver the same macroscopic response (e.g., force-displacement curve: convergence!)
- All microstructures are pre-accounted for by the relaxed problem (no physics lost)
- Microstructures can be reconstructed from the solution of the relaxed problem (no loss of information: return option!)

Relaxation is an ‘optimal’ multiscale method!

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Time-dependent microstructure

Copper single crystal
(Mughrabi, Phil. Mag. 23, 869, 1971)

1% deformation

90% cold-rolled Ni (Hansen, Huang and Hughes, Mat. Sci. Engin. A 317, 3, 2001)

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Time-dependent problems

- Time-dependent problems: \( \partial \psi(u, \dot{u}) + D E(t, u) = 0 \)

- Energy-dissipation functional: 
  \[
  F_\epsilon(u) = \int_0^T e^{-t/\epsilon} \left[ \frac{1}{\epsilon} E(t, u) + \psi(u, \dot{u}) \right] dt \rightarrow \infty!
  \]

- Rate-independence + monotonic loading:
  \[
  \psi(u(t), \dot{u}(t)) = \frac{d}{dt} P(u(t))
  \]

- Deformation theory: 
  \[
  F_\epsilon(u) = \int_0^T e^{-t/\epsilon} \left[ E(t, u) + P(u) \right] \frac{dt}{\epsilon} \rightarrow \infty!
  \]

  \[
  u(t) \in \operatorname{argmin} \left( E(t, \cdot) + P(\cdot) \right)
  \]

Application to crystal plasticity

- Elastic energy: \[ E(u, \gamma) = \int_\Omega W^e(\nabla u - \sum \gamma s \otimes m) \, dx \]
- Plastic work: \[ P(\gamma) = \int_\Omega W^p(\gamma) \, dx \quad \text{non-convex!} \]
- Monotonicity: \[ \gamma(t_2) > \gamma(t_1), \text{ if } t_2 > t_1 \]
Strong latent hardening

- Strong latent hardening: Crystals much 'prefer' to activate a single slip system at each material point, though the active system may vary from point to point.

Latent hardening experiments

Non-convexity - Strong latent hardening

- Linear hardening: \( W^p = \tau_0 \sum_\alpha \gamma^\alpha + \sum_\alpha \sum_\beta h_{\alpha\beta} \gamma^\alpha \gamma^\beta \)

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

\( \beta^p \in \gamma s \otimes m + so(3) \)  
(Single slip)

- \( W(\nabla u) \) non-convex!

(Ortiz and Repetto, *JMPS*, 47(2) 1999, p. 397)
Strong latent hardening & microstructure

affine boundary conditions
\[ u_1 = \gamma x_2 \]
uniform double slip

FCC crystal deformed in simple shear on (001) plane in [110] direction

(M Ortiz, EA Repetto and L Stainier
*JMPS*, **48**(10) 2000, p. 2077)
Strong latent hardening & microstructure

 boundary layer

 dislocation walls

 FCC crystal deformed in simple shear on (001) plane in [110] direction

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*JMPS*, *48*(10) 2000, p. 2077)
Strong latent hardening & microstructure

Microstructural refinement!

FCC crystal deformed in simple shear on (001) plane in [110] direction

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Strong latent hardening & microstructure

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• $W^p$ with linear growth
• Explicit lamination-type construction delivers:
  - Quasi-convex envelop $W_0$ in close form: ideal plasticity + no latent hardening
  - Optimal microstructures as post-processing step
• Some variants take the form of slip lines...

Conti, S. & MO, ARMA, 2005
Example – Single-crystal indentation

Indentation of [001] surface of BCC single crystal
32,000 nodes
27,436 hexahedral elements

Conti, S., Hauret, P. and MO,
*SIAM Multiscale Model. Simul.*, 2005
Example – Single-crystal indentation

rank 2/2, $|\gamma|_\infty = 0.0025$

rank 4/14, $|\gamma|_\infty = 0.43$

rank 4/12, $|\gamma|_\infty = 0.02$

rank 4/6, $|\gamma|_\infty = 0.026$

rank 4/16, $|\gamma|_\infty = 0.21$

Conti, S., Hauret, P. and MO, SIAM Multiscale Model. Simul., 2005
Example – Single-crystal indentation

Conti, S., Hauret, P. and MO, SIAM Multiscale Model. Simul., 2005
Application to High Explosives (HE)

- Detonation sensitivity: Ease with which an explosive can be detonated
- What factors determine detonation sensitivity?
- In high explosives localized **hot spots** cause detonation initiation

Detonation of high-explosive (RDX, PETN, HMX)

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High-Explosives - Initiation

- Can hot spots arise as a result of localized plastic deformation?
- Can small-scale details of the deformation pattern (partially) explain detonation sensitivity?
- Need to predict deformation microstructures, extreme events! (not just average behavior)

HE initiation – Multiscale modeling

first-principles & atomistic calculations

material properties

relaxation

post-processing

microstructure reconstruction

effective properties

Direct Numerical Simulation (DNS)

full chemistry

boundary conditions

Rimoli, J.J. and MO, Phys. Rev. E, 2010

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PETN – Elastic constants

Body Centered Tetragonal Lattice

- Elastic Constants (GPA): (Winey and Gupta, 2001)
  
  \[ C_{11} = 17.22 \quad C_{33} = 12.17 \]
  
  \[ C_{44} = 5.04 \quad C_{66} = 3.95 \]
  
  \[ C_{12} = 5.44 \quad C_{13} = 7.99 \]

- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

  \[ C_{ij}(\theta, p) = \frac{\theta - \theta_{melt}(p)}{\theta_0 - \theta_{melt}(p)} \]

- Menikoff and Sewell (2002):

  \[ \theta_{melt}(\rho) = \theta_{melt}(p_0) \left(1 + \frac{a \Delta V}{V_0}\right) \]

  where \( a = 2(\Gamma - 1/3) \), \( \Gamma \sim 1.2 \) = Grüneisen constant

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PETN – Slip systems

\[ \tau_c (\theta) \] fitted to data of Amuzu et al. (1976) and:

\[ a = b = 9.380\text{Å} \quad c = 6.710\text{Å} \]

<table>
<thead>
<tr>
<th>Slip System</th>
<th>( s^a )</th>
<th>( m^a )</th>
<th>( \tau_c ) [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3</td>
<td>( \pm [1\bar{1}1] ) (110)</td>
<td>( [1\bar{1}1] ) (110)</td>
<td>1.0</td>
</tr>
<tr>
<td>B4</td>
<td>( \pm [1\bar{1}1] ) (110)</td>
<td>( [1\bar{1}1] ) (110)</td>
<td>1.0</td>
</tr>
<tr>
<td>A1</td>
<td>( [111] ) (1\bar{1}0)</td>
<td>( [111] ) (1\bar{1}0)</td>
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</tr>
<tr>
<td>A2</td>
<td>( \pm [1\bar{1}1] ) (110)</td>
<td>( [1\bar{1}1] ) (110)</td>
<td>1.0</td>
</tr>
<tr>
<td>B6</td>
<td>( [1\bar{1}0] ) (1\bar{1}0)</td>
<td>( [1\bar{1}0] ) (1\bar{1}0)</td>
<td>2.0</td>
</tr>
<tr>
<td>A5</td>
<td>( \pm [1\bar{1}1] ) (110)</td>
<td>( [1\bar{1}1] ) (110)</td>
<td>2.0</td>
</tr>
</tbody>
</table>

P. Xu, S. Zybin, S. Dasgupta, and W. A. Goddard III, private communication
PETN – Chemistry

- Single-step reaction kinetics (Caspar et al., 1998):
  \[
  \frac{d\lambda}{dt} = Z(1 - \lambda)\exp\left(-\frac{ER}{\theta}\right)
  \]

- Activation energy \( E \) and rate constant \( Z \) from Rogers (1975):

| \( R \) | 8.314 J/mol/K |
| \( E \) | 196,742 \times 10^3 J/mol |
| \( Z \) | 6.3 \times 10^{19} s^{-1} |

- Temperature computed assuming adiabatic heating, full conversion of plastic work to heat, heat capacity
PETN – Plate impact test

Flyer plate

PETN target plate

Computational domain

Plate-impact configuration

High-Explosives Detonation Initiation

Polycrystal model and grain boundaries
PETN plate impact - Velocity
PETN plate impact - temperature
PETN plate impact – Subgrain microstructures

Microstructure evolution at selected material points
PETN plate impact – Hot-spot analysis

direct numerical simulation of polycrystalline PETN

reconstructed microstructure at selected material points

chemical analysis of hot-spots with B.C. from microstructure

Rimoli, J.J. and MO, Phys. Rev. E, 2010
PETN plate impact - temperature and reaction evolution at selected hot spot

- Temperature vs. Time
- Reacted molar fraction vs. Time

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PETN plate impact - Number of hot spots

![Graph showing the number of hot spots as a function of reacted molar fraction exceeded.](image)

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PETN plate impact - Number of hot spots

![Graph showing the number of hot spots vs. pressure exceeded (GPa) for different velocities (500n/s, 600n/s, 700n/s, 800n/s).](image)

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PETN plate impact - Number of hot spots

Temperature exceeded (Gpa) vs. Number of hot spots

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PETN plate impact – pop-plots

Impact velocity (m/s)

Exponent ~ 2.91

1/Number of hot-spots

Impact velocity (m/s)

Distance to detonation (mm)

Input pressure (Gpa)

Multiscale model

S.A. Sheffield and R. Engelke (2009)

Experimental exponent ~ 2.01–2.58


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Concluding remarks

• Relaxation: Optimal theory of Multiscale Analysis with a clear sense of ‘convergence’: Exactness of macroscopic response for all applied loadings

• Relaxation eliminates fine-scale microstructural features from consideration in macroscopic calculations, but provides a ‘return option’: The optimal microstructures can be reconstructed at post-processing stage

• Return option is important when the extreme values of the solution, and not just averages, are of concern: failure, nucleation, initiation...

• Application to HE initiation would not have been possible without relaxation scheme...
Micro to Macro (and back again)

Thank you!