Optimal scaling
in plasticity and fracture

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Workshop on Analysis and Computation of Microstructure in Finite Plasticity
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The Genesis of the program: Mathematicians and engineers puzzle over microplasticity...
The framework: Multiscale physics

Objectives: Increase fidelity of material models, reduce empiricism and uncertainty

Foundational theory: Atomistic models (QM, MD, SM...)

- Lattice defects
- Dislocation dynamics
- Subgrain structures
- Polycrystals

Application
The question: Evolving microstructures

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

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

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

Can analysis shed light on the experimental record? (e.g., can some of the observed microstructures be understood as energy minimizers?)

Can analysis inform modeling and simulation? (e.g., homogeneization, multiscale modeling, relaxation, acceleration...)
Ten Years Later...

The well-understood setting:
Rate-independent, proportional loading and local behavior (deformation theory of plasticity + relaxation)

Still open:
Rate-dependent, non-proportional loading and non-local or localized behavior
Crystal plasticity – Linearized kinematics

- Kinematics: \( \varepsilon^p(\gamma) = \frac{1}{|\Omega|} \int_{J_u} [u] \otimes m \, d\mathcal{H}^2 \equiv \sum \gamma s \otimes m \)

- Energy: \( E(u, \gamma) = \int_{\Omega} \left[ W^e(\nabla u - \varepsilon^p(\gamma)) + T |\nabla \gamma \times m| \right] \, dx \)

- Dissipation: \( \psi(\dot{\gamma}) = \begin{cases} \tau_c |\dot{\gamma}|, & \text{single slip,} \\ +\infty, & \text{otherwise.} \end{cases} \)
Crystal plasticity – Deformation theory

- Energy-dissipation functional\(^1\):

\[
F_\varepsilon(u, \gamma) = \int_0^T e^{-t/\varepsilon} \left[ \psi(\dot{\gamma}(t)) + \frac{1}{\varepsilon} E(u(t), \gamma(t)) \right] dt \to \infty!
\]

- Assume: \(\gamma(t)\) monotonic (proportional loading).

- Plastic work density: \(W^p(\gamma) = \begin{cases} \sum \tau_c \gamma, & \text{single slip,} \\ +\infty, & \text{otherwise.} \end{cases} \)

- Then: \(\psi(\dot{\gamma}(t)) = \frac{d}{dt} \int_\Omega W^p(\gamma(t)) \, dx = \frac{d}{dt} P(\gamma(t))\)

- Energy-dissipation functional: \textbf{minimize pointwise!}

\[
F_\varepsilon(u, \gamma) = \int_0^T e^{-t/\varepsilon} \left[ E(u(t), \gamma(t)) + P(\gamma(t)) \right] dt \to \infty!
\]

Crystal plasticity – Deformation theory

- Incremental flow rule: $\varepsilon^p(\gamma) = \sum \gamma_s \circ m$

- Pseudo-elastic strain energy density:
  $$W(\varepsilon) = \inf_\gamma \{ W^e(\varepsilon - \varepsilon^p(\gamma)) + W^p(\gamma) \}$$

- Variational problem (static equilibrium):
  $$F(u) = \int_\Omega W(\varepsilon(u)) \, dx \to \inf!$$
Crystal plasticity – Non-convexity\textsuperscript{1}

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

- Pseudo-elastic energy density:
  \[ W = \begin{cases} 
  \text{linear,} & \text{if } \epsilon = \gamma s \odot m \\
  \text{quadratic,} & \text{otherwise.} 
\end{cases} \]

- \( W(\epsilon) \) non-convex! \( \Rightarrow \) Relaxation!

\textsuperscript{1}M. Ortiz and E. A. Repetto, JMPS, 47(2) 1999, p. 397.
Crystal plasticity – Relaxation

\[ s c^{-} F(u) = \int_{\Omega} W^{**}(\epsilon(u)) \, dx + \int_{\Omega} W^{\infty} \left( \frac{E_{s} u}{|E_{s} u|} \right) \, d|E_{s} u| \]

ideal plasticity

slip-line energy


(Crone and Shield, *JMPS*, 2002)

\(^1\)S. Conti and M. Ortiz, *ARMA*, 176 (2005), pp. 103–147
Crystal plasticity – Lamellar structures

Lamellar dislocation structure
in 90% cold-rolled Ta
(DA Hughes and N Hansen, Acta Materialia, 44 (1) 1997, pp. 105-112)

Lamellar structure
in shocked Ta

Lamellar dislocation structures at large strains

Polycrystals – Concurrent multiscale (C³)

Problem: Too slow!
Need to accelerate!
Acceleration: Phase-space interpolation

- RVE problem must supply $P(F, \dot{F}, T)$
- Replace by interpolant $P_h(F, \dot{F}, T)$!

- Simplicial interpolation in high-dimensional spaces
- One single RVE calculation per boundary crossing
- Speed-up = #steps/simplex @ constant accuracy

Acceleration: Phase-space interpolation

- Dynamic extension of tensile neo-Hookean specimen
- Explicit Newmark integration
- Hexahedral finite elements
- Quadratic: \( W(F) \rightarrow W_h(F) \)

\[ \dot{\varepsilon} = 1 \text{s}^{-1} \]

\[ \dot{\varepsilon} = 100 \text{s}^{-1} \]

Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.
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and local behavior (deformation theory of
plasticity + relaxation)

Still open:
Rate-dependent, non-proportional loading
and non-local behavior
Pitfalls

‘Standard program’ may fail due to:

Non-proportional loading (unloading, cycling loading, change of loading path direction) leading to microstructure evolution

Departures from volume scaling (size effect, domain dependence, localization) leading to failure of homogenization and relaxation
Crystal plasticity – Scaling laws

**Taylor hardening**

**Hall-Petch scaling**

**Taylor scaling**
(SJ Basinski and ZS Basinski, Dislocations in Solids, FRN Nabarro (ed.) North-Holland, 1979.)

Classical scaling laws of crystal plasticity
Crystal plasticity – Effect of boundaries

Dislocation pile-up at Ti grain boundary (I. Robertson)

LiF plate impact experiment. Dislocation pile-ups at surfaces and grain boundaries (G Meir and RJ Clifton, J. Appl. Phys., 59 (1) 1986, pp. 124-148)

Dislocation pile-ups at grain boundaries, surfaces
Crystal plasticity – Size effect

Evolution of dislocation structures in Cu specimen. Lamellar width: \( l \sim \gamma^{-0.65} \)
Crystal plasticity – Size effect

Pure nickel cold rolled to 90%

Scaling of lamellar width and misorientation angle with deformation

Non-local microplasticity

Scaling laws such as Hall-Petch suggest the existence of an intrinsic material length scale.

Modeling assumption: Account for dislocation self-energy using a line-tension approximation.

The resulting deformation-theoretical energy is non-local (specifically, depends on $\nabla \gamma$).

Intrinsic length-scale: Burgers vector.
Crystal plasticity – Linearized kinematics

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- Energy: $E(u, \gamma) = \int_{\Omega} \left[ W^e(\nabla u - \varepsilon^p(\gamma)) + T |\nabla \gamma \times m| \right] dx$

- Dissipation: $\psi(\dot{\gamma}) = \begin{cases} \tau_c |\dot{\gamma}|, & \text{single slip}, \\ +\infty, & \text{otherwise}. \end{cases}$
Crystal plasticity – Optimal scaling

**Theorem** [Conti & MO, ARMA, 2005] There are constants \(c\) and \(c'\) such that

\[
cE_0(T, \gamma, \tau_0, \mu, d) \leq \inf E \leq c'E_0(T, \gamma, \tau_0, \mu, d)
\]

where

\[
\frac{E_0(T, \gamma, \tau_0, \mu, d)}{G\gamma^2 d^3} = \min \left\{ 1, \frac{\mu}{G}, \frac{\tau_0}{G\gamma} + \left(\frac{\mu}{G}\right)^{1/2} \left(\frac{T}{G\gamma bd}\right)^{1/2}, \frac{\tau_0}{G\gamma} + \left(\frac{T}{G\gamma bd}\right)^{2/3} \right\}
\]

- Upper bounds determined by construction
- Lower bounds: Rigidity estimates, ansatz-free lower bound inequalities (Kohn and Müller ’92, ’94; Conti ’00)

S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147
Optimal scaling – Laminate construction

- Energy:
  \[ W \equiv \frac{E_0}{d^3} \sim \tau_0 \gamma + \left(\frac{\mu T \gamma^3}{bd}\right)^{1/2} \]

- Yield stress:
  \[ \tau \equiv \frac{\partial W}{\partial \gamma} \sim \tau_0 + \frac{1}{2} \left(\frac{\mu T \gamma}{bd}\right)^{1/2} \]

parabolic hardening +

Hall-Petch scaling

- Lamellar width:
  \[ l \sim \left(\frac{\mu T d}{\mu \gamma b}\right)^{1/2} \]

S. Conti and M. Ortiz, *ARMA*, 176 (2005), pp. 103–147
Optimal scaling – Branching construction

- Energy:
  \[ W \sim \tau_0 \gamma + G \left( \frac{T \gamma^2}{Gbd} \right)^{2/3} \]
- Yield stress:
  \[ \tau \sim \tau_0 + \left( \frac{T}{bd} \right)^{2/3} (G \gamma)^{1/3} \]
- Microstructure size:
  \[ l \sim \left( \frac{T d^2}{G \gamma b} \right)^{1/3} \]

S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147
Optimal scaling – Microstructures

Dislocation structures corresponding to the lamination and branching constructions

S. Conti and M. Ortiz, *ARMA*, 176 (2005), pp. 103–147
Optimal scaling – Phase diagram

\[ \left( \frac{T}{G\gamma bd} \right) \]

- Rigid
- Elastic
- Lamellar
- Branching

T = dislocation energy
G = shear modulus
\( \gamma \) = deformation
b = Burgers vector
d = grain size
\( \mu \) = GB strength

S. Conti and M. Ortiz, *ARMA*, 176 (2005), pp. 103–147
Polycrystals – Concurrent multiscale (C³)

Problem: Relaxation is domain dependent!
Pitfalls

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Localization – Fracture scaling

- Ductile fracture in metals occurs by void nucleation, growth and coalescence
- Fractography of ductile-fracture surfaces exhibits profuse dimpling, vestige of microvoids
- Ductile fracture entails large amounts of plastic deformation (vs. surface energy) and dissipation.

Fracture surface in SA333 steel, room temp., $d\varepsilon/dt = 3 \times 10^{-3} \text{s}^{-1}$
Localization – Fracture scaling

- Fracture energy scales with crack area: $E \sim L^2$
- A number of ASTM engineering standards are in place to characterize ductile fracture properties (J-testing, Charpy test)
- In general, the specific fracture energy for ductile fracture is greatly in excess of that required for brittle fracture...

1Heller, A., Science & Technology, LLNL, pp. 13-20, July/August, 2002
2Tanguy et al., Eng. Frac. Mechanics, 2005
Naïve model: Local plasticity

- Deformation theory: Minimize
  \[ E(y) = \int_{\Omega} W(Dy(x)) \, dx \]
- Growth of \( W(F) \)?
- Assume power-law hardening:
  \[ \sigma \sim K\epsilon^n = K(\lambda - 1)^n \]

- Nominal stress: \( \partial_\lambda W = \sigma/\lambda = K(\lambda - 1)^n/\lambda \)
- For large \( \lambda \): \( \partial_\lambda W \sim K\lambda^{n-1} \Rightarrow W \sim K\lambda^n \)
- In general: \( W(F) \sim |F|^p, \ p = n \in (0, 1) \)

\[ \Rightarrow \text{Sublinear growth!} \]
Naïve model: Local plasticity

- Energies with sublinear growth relax to 0.
- Example: Uniaxial extension
- Energy: \( E_h \sim h \left( \frac{2\delta}{h} \right)^p \)
- For \( p < 1 \): \( \lim_{{h \to 0}} E_h = 0 \)

- For hardening exponents in the range of experimental observation, local plasticity yields no useful information regarding ductile fracture properties of materials!
- Need additional physics, structure...
Strain-gradient plasticity

- The yield stress of metals is observed to increase in the presence of strain gradients.
- Deformation theory of strain-gradient plasticity:
  \[ E(y) = \int_{\Omega} W\left(Dy(x), D^2y(x)\right) \, dx \]
  \( y : \Omega \rightarrow \mathbb{R}^n \), volume preserving

- Strain-gradient effects may be expected to oppose localization.
- Question: Can fracture scaling be understood as the result of strain-gradient plasticity?
Strain-gradient plasticity

- Growth of $W(F, \cdot)$?
- For fence structure:
  $$F^{\pm} = R^{\pm} (I \pm \tan \theta \, s \otimes m)$$
- Across jump planes:
  $$|\|F\|| = 2 \sin \theta$$
- Dislocation-wall energy:
  $$E = \frac{T}{b} 2 \sin \theta = \frac{T}{b} |\|F\||$$
  $$\Rightarrow W(F, \cdot) \text{ has linear growth!}$$
Optimal scaling – Ductile fracture

- Approach: Optimal scaling
- Slab: $\Omega = [0, L]^2 \times [-H, H]$, periodic
- Uniaxial extension: $y_3(x_1, x_2, \pm H) = x_3 \pm \delta$
Optimal scaling – Ductile fracture

- $y : \Omega \rightarrow \mathbb{R}^3$, $[0, L]^2$-periodic, volume preserving
- $y \in W^{1,1}(\Omega; \mathbb{R}^3)$, $Dy \in BV(\Omega; \mathbb{R}^{3 \times 3})$
- Growth: For $p \in (0, 1)$, intrinsic length $\ell > 0$,
  \[
  E(y) \sim K \left( \int_{\Omega} \left( |Dy|^p - 3^{p/2} \right) dx + \ell \int_{\Omega} |D^2y| dx \right)
  \]

**Theorem** [Fokoua, Conti & MO, ARMA, 2013]. For $\ell$ sufficiently small, $p \in (0, 1)$, $0 < C_L(p) < C_U(p)$,
\[
  C_L(p)L^2\ell^{\frac{1-p}{2-p}}\delta^{2-p} \leq \inf E \leq C_U(p)L^2\ell^{\frac{1-p}{2-p}}\delta^{2-p}
\]
Fracture!

Optimal scaling – Upper bound


Optimal scaling – Upper bound

- In every cube:

- Calculate, estimate: \( E \leq C L^2 \left( a^{1-p} \delta^p + \ell \delta / a \right) \)

- Optimize: \( a = (\ell \delta^{1-p})^{1/(2-p)} \Rightarrow E \leq C_U L^2 \ell^{1-p} \delta^{2-p} \)

Numerical implementation
Material-point erosion

- $\epsilon$-neighborhood construction:
  Choose $h \ll \epsilon \ll L$

- Erode material point if
  \[
  \frac{h^2}{|K_\epsilon|} \int_{K_\epsilon} W(\nabla u) \, dx \geq J_c
  \]

- For linear elasticity, proof of $\Gamma$-convergence to Griffith fracture

**Theorem**\(^1\): Suppose $\epsilon = \epsilon(h)$ and $h/\epsilon(h) \to 0$ as $h \to 0$. Then, $\Gamma - \lim_{h \to 0} E_{h, \epsilon(h)} = \text{Griffith energy}$

Application to hypervelocity impact

Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

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Fracture of polymers

- Polymers undergo entropic elasticity and damage due to chain stretching and failure.
- Polymers fracture by means of the crazing mechanism consisting of fibril nucleation, stretching and failure.
- The free energy density of polymers saturates in tension once the majority of chains are failed: $p=0$.
- Crazing mechanism is incompatible with strain-gradient elasticity.

Crazing in 800 nm polystyrene thin film (C. K. Desai et al., 2011)
Fracture of polymers - Topology

Formation of fibers from solid polymer entails a topological transition

Fracture of polymers

- Suppose: For $K_U > 0$, intrinsic length $\ell > 0$,
  \[ E(y) \leq K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) \, dx + \ell \int_{\Omega} |D^2y| \, dx \right) \]
- If $E(y) < +\infty \Rightarrow y$ continuous on a.e. plane!
- Crazing is precluded by the continuity of $y$!
- Instead suppose: For $\sigma \in (0, 1)$,
  \[ E(y) \leq K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) \, dx + \ell^{\sigma} |y|_{W^{1+\sigma,1}(\Omega)} \right) \]

**Theorem** [Conti & MO, ARMA]. For $\ell$ sufficiently small, $p = 0$, $\sigma \in (0, 1)$, $0 < C_L < C_U$,
\[
C_L L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}} \leq \inf E \leq C_U L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}}
\]
Optimal scaling – Upper bound

Crazing in 800 nm polystyrene thin film (C. K. Desai et al., 2011)

S. Conti and M. Ortiz, ARMA (submitted for publication).
Optimal scaling – Upper bound

- In every cube:

S. Conti and M. Ortiz, *ARMA* (submitted for publication).
Taylor-anvil tests on polyurea

Shot #854:
R₀ = 6.3075 mm,
L₀ = 27.6897 mm,
v = 332 m/s

Experiments conducted by W. Mock, Jr. and J. Drotar, at the Naval Surface Warfare Center (Dahlgren Division) Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

S. Heyden et al., JMPS, 74 (2015) 175.
Experiments and simulations

Shot #861:
R₀ = 6.3039 mm,
L₀ = 27.1698 mm,
v = 424 m/s

Experiments conducted by W. Mock, Jr. and J. Drotar,
at the Naval Surface Warfare Center (Dahlgren Division)
Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA
S. Heyden et al., JMPS, 74 (2015) 175.
Concluding remarks

Can analysis shed light on the experimental record? (e.g., can some of the observed microstructures be understood as energy minimizers?)

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The Apotheosis of the program: Mathematicians and engineers still puzzle over microplasticity...
Thanks!