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The construction of an atomistic **J**-integral via estimates of continuum fields

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7.3 Recent Developments in Nanoscale Modeling of Materials

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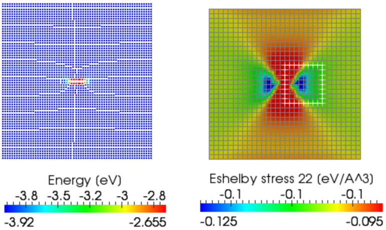
Outline

Crack in periodic box



- significant surface energy unlike in most continuum solutions
- a displacement pattern characteristic of linear elastic fracture mechanics (LEFM)
- the recovered Eshelby stress field is smooth

Motivation

This work is based on the simple premise:

- consistent fields from MD
- continuum theory

$\Big\} \rightarrow$ nanoscale results

i.e. first connect atomistic statics or dynamics to continuum fields in a manner consistent with balances then use continuum theory to analyze the process.

There are many technologically relevant examples of the validity of this approach down to the length-scale of nanometers and hundreds of atoms.

In particular atomistic simulation is particularly suited to the analysis of configurational forces.

Background

Connection between particle & continuum mechanics:

- [Irving&Kirkwood *JChemPhys* 1950], [Noll *JRatMechAnal* 1955] correspondence of particle trajectories & continuum fields through balance laws
- [Hardy *JChemPhys* 1982], [Murdoch *IJEngSci* 1993] Extension of I&K to smooth kernels
- [Zimmerman *JCompPhys* 2010] referential/material correspondence

Background

In addition to the well-known work of Eshelby(1951), Rice(1968), Peach & Koehler (1950), there is history work on an atomistic **J**-integral:

- [Inoue *IJFrac* 1994] path-dependent approximation to the **J**-integral
- [Nakatani *AIAAJ* 1998], [Jin *JNSNT* 2005], [Khare *PRB* 2007] domain integral approach, examine appropriate reference configuration.
- [Xu *IJFrac* 2004] finite-difference approximation of energy release rate
- [Choi *PhilMag* 2007] alternative contour integral & emphasis on cohesive zone development
- [Jones *JMechPhysSol* 2010] path-independent, $T = 0$ atomistic **J**-integral
- [Jones *JPhysCondMat* 2011] finite T, quasistatic **J**-integral

Eshelbian mechanics

The energy release rate relative to a process with a fixed reference configuration

$$\dot{\Pi}(\varphi_t(\mathbf{X}), \chi, \mathbf{F}) - \dot{\Pi}(\mathbf{X}, \chi, \mathbf{F}) = \int \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{expl} \cdot \dot{\varphi}\, dV$$

where $\varphi_t(\mathbf{X})$ is a map describing the configurational change in the reference, and

$$\left.\frac{\partial W}{\partial \mathbf{X}}\right|_{expl} \equiv \frac{\partial W(\mathbf{X}, \mathbf{F})}{\partial \mathbf{X}} = \frac{\partial W(\mathbf{X}, \mathbf{F}(\mathbf{X}))}{\partial \mathbf{X}} - \frac{\partial W(\mathbf{X}, \mathbf{F}(\mathbf{X}))}{\partial \mathbf{F}} : \nabla_{\mathbf{X}} \mathbf{F} = \nabla_{\mathbf{X}} \cdot \mathcal{S}$$

is work conjugate to the configurational change.

$\mathcal{S}$ is the Eshelby stress and the **J**-integral is the resultant force

$$\mathbf{J} = \int_{\partial \Omega} \mathcal{S} \mathbf{N}\, dA = \left.\frac{d\Pi}{d\mathbf{X}}\right|_{expl}$$

Eshelbian mechanics

Eshelby stress is

$$\mathcal{S} = \Psi \mathbf{I} - \mathbf{F}^T \mathbf{P}$$

where

- Ψ is the (Helmholtz) free energy,
- $\mathbf{F} = \nabla_{\mathbf{X}} \chi$ is the deformation gradient,
- $\mathbf{P}$ is the 1st Piola-Kirchhoff stress

notice these are a work-conjugacy triplet.

At zero temperature equilibrium

$$\mathbf{J} = \int_{\partial\Omega} \mathcal{S}\, \mathbf{N}\, dA = \int_{\partial\Omega} \Psi \mathbf{N} - \mathbf{F}^T \mathbf{P} \mathbf{N}\, dA = \int_{\partial\Omega} W \mathbf{N} - \mathbf{H}^T \mathbf{P} \mathbf{N}\, dA$$

where W is the internal energy, and $\mathbf{H} = \nabla_{\mathbf{X}} \mathbf{u}$ is the displacement gradient.

Hardy coarse-graining

Take Newton's law

$$m_\alpha \ddot{\mathbf{u}}_\alpha = \mathbf{f}_\alpha$$

with mass m_α, displacement $\mathbf{u}_\alpha$ and force $\mathbf{f}_\alpha = \partial_{\mathbf{x}_\alpha} \Phi$, and localize with kernel $\psi = \psi(\mathbf{x})$

$$\int m_\alpha \ddot{\mathbf{u}}_\alpha \, \psi \, dV = \int \mathbf{f}_\alpha \, \psi \, dV$$

The left-hand side can be identified with a change in momentum

$$\mathbf{p}(\mathbf{X}, t) = \int m_\alpha \dot{\mathbf{u}}_\alpha(t) \, \psi(\mathbf{X}_\alpha - \mathbf{X}) \, dV$$

and the right-hand side with a divergence of stress

$$\boldsymbol{\nabla}_{\mathbf{X}} \cdot \mathbf{P} = \int \mathbf{f}_\alpha \, \psi(\mathbf{X}_\alpha - \mathbf{X}) \, dV = \sum_{\alpha\beta} \psi_\alpha \mathbf{f}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta} (\psi_\alpha - \psi_\beta) \mathbf{f}_{\alpha\beta} = \dots$$

Hardy

Instead of a truncated expansion for $\Delta\psi = \psi_\alpha - \psi_\beta$, define an exact relation

$$\Delta\psi = \boldsymbol{\nabla}_{\mathbf{X}}\psi \cdot \Delta\mathbf{X} + \ldots = \boldsymbol{\nabla}_{\mathbf{X}} B \cdot \Delta\mathbf{X}$$

via $B_{\alpha\beta}(\mathbf{X}) = \int_0^1 \psi\left(\lambda(\mathbf{X}_\alpha - \mathbf{X}) + (1-\lambda)(\mathbf{X}_\beta - \mathbf{X})\right) d\lambda$ to obtain a stress

$$\mathbf{P}(\mathbf{X}, t) = \int \mathbf{f}_{\alpha\beta} \otimes \mathbf{X}_{\alpha\beta}\, B_{\alpha\beta}(\mathbf{X})\, \mathrm{d}V$$

which is unique up to a solenoidal field.

Consistent fields

The estimation of three fields are necessary

- (stored) energy density:

$$W(\mathbf{X},t) = \sum_{\alpha} \phi_\alpha(t)\,\psi(\mathbf{X}-\mathbf{X}_\alpha) - W(\mathbf{X})$$

where $W(\mathbf{X}) = \sum_\alpha \phi_\alpha^X \psi(\mathbf{X}-\mathbf{X}_\alpha)$ and $\phi_\alpha^X = \phi_\alpha(\{\mathbf{X}_\beta\})$ is the PE in a *fixed reference configuration* $\{\mathbf{X}^\beta\}$.

- displacement gradient defined in *mass-weighted* fashion

$$\mathbf{u}(\mathbf{X},t) = \frac{\sum_\alpha (\mathbf{x}_\alpha(t)-\mathbf{X}_\alpha)\, m_\alpha \psi(\mathbf{X}_\alpha - \mathbf{X})}{\sum_\alpha m_\alpha \psi(\mathbf{X}_\alpha - \mathbf{X})},$$

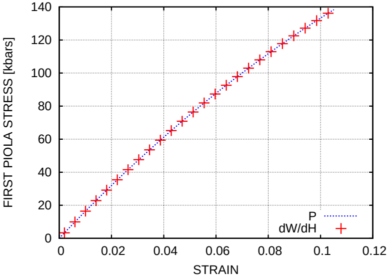
consistent with momentum density $\mathbf{p}$. With *interpolation* $\mathbf{u} = \sum_I \mathbf{u}(\mathbf{X}_I,t) N_I(\mathbf{X})$ leads directly to

$$\mathbf{H} = \nabla_{\mathbf{X}} \mathbf{u} = \sum_I \mathbf{u}_I(t) \nabla_{\mathbf{X}} N_I(\mathbf{X})\ .$$

- stress

$$\mathbf{P}(\mathbf{X},t) = -\sum_{\alpha<\beta} \mathbf{f}_{\alpha\beta}(t) \otimes \mathbf{X}_{\alpha\beta} B_{\alpha\beta}(\mathbf{X})$$

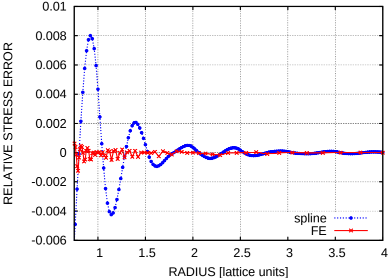
Consistency and Accuracy



The Hardy measures satisfy

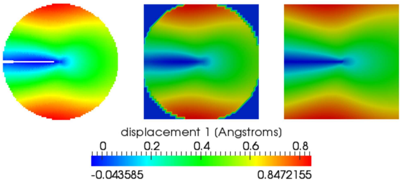
$$\mathbf{P} = \nabla_{\mathbf{F}} \Psi$$

i.e. there is (thermodynamic) consistency between the energy, stress and deformation measures.

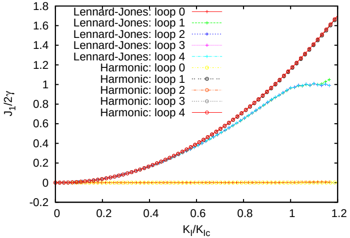


Also our use of partition of unity/FE kernels (and interpolation) can lead to faster and more accurate estimates than with traditional kernels.

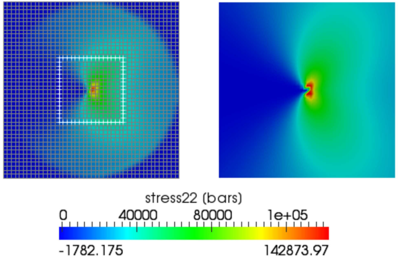
Crack tip with far field boundary conditions



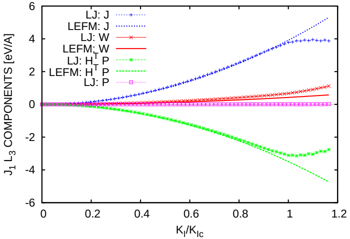
displacement: atomic, Hardy, LEFM



path independence & expected limit



stress: Hardy, LEFM



even components match theory

Finite temperature

At finite temperatures we need to revisit

$$\mathbf{J} = \int_{\partial\Omega} \langle \Psi \rangle \mathbf{N} - \langle \mathbf{F}^T \mathbf{P} \rangle \mathbf{N} \, dA = \int_{\partial\Omega} \langle \Psi \rangle \mathbf{N} - \langle \mathbf{H}^T \mathbf{P} \rangle \mathbf{N} \, dA$$

and

$$\mathbf{P} = \partial_{\mathbf{F}}\big|_T \Psi$$

The free-energy Ψ is hard to calculate directly, instead we chose a quasi-harmonic model

$$\Psi_{QH} = \Phi_0 + \frac{k_B T}{V} \log \prod_{i=1}^{n} \frac{\hbar \omega_i}{k_B T}$$

based on an assumed partition function, i.e. $\prod \omega_i = \sqrt{\det \mathbb{D}}$, and dynamical matrix

$$\mathbb{D}_{\alpha\beta} \equiv \frac{V}{\sqrt{m_\alpha m_\beta}} \frac{\partial^2 \Phi}{\partial \mathbf{u}_\alpha \partial \mathbf{u}_\beta},$$

Consistency

In mechanical $\nabla_{\mathbf{X}} \cdot \mathbf{P} = \mathbf{0}$ and thermal equilbrium $\nabla_{\mathbf{X}} T = \mathbf{0}$, we get

$$\mathbf{J}_T = \int_{\partial\Omega} \Phi_0 \mathbf{N} - \langle \mathbf{H}^T \mathbf{P} \rangle \mathbf{N} - \langle \Theta \rangle \mathbf{N} \, dA = \mathbf{J}_0 - \int_{\partial\Omega} \langle \Theta \rangle \mathbf{N} \, dA$$

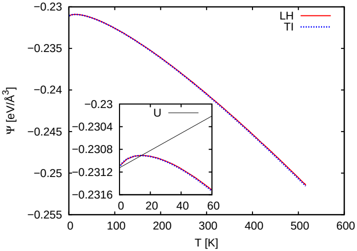
Thus, we can decompose the free-energy into the stored energy Φ we used before plus a correction

$$\Psi_{LH} = \Phi_0 + \Theta_{LH}$$

where

$$\Theta_{LH} = \frac{k_B T}{V_\alpha} \log \left(\left(\frac{\hbar}{k_B T} \right)^3 \sqrt{\det \mathbb{D}_{LH}} \right)$$

Consistency



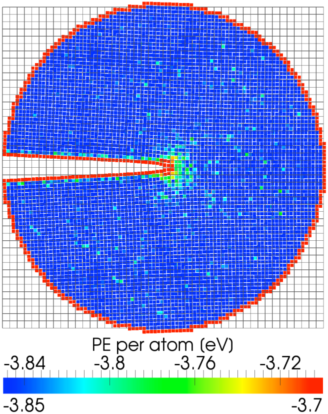
Using thermodynamic integration

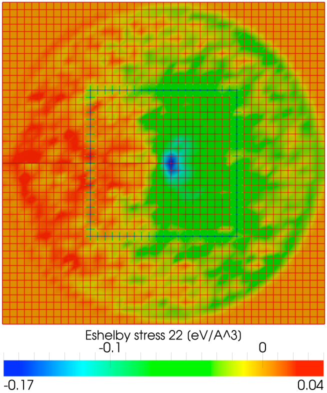
$$\Psi_1 - \Psi_0 = \int_0^1 \mathbf{P} \cdot \mathrm{d}\mathbf{F} + \int_0^1 S \, \mathrm{d}T$$

and a variety of (homogenous) loading conditions we verified that the local harmonic model was sufficiently accurate for our application.

Finite temperature crack

Using thermalization of a sequence minimized states with far field loading

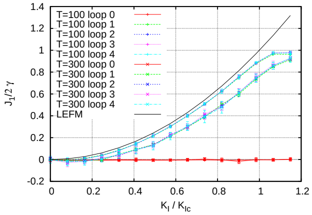




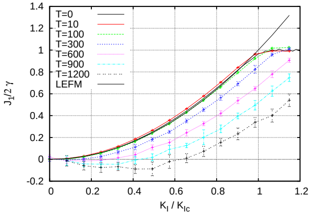
we obtain fields that show localization together with thermal noise.

Finite temperature crack

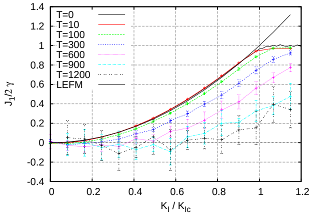
path independence



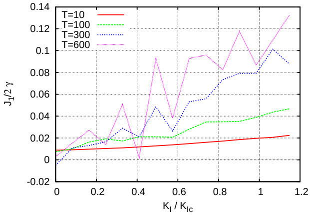
results based on internal energy



temperature dependence



differences



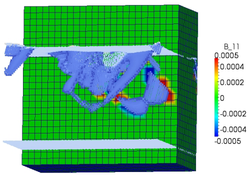
Future work

The present work

- shows path-independence
- good agreement with theory
- straight-forward implementation

Present work could be extended to:

- full dynamics
- other potentials
- more accurate QH models
- amorphous solids

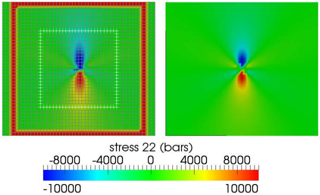


dislocation density

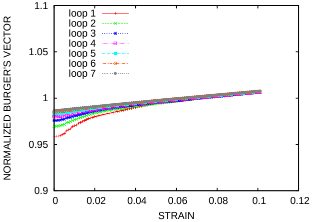
Right now we are working on connecting atomistic processes to continuum plasticity , e.g. plastic strain, dislocation density with a statistical ensemble of dislocations in MD.

Edge dislocation

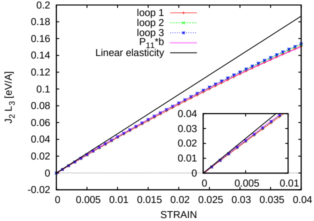
stress: Hardy vs. LEFM



Burgers vector



climb



slip