Multiscale Modeling: Continuum–Atomistic Coupling via Spacetime Discontinuous Galerkin Methods

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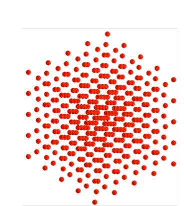
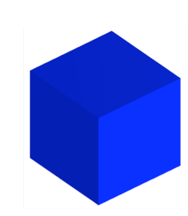
Background

Atomistic vs. Continuum Modeling

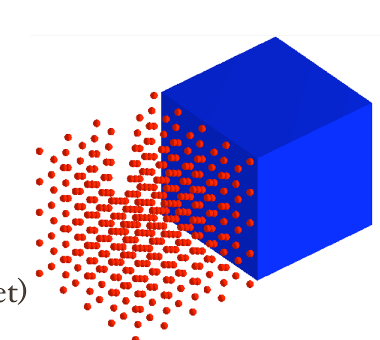




Atomistic	Continuum
• Discrete	• Continuous fields
◦ mass, momentum	◦ mass, momentum density
◦ position, velocity	◦ position, velocity
◦ fixed length scale	◦ variable length scales
• Finite number d.o.f.	• Infinite number d.o.f.
• Non–local interactions	• Localized stress, strain
◦ empirical or *ab initio*	◦ macroscopic, homogenized
• "Correct" description of defects	• Constitutive models describe cohesion, plasticity, damage, ...
• Finite differences in time	• Finite elements in space(time)

Objectives

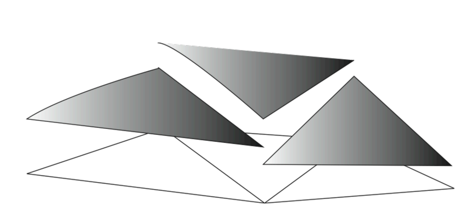
- Address full set of mechanics relations
- Eliminate non-physical reflections at interface
- O(*N*) computational complexity and parallelizable
- Modular with popular MD algorithms (velocity Verlet)
- Unified mathematical framework

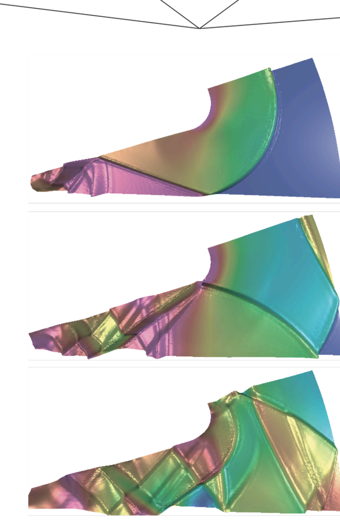


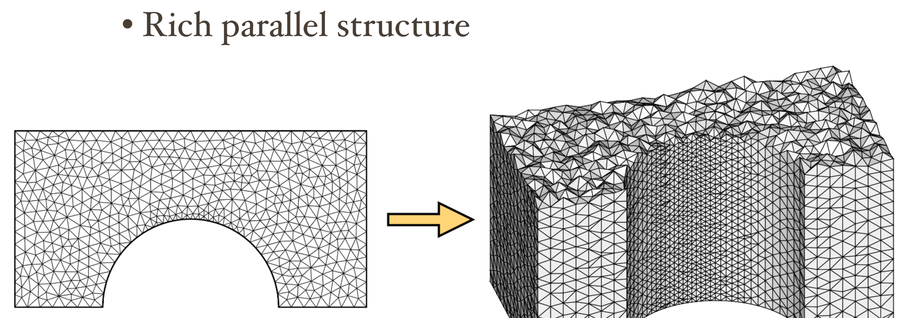
Simulation Details

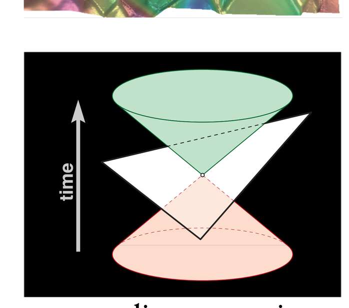
Spacetime Discontinuous Galerkin Method

- Inter–element discontinuous basis functions
  - Weak enforcement of balance/conservation jump conditions (e.g., Rankine–Hugoniot)
  - Enables exact conservation per element and O(*N*) complexity for hyperbolic problems
- Direct discretization of spacetime
  - Unstructured spacetime mesh for variable time step
  - Causality constraint for patch–by–patch solution procedure
  - Rich parallel structure



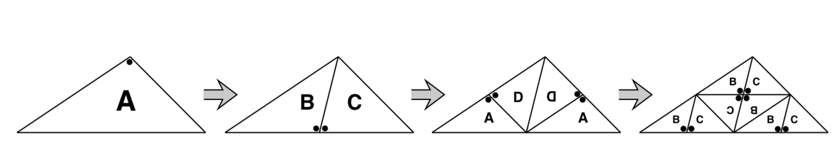


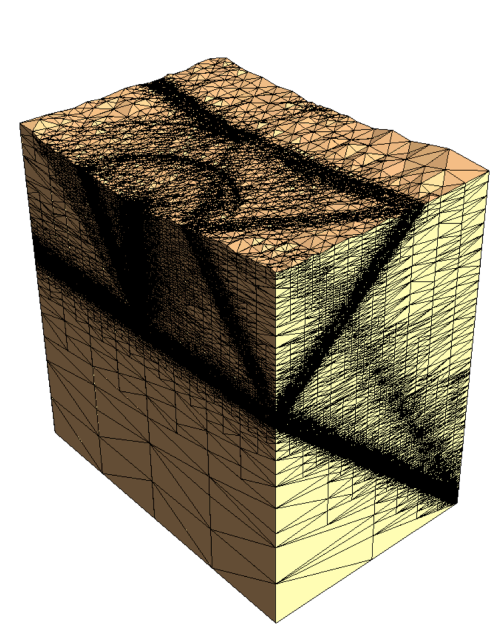


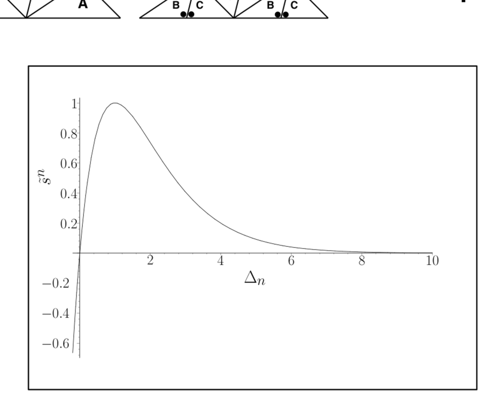


causality constraint

Adaptive Analysis

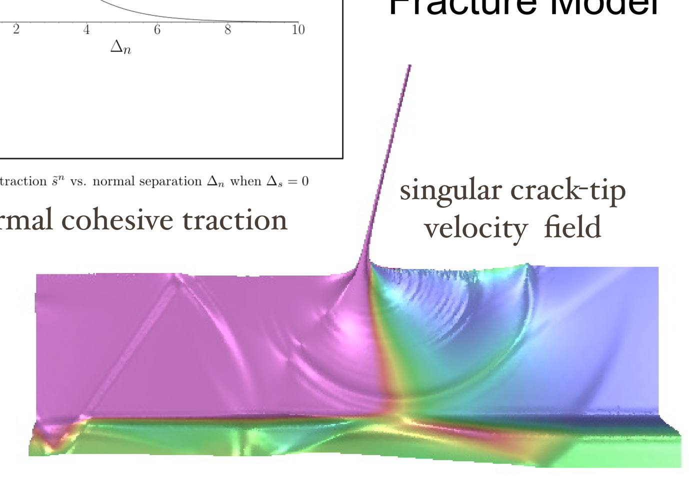






normal cohesive traction

Cohesive Fracture Model



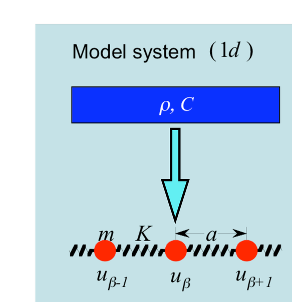
singular crack-tip velocity field

Two–Field SDG Formulation for **u, v**

$$\int_Q \{\mathbf{i}\hat{\mathbf{v}} \wedge (\mathbf{dM} + \rho\mathbf{b}) + \mathbf{d}\boldsymbol{\varepsilon} \wedge \mathbf{i}\hat{\boldsymbol{\sigma}} + k^Q \hat{\mathbf{u}}_0 \wedge (\dot{\mathbf{u}} - \mathbf{iv})\,\boldsymbol{\Omega}\}$$
$$+ \int_{\partial Q} \{\mathbf{i}\hat{\mathbf{v}} \wedge (\mathbf{M}^* - \mathbf{M}) + (\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}) \wedge \mathbf{i}\hat{\boldsymbol{\sigma}} + k^Q \hat{\mathbf{u}}_0 \wedge (\boldsymbol{u}^* - \mathbf{u})\,\mathbf{i}\boldsymbol{\Omega}\}$$
$$= 0 \quad \forall\, (\hat{\mathbf{u}}, \hat{\mathbf{v}}) \in \mathcal{V}_{\mathbf{u}} \times \mathcal{V}_{\mathbf{v}}$$

Localize to Discrete Atomic Fields

$$\rho(\mathbf{x},t) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) m_\alpha$$
$$\mathbf{u}(\mathbf{x},t) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) \mathbf{u}_\alpha(t)$$
$$\mathbf{v}(\mathbf{x},t) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) \mathbf{v}_\alpha(t)$$
$$\mathbf{dp}(\mathbf{x},t) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) m_\alpha \dot{\mathbf{v}}_\alpha(t)\Omega$$
$$\rho(\mathbf{x},t)\mathbf{b}(\mathbf{x},t) = \sum_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) \mathbf{F}_\alpha(\{\mathbf{x}_\beta(t)\})\,\Omega$$



- Undefined atomistic stess and strain set to zero
- Uniform time step (spacetime slabs)
- Integrate over slab

Explicit Position Update

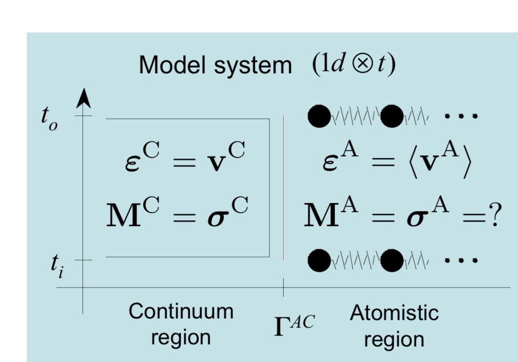
$$\mathbf{u}_\alpha(t_\mathrm{o}) = \mathbf{u}_\alpha^{\mathrm{prev}}(t_\mathrm{i}) + \mathbf{v}_\alpha^{\mathrm{prev}}(t_\mathrm{i})\Delta t + \frac{\mathbf{F}_\alpha^{\mathrm{prev}}(t_\mathrm{i})}{2m_\alpha}\Delta t^2; \quad \Delta t = t_\mathrm{o} - t_\mathrm{i}$$

Implicit Velocity Update

- Forces from explicit displacement update; assume linear in time
- Integrate quadratic atomic velocities with Simpson's rule
- Yields standard Verlet velocity update

$$\mathbf{v}_\alpha(t_\mathrm{i}) = \mathbf{v}_\alpha^{\mathrm{prev}}(t_\mathrm{i})$$
$$\dot{\mathbf{v}}_\alpha(t_\mathrm{i}) = \frac{\mathbf{F}_\alpha(t_\mathrm{i})}{m_\alpha} =: \mathbf{a}_\alpha(t_\mathrm{i})$$
$$\dot{\mathbf{v}}_\alpha(t_\mathrm{o}) = \frac{\mathbf{F}_\alpha(t_\mathrm{o})}{m_\alpha} =: \mathbf{a}_\alpha(t_\mathrm{o})$$
$$\Rightarrow \mathbf{v}_\alpha(t_\mathrm{o}) = \mathbf{v}_\alpha^{\mathrm{prev}}(t_\mathrm{i}) + \frac{1}{2}\left[\mathbf{a}_\alpha(t_\mathrm{i}) + \mathbf{a}_\alpha(t_\mathrm{o})\right]\Delta t$$

Coupling Scheme

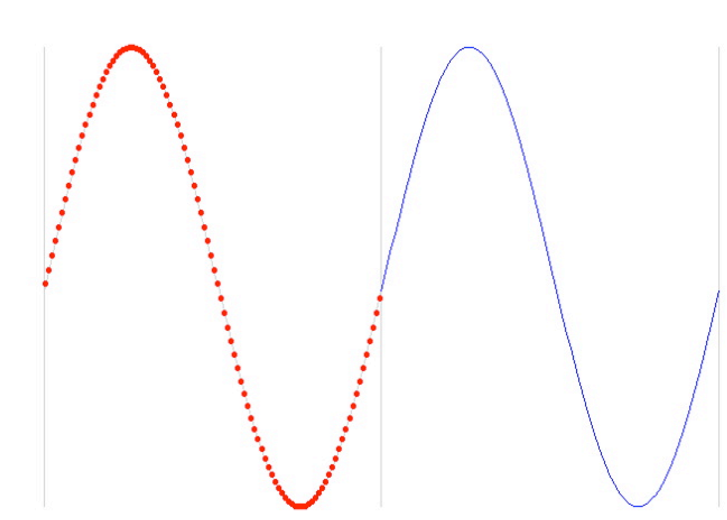


- Equip atomistic boundary with:
  - Homogenized velocity field
  - Unknown tractions represent interactions with missing atoms
  - Tractions distribute to atomic forces dual to homogenization scheme
- Extra boundary term:

$$\int_{\Gamma^{AC}} \left\{\langle\hat{\mathbf{v}}^A\rangle \wedge (\boldsymbol{\sigma}^* - \boldsymbol{\sigma}^A) + (\mathbf{v}^* - \langle\mathbf{v}^A\rangle\mathbf{d}t) \wedge \mathbf{i}\hat{\boldsymbol{\sigma}}^A\right\}$$

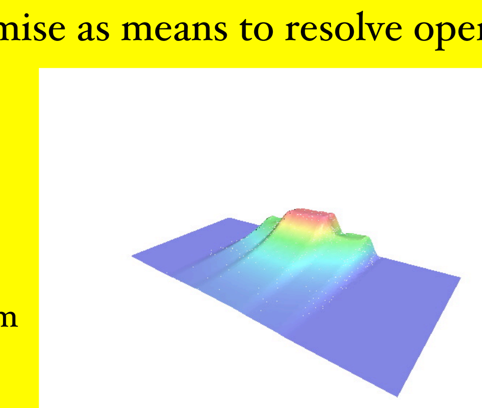
Results

- Potentials (free to choose)
  - Mass spring
  - Morse
- Reflection–free coupling in long wavelength limit
  - Periodic boundary conditions
  - Morse
- 100–atom, nearest–neighbor model
- Weak enforcement of
  - Momentum balance
  - Velocity compatibility



Conclusions

- Unified mathematical framework shows promise as means to resolve open problems in multiscale simulation
- Current and continuing work
  - Self–equilibrating interaction forces
  - Implementation in two space dimensions
  - Energy balance using thermomechanical continuum
    - non-Fourier (MCV) hyperbolic thermal model



Acknowledgements

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