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

Robert Haber, Duane Johnson, Brent Kraczek and Scott Miller

Departments of Materials Science & Engineering, Physics and Theoretical & Applied Mechanics
University of Illinois at Urbana–Champaign

Supported by the National Science Foundation under Award Number DMR-03-25930 (ITR) by the Materials Computational Center at the University of Illinois at Urbana-Champaign
Principal Investigators: Duane D. Johnson and Richard M. Martin

Background

Atomistic vs. Continuum Modeling

- Discrete
  - mass, momentum
  - position, velocity
  - fixed length scale
  - Finite number d.o.f.
  - Non-local interactions
  - empirical or at state
  - "Caustic" description of defects
- Continuous fields
  - mass, momentum density
  - position, velocity
  - variable length scales
  - Infinite number d.o.f.
  - Localized stress, strain
  - Macroscopic, homogenized
  - Constitutive models

Objectives

- Address full set of mechanics relations
- Eliminate non-physical reflections at interface
- ONS-computational complexity and parallellizable
- Module 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 ONS-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

Two-Field SDG Formulation for \(u, v\)

\[
\begin{align*}
\frac{d\mathbf{x}(t)}{dt} &= \mathbf{u}(\mathbf{x}(t)) \\
\frac{d\mathbf{v}(t)}{dt} &= \mathbf{v}(\mathbf{x}(t))
\end{align*}
\]

Localization to Discrete Atomic Fields

- Uniform atomic stress and strain set to zero
- Uniform time step (spacetime slab)
- Integrate over slab

Explicit Position Update

\[
v(t+\Delta t) = v(t) + \Delta t \dot{v}(t)
\]

Implicit Velocity Update

\[
v(t+\Delta t) = \frac{v(t) + \Delta t \dot{v}(t)}{1 + \Delta t a(t)}
\]

Fracture Model

- Cohesive traction model
- Non-zero traction at interface
- Homogenized traction

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 terms

Results

- Potentials (free to choose)
  - Mass spring
  - Morse
  - Reflection-free coupling in long wavelength limit
  - Periodic boundary conditions
  - Morse
  - 10^{10} 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

This work is supported by the ACS Petroleum Research Fund under Grant No. 38543-G7 and by the NSF through ITR grants (DMR-03-25930 and DMR-01-21695) via the Materials Computational Center and the Center for Process Simulation & Design at the University of Illinois at Urbana-Champaign.