Hybrid Particle-Continuum Simulation

Aiichiro Nakano
Collaboratory for Advanced Computing & Simulations
Department of Computer Science
Department of Physics & Astronomy
Department of Chemical Engineering & Materials Science
Department of Biological Sciences
University of Southern California
Email: anakano@usc.edu

Adaptively manage accuracy-cost trade-off; coarse-graining by heuristics (i.e., switching to different abstract)
The Nobel Prize in Chemistry 2013 was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel “for the development of multiscale models for complex chemical systems”.

A. Warshel & M. Levitt, *J. Mol. Biol.* **103**, 227 (’76)

Find multiscale modeling in your area!
Adaptive Multiscale Dynamics

Oxidation of Si

L. Lidorikis et al., *Phys. Rev. Lett.* **87**, 086104 (’01)

QMD/MD/FED:
quantum molecular dynamics/
molecular dynamics/
finite-element dynamics simulation

High-energy beam oxidation of Si (SIMOX)
H. Takemiya et al., *IEEE/ACM Supercomputing* (SC06)
Multiscale FED/MD/QMD Simulation

- Embed high-accuracy computations only when & where needed
- Train coarse simulations by fine simulations

Multiscale simulation to seamlessly couple:
- Finite element (FE) dynamics based on continuum elasticity
- Atomistic molecular dynamics (MD) simulation
- Quantum molecular dynamics (QMD) based on the density functional theory (DFT)
Hierarchical Atomistic Simulation Methods

First principles-based reactive force-fields

- Reactive bond order \( \{BO_{ij}\} \)
  \( \rightarrow \) Bond breakage & formation

- Charge equilibration (QEq) \( \{q_i\} \)
  \( \rightarrow \) Charge transfer

[Brenner; Streitz & Mintmire; van Duin & Goddard; Vashishta et al.]
Additive hybridization [Morokuma et al., ’96]

- Extrapolation in meta-model space (accuracy vs. size)
- Modular
  → Reuse of existing MD & QM (density functional theory) codes
  → Minimal inter-model dependence/communication

Divide-\&-conquer DFT embedded in MD

\[ E_{\text{MD/QM}} = E_{\text{system}}^{\text{MD}} + \sum_{\text{cluster}} [E_{\text{QM}}^{\text{cluster}}(\{r_{\text{QM}}\}, \{r_{\text{HS}}\}) - E_{\text{MD}}^{\text{cluster}}(\{r_{\text{QM}}\}, \{r_{\text{HS}}\})] \]
Environmental Effect on Fracture

Reaction of H$_2$O molecules at a Si crack tip

Collaborators: S. Ogata (NIT), F. Shimojo (Kumamoto)

Significant dependence of the reaction on stress intensity factor
Atomistic Simulations of Nanodevices
Hybrid FE/MD Algorithm

- FE nodes & MD atoms coincide in the handshake region
- Additive hybridization

Si/Si$_3$N$_4$ nanopixel
Si(111)/Si$_3$N$_4$(0001) Nanopixel

Displacement from equilibrium positions

Si$_3$N$_4$  Interface

Si

Full MD

Hybrid FE/MD

$|\Delta r|$ [Å]

$|\Delta z|$ [ nm]

$|\Delta y|$ [ nm]

Displacement [Å]

• full MD  — Hybrid

HS

Int.
Dynamics Test & Demonstration: Projectile Impact on Silicon

Waves propagate seamlessly into the FE region
Application of Multiscale Simulations

Oxidation dynamics on Si surface

QMD/MD/FED:
Quantum molecular dynamics/molecular dynamics/finite-element dynamics
“Learning on the Fly” MD/QM

- Use parameterized interatomic potential, with parameters varying atom-by-atom
- Runtime refit of the parameters in chemically reactive regions by performing small quantum-mechanical calculations

![Diagram: Atoms selected for quantum treatment (defect at 3)]

QM Cluster 1 → F₁  QM Cluster 5 → F₅

G. Csanyi et al., Phys. Rev. Lett. 93, 175503 ('04); Nature 455, 1224 ('08)

- Use expressive machine-learning (ML) potential like neural network (NN)¹ or Gaussian approximation potential (GAP)²
- Active learning to use uncertain quantification (UQ) of the ML potential to re-train the model only when needed³,⁴

¹ J. Behler & M. Parrinello, Phys. Rev. Lett. 98, 146401 ('07); IJQC 115, 1032 ('15)
⁴ J. Vandermause et al., arXiv:1904.02042v1a ('19)
Coarse Grained Molecular Dynamics

• Coarse graining: \( u_j = \sum_\mu f_{j\mu} u_\mu \), cf. wavelet smoothing

• Reduced (constrained) Hamiltonian → equations-of-motion for \( u_j \)’s

\[
E(u_k, \dot{u}_k) = \langle H_{MD} \rangle u_k, \dot{u}_k
\]

\[
= \int dx_\mu dp_\mu H_{MD} e^{-\beta H_{MD}} \Delta / Z,
\]

\[
\Delta = \prod_j \delta \left( u_j - \sum_\mu u_\mu f_{j\mu} \right) \delta \left( \dot{u}_j - \sum_\mu \frac{p_\mu f_{j\mu}}{m_\mu} \right),
\]


Coarse Graining Using Wavelets

J.-S. Chen et al., *Finite Elements in Analysis & Design* 43, 346 ('07)

Fig. 11. Effective bond potential based on wavelet multi-scale projection of fine scale bond potential.
Quasicontinuum Method

- Piecewise interpolation of the deformation of a selected subset of atoms

\[ \mathbf{x}_\mu = \sum_j N_j(\mathbf{x}_\mu) \mathbf{x}_j \]

- Coarse graining as numerical quadrature

\[ E_{\text{total}} = \sum_j w_j E_j \]

- Summation weight locally determined by a cluster of atoms centered at the “representative atoms”


Iterate:
1. Perform a small # of steps of conventional (e.g., CG) energy minimization
2. Perform one step where solid is described by elastic theory
   a. Calculate the forces acting on the atoms
   b. Transfer the atomic forces onto a computational grid
   c. Solve linear elastic eq. with a multigrid method to obtain the displacement field
   d. Get the atomic displacements by interpolating the displacement field
   e. Move the atoms along the displacement directions

TABLE I. Number of force evaluations \( n_f \) and CPU time \( T \) in seconds for the conjugate gradient (CG) and the linear scaling (SC) method for a divacancy in silicon.

<table>
<thead>
<tr>
<th>Number of atoms</th>
<th>( n_f ) (CG)</th>
<th>( n_f ) (LS)</th>
<th>( T ) (CG)</th>
<th>( T ) (LS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>510</td>
<td>102</td>
<td>106</td>
<td>0.41</td>
<td>0.50</td>
</tr>
<tr>
<td>998</td>
<td>124</td>
<td>106</td>
<td>0.90</td>
<td>0.93</td>
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<tr>
<td>1726</td>
<td>146</td>
<td>109</td>
<td>1.7</td>
<td>1.6</td>
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<td>4094</td>
<td>184</td>
<td>115</td>
<td>5.1</td>
<td>4.2</td>
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<tr>
<td>13822</td>
<td>260</td>
<td>115</td>
<td>24.0</td>
<td>14.0</td>
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<tr>
<td>110592</td>
<td>502</td>
<td>115</td>
<td>373.0</td>
<td>135.0</td>
</tr>
<tr>
<td>884734</td>
<td>934</td>
<td>117</td>
<td>5586.0</td>
<td>1147.0</td>
</tr>
</tbody>
</table>

[100 million-atom molecular dynamics simulation of a crack tip in GaAs]

S. Goedecker et al., *Phys. Rev. B* **64**, 161102(R) ('01)
Dissipative Particle Dynamics

\[
\frac{d^2 \mathbf{r}_i}{dt^2} = \sum_{j(\neq i)} \left( f_{ij}^C + f_{ij}^D + f_{ij}^R \right)
\]

\[
\begin{align*}
  f_{ij}^C &= a_{ij} (1 - r_{ij}) \hat{r}_{ij} \Theta(1 - r_{ij}) & \text{coarse interaction} \\
  f_{ij}^D &= -g(1 - r_{ij})^2 \Theta(1 - r_{ij}) (\mathbf{v}_{ij} \cdot \hat{r}_{ij}) \hat{r}_{ij} & \text{friction} \\
  f_{ij}^R &= \sqrt{2gk_B T} (1 - r_{ij}) \Theta(1 - r_{ij}) \text{rnd}_{ij} \hat{r}_{ij} & \text{random force}
\end{align*}
\]

- Generalized Langevin equation (Liouville equation & Mori-Zwanzig projection operator) for first-principles derivation of coarse forces

Lattice Boltzmann + Atomistic

- Coupling fluid dynamics + atomistics/chemical reactions
- Possible breakdown of hydrodynamics at small length scales: Boltzmann equation for $f(x, v, t)$

S. Succi, O. Filippova, G. Smith & E. Kaxiras, Comp. Sci. Eng. 3(6), 26 ('01)
Y. Kwak et al., Int'l J. Comput. Sci. 3, 579 ('09)
Spatio-Temporal Interpolation

- Interpolation in both space & time (coarse model can be “equation free”)
- Fine simulations only in small space-time patches

J. M. Hyman, *Comp. Sci. Eng.* **7**(3), 47 (’05)