FRG: Multiscale Simulation of Atomistic Processes in Nanostructured Materials

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1. Multiscale finite-element/molecular-dynamics /quantum-mechanical simulation on a computational Grid

2. Immersive & interactive visualization of billion-atom systems

3. Multimillion atom MD simulations of fracture & nanoindentation in crystalline, amorphous & nanophase materials & ceramic nanocomposites

4. New educational and outreach programs
Multiscale FE/MD/QM Simulation

Multiscale simulation to seamlessly couple:
- Finite-element (FE) calculation
- Atomistic molecular-dynamics (MD) simulation
- Quantum-mechanical (QM) calculation based on the density functional theory (DFT)
Molecular Dynamics Simulation

- Newton’s equations of motion
  \[ m_i \frac{d^2 \vec{r}_i}{dt^2} = - \frac{\partial V(\vec{r}^N)}{\partial \vec{r}_i} \quad (i = 1, \ldots, N) \]

- Interatomic potential
  \[ V = \sum_{i<j} u_{ij}(r_{ij}) + \sum_{i,j<k} v_{ijk}(\vec{r}_{ij}, \vec{r}_{ik}) \]

- \(N\)-body problem
  long-range electrostatic interaction—\(O(N^2)\)
  \[ \text{Evaluate } V_{es}(\mathbf{x}) = \sum_{i=1}^{N} \frac{q_i}{|\mathbf{x} - \mathbf{x}_i|} \text{ at } \mathbf{x} = \mathbf{x}_j \quad (j = 1, \ldots, N) \]

- Efficient \(O(N)\) solution—space-time multiresolution algorithm
  1. Fast Multipole Method (FMM) (Greengard & Rokhlin, 87)
  2. Symplectic Multiple Time-Scale (MTS) method (Tuckerman et al., 92)
Quantum Mechanical Calculation

Density functional theory (DFT)

\[ \psi(r_1, r_2, \ldots, r_{N_{el}}) \rightarrow \{ \psi_n(r) | n = 1, \ldots, N_{el} \} \]

\( O(C^N) \)  \hspace{2cm} \( O(N^3) \)

Constrained minimization problem:
- Minimize \( E[\{\psi_n\}] \) with orthonormal constraints,
  \[ \int d\mathbf{r} \psi_m^*(\mathbf{r}) \psi_n(\mathbf{r}) = \delta_{mn} \]

Efficient parallelization: real-space approaches
- Finite difference (Chelikowsky, Troullier, Saad, 94) & multigrid acceleration (Bernholc, 96)

\( O(N) \) algorithm (Kim, Mauri & Galli, 95)
- Asymptotic decay of density matrix:
- Localized functions:

\[ \rho(\mathbf{r}, \mathbf{r}') \equiv \sum_{n=1}^{N_{el}} \psi_n^*(\mathbf{r}) \psi_n(\mathbf{r}') \propto \exp(-C | \mathbf{r} - \mathbf{r}'|) \]

\[ \phi_m(\mathbf{r}) = \sum_n \psi_n(\mathbf{r}) U_{nm} \]

- Unconstrained minimization—Lagrange multiplier
Scalable Scientific Algorithm Suite

1,024 IBM SP3 & Cray T3E processors at NAVO

On 1,024 IBM SP3 processors:
- 6.44-billion-atom MD of SiO$_2$
- 444,000-electron DFT of GaAs

IEEE/ACM Supercomputing 2001
Best Paper Award
Hybrid MD/QM Algorithm

MD simulation embeds a QM cluster described by a real-space multigrid-based density functional theory

Additive hybridization
Reuse of existing MD & QM codes
(Morokuma et al., ‘96)

\[ E \equiv E_{\text{system}} = E_{\text{MD}} + E_{\text{QM}} - E_{\text{MD \ cluster}} \]

Scaled-position link atoms
Seamless coupling of MD & QM systems
Hybrid FE/MD Algorithm

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

Si/Si$_3$N$_4$ nanopixel
FE/MD/QM Simulation: Oxidation on Si Surface

Dissociation energy of $O_2$ on a Si (111) surface dissipated seamlessly from the QM cluster through the MD region to the FE region
Stress Corrosion in Si

Reaction of $\text{H}_2\text{O}$ molecules at a Si(110) crack tip

237 QM atoms

Yellow: QM-H
Red: QM-O
Green: QM-Si
Blue: HS-Si
Gray: MD-Si
Stress Corrosion in Si

Significant effects of stress intensity factor on the reaction

Yellow: H
Red: O
Green: Si
Distributed Cluster Computing

Additive hybridization; multiple QM clustering

• Globus/MPICH-G2 — Ian Foster (ANL)
• S. Ogata (Yamaguchi), F. Shimojo (Hiroshima), K. Tsuruta (Okayama), H. Iyetomi (Niigata)
Multiscale Simulation on a Grid

- Scaled speedup, $P = 1 + 8n$ ($n =$ number of clusters)
- Efficiency = 94.0% on 25 processors in the US & Japan
Immersive & Interactive Visualization

- Octree-based fast view-frustum culling
- Parallel/distributed processing
Parallel & Distributed Visualization

Nearly real-time walkthrough for 1 billion atoms on an SGI Onyx2 (2 MIPS R10K, 4GB RAM) connected to a PC cluster (4 800MHz P3)
Outline

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Fracture in Glasses, Nanophase Ceramics & Nanocomposites

Systems
- Nanophase Si$_3$N$_4$, SiC, Al$_2$O$_3$
- SiO$_2$ glass
- Nanocomposite - SiC fibers in a Si$_3$N$_4$ matrix

Issues
- Atomistics of crack propagation
- Mechanisms of energy dissipation
- Scaling properties of fracture surfaces
Validation of Interatomic Potential

Amorphous SiO$_2$

MD results for elastic moduli also agree well with experiments
Fracture in Amorphous Silica: 15 Million Atom MD Simulations

Fracture Toughness

\[ K_{IC} = 1 \text{ MPa.m}^{1/2} \text{ (MD)} \]

\[ 0.8 \text{ MPa.m}^{1/2} < K_{IC} < 1.2 \text{ MPa.m}^{1/2} \text{ (Experiment)} \]
Experiment by Bouchaud et al.

Cavity formation & coalescence with crack in a glass
(Top) AFM study in a glass: (a) nanometric cavities before the crack advances; (b) growth of cavities; (c) crack propagation via the coalescence of cavities.

(Bottom) MD results showing the same phenomenon in a-SiO$_2$
Dynamic Fracture in Nanophase $\text{Si}_3\text{N}_4$

Nanophase $\text{Si}_3\text{N}_4$ is much tougher than $\text{Si}_3\text{N}_4$ crystal

Crack Deflection  Pore Coalescence

Toughening Mechanism: Crack deflection, branching & coalescence with nanopores
Morphology & Scaling Behavior of Fracture Surfaces

Fracture surfaces are anisotropic & statistically invariant under an affine transformation

\[
(x, y, z) \rightarrow (b^\zeta x, by, bz)
\]

\[
\Delta h(r) = \left\langle (x(z + r) - x(z))^2 \right\rangle_z^{1/2}
\]

\[
\Delta h(r) \propto r^\zeta
\]

\(\zeta\) is called the roughness exponent
Scaling Behavior of Cracks

Two regimes with roughness exponents 0.5 & 0.8

P. Daguier, B. Nghiem, E. Bouchaud & F. Creuzet (1997)
MD results for roughness exponents agree with experiments

MD results reveal that the smaller roughness exponent is due to intrapore correlations and the larger one due to coalescence of pores and cracks.
Fracture in a Nanocomposite

1.5-billion-atom MD on 1,024 IBM SP3 processors

Color code: $\text{Si}_3\text{N}_4$; SiC; SiO$_2$

Silicon nitride matrix-silicon carbide fiber nanocomposite

0.3 mm
Nanoindentation in $\text{Si}_3\text{N}_4$

Nanoindentation allows for the measurement of hardness, which in turn provides important information about elastic and plastic deformation. Multi-million atom MD simulations can be used to model such phenomena.
Indentation Fracture & Amorphization

Indentation fracture at indenter diagonals

Amorphous pile-up at indenter edges

Anisotropic fracture toughness
Hardness of Silicon Nitride

Load-displacement curve

- $\alpha$-crystal (0001): 50 GPa
- Amorphous: 32 GPa

Microindentation experiments on $\alpha$-crystal (0001): 31-48 GPa
Summary

- Parallel multiscale MD/QM simulation methodology
- Interactive visualization of billion atoms
- Multimillion atom MD simulations
  - fracture in silica glass, nanophase ceramics & nanocomposite
  - nanoindentation in crystalline & amorphous Si$_3$N$_4$
Graduate Education

Dual-Degree Program
Ph.D. in the physical sciences & M.S. in computer science

International course on computational physics
- LSU/USC
- TU Delft, The Netherlands
- Niigata Univ., Japan

Experimental training
- Synthesis
- Characterization
- Property measurements
Undergraduate Outreach Activities

Computational Science Workshop for Underrepresented Groups

- 19 participants from 11 institutions — Hampton, Clark-Atlanta, Morehouse, Jackson State, Mississippi State, Texas Southern, Univ. of Texas — Pan American, Xavier, Grambling, Southern & Univ. of Louisiana in Monroe
- Activities: Construction of a PC cluster from off-the-shelf components & using this parallel machine for algorithmic and simulation exercises.