A Metascalable Computing Framework for Large-Scale Atomistic Simulations

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Advanced Atomistic Simulation Methods

- **Molecular Dynamics (MD)**
- **ReaxFF**: First principles-based reactive force-field
- **QM—Density functional theory (DFT)**
- **Electron wave function**

O(N) Scalable Simulation Algorithm Suite

- **N-body problem**: \(O(N^2) \rightarrow O(N)\)
  - Space-time multiresolution molecular dynamics (MRMD): Fast multipole method & symplectic multiple time stepping
- **Variable N-charge problem**: \(O(N^3) \rightarrow O(N)\)
  - Fast reactive force-field (F-ReaxFF) MD: Multilevel preconditioning
- **Quantum N-body problem**: \(O(C^3) \rightarrow O(N)\)
  - D&C density functional theory (DC-DFT): Adaptive multigrids
- **Multiscale QM (DC-DFT)/MD simulation**

Benchmark Results: Internode Weak/Strong Scalability

- Weak-scaling internode parallel efficiency 0.985 on 212,992 CPUs BlueGene/L at LLNL on 131,072 CPUs BlueGene/P at ANL

Benchmark Results: Hybrid MPI/threads/SIMD Optimization

- Internode scalability: Superlinear speedup on Xeon 128 CPUs
- Intercore scalability: Efficiency 0.811
- Intracore optimization: 5.9 Gflops (55% of the peak performance) with SIMD on Nehalem