intel Look Inside™

Newer version coming

Large-Scale Hydrodynamic Brownian Simulations on Intel Xeon Phi

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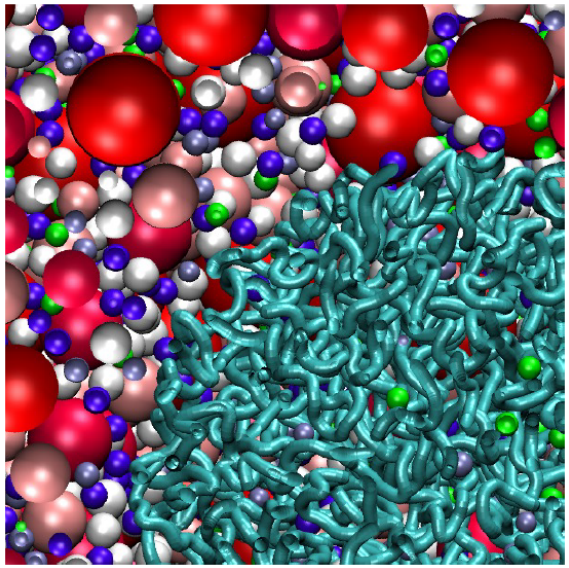
What's unique about my tuning work

- **Application: Hydrodynamic Brownian Simulations**
  - Computational method for simulating the motion of particles, such as macromolecules and nanoparticles, in a fluid environment.
  - Widely used in biology, biochemistry, chemical engineering and materials science
- **Application domain**
  - Computational biology; Molecular simulation
- **Execution mode**
  - Hybrid CPU+MIC
- **Tools used**
  - Intel VTune



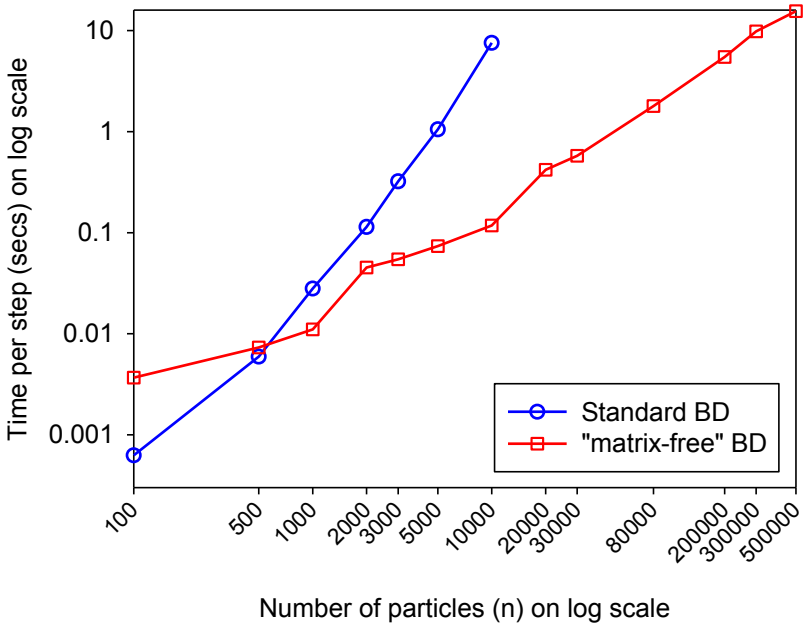
Performance

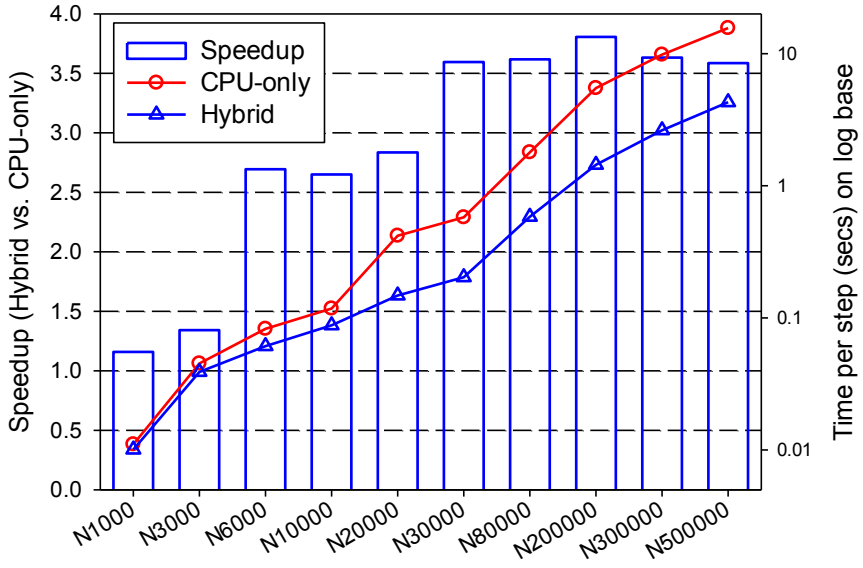
- **Hybrid CPU-Phi (2 Xeon + 2 MIC) implementation is >3.5X faster than CPU-only code (2 Xeon)**
  - > 90% offload efficiency
- **Optimizations: on Xeon >3x, on MIC >5x**
  - SIMDization: on Xeon 2.2x, on MIC 4.3x
  - Load balancing: on Xeon 1.05x, on MIC 1.3x
  - Prefetching: on Xeon 1.05x, on MIC 1.2x
- **With the above optimizations as well as algorithm improvement, simulations with 500,000 particles can now be accomplished on a single Intel Xeon Phi card**
  - Previous codes are limited to 3,000 particles

Performance Cont.

standard BD: standard algorithm for Brownian dynamics simulations

"matrix-free" BD: our algorithm for Brownian dynamics simulations with MIC optimizations





Insights

- **Potential performance issues on MIC**
  - Low SIMD efficiency
  - Load imbalance
  - Memory/Cache latency
- **Potential performance issues of hybrid computing**
  - Load imbalance between CPU and MIC
  - Kernel launching/PCI-e communication overheads
- **Questions?**
  - What's the best practice for implementing a dynamic scheduler between CPU and MIC?
  - How to estimate the PCI-e communication overheads?