September 18, 2012

Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations

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XSEDE

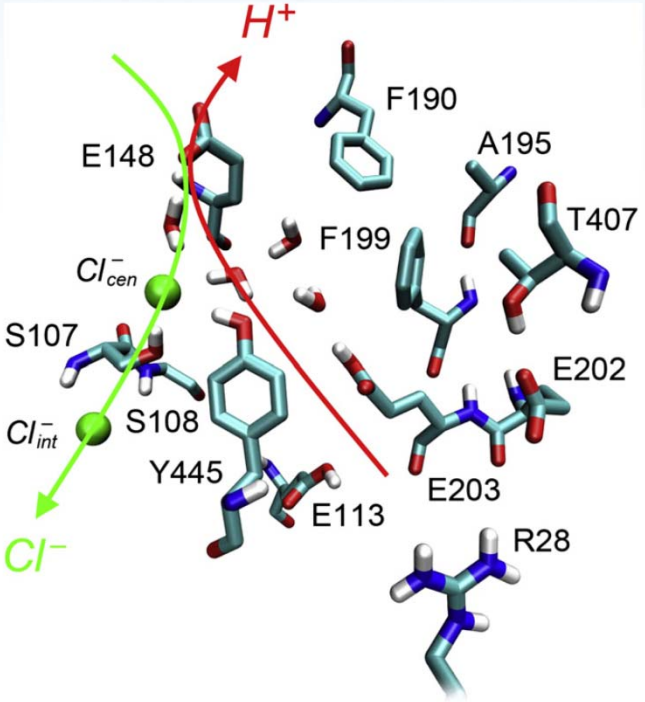
Extreme Science and Engineering Discovery Environment

Outline

- Proton Solvation and Transport and Multiscale Reactive Molecular Dynamics
- Reactive MD Challenges
- Choice of New Code
- Parallel Strategies
- Project Challenges
- Results
- Future Work

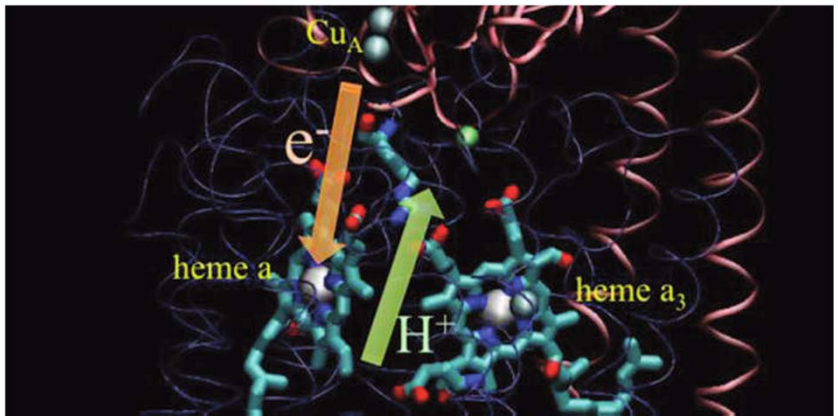
Proton Solvation and Transport

Unraveling proton transport pathways in chloride transport membrane proteins.



*Wang and Voth, Biophys. J, **97**, 121 (2009)*

Electron-coupled proton transport in Cytochrome c Oxidase



*Yamashita and Voth, J. Am. Chem. Soc., **134**, 1147 (2011)*

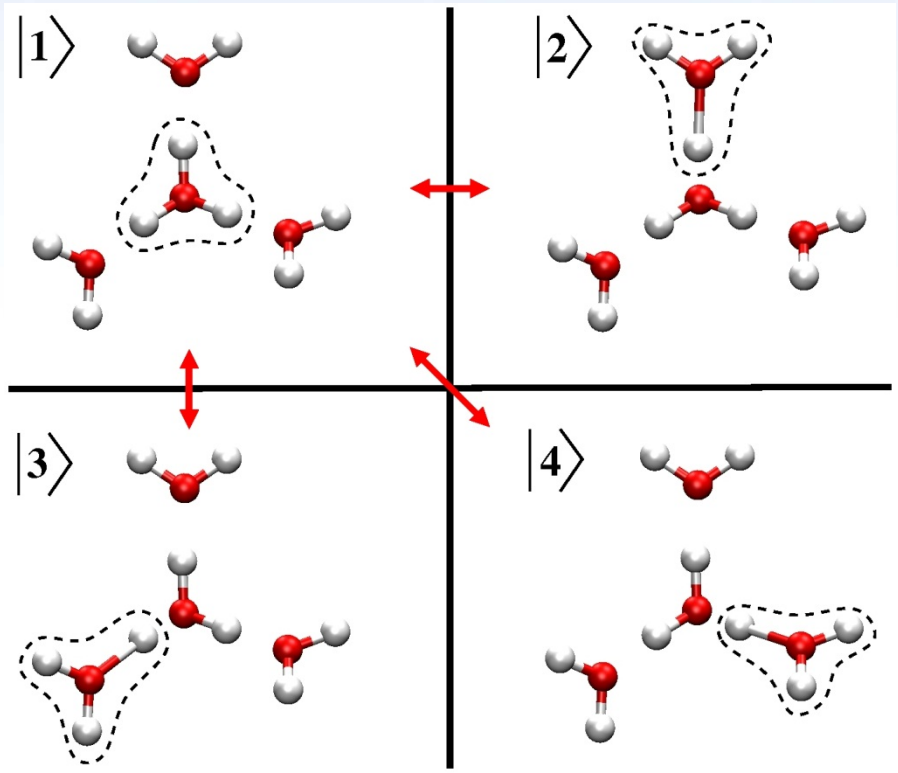
Multiscale Reactive Molecular Dynamics

*Swanson et. al., J. Phys. Chem. B, **111**, 4300 (2007)*

*Knight and Voth, Acc. Chem. Res., **45**, 101 (2012)*

- A linear combination of bonding topologies can be used to describe the variable bond topology of a reactive complex.

$$\mathbf{H} = \begin{pmatrix} V_{11} & V_{12} & V_{13} & V_{14} \\ V_{12} & V_{22} & 0 & 0 \\ V_{13} & 0 & V_{33} & 0 \\ V_{14} & 0 & 0 & V_{44} \end{pmatrix}$$



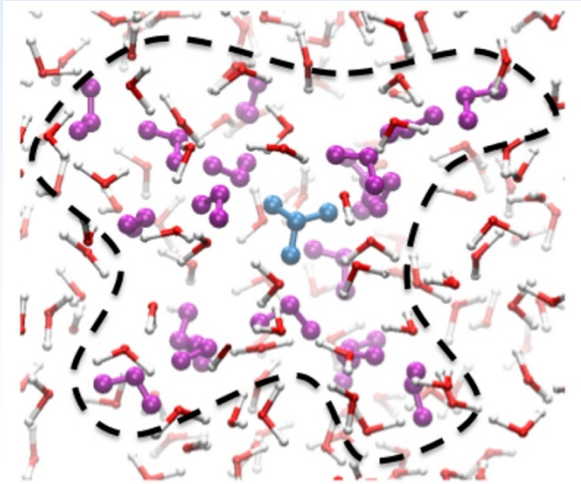
All interactions are parameterized by fitting to QM or AIMD data.

Algorithmic Challenges and Parallel Scaling

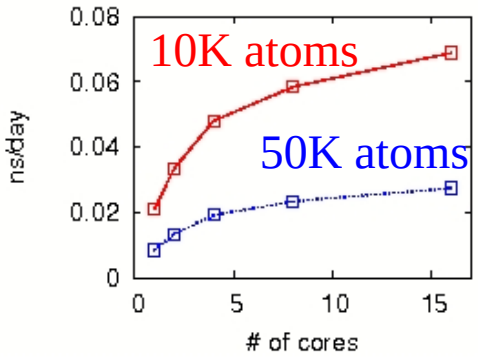
- Efficiently calculate Hamiltonian matrix

- Complex is all possible bond topologies (states) for a given proton.
- As many as 30+ states in a given complex

  - environment — environment
  - complex — environment
  - complex — complex



- Poor parallel scaling (DL_EVB)



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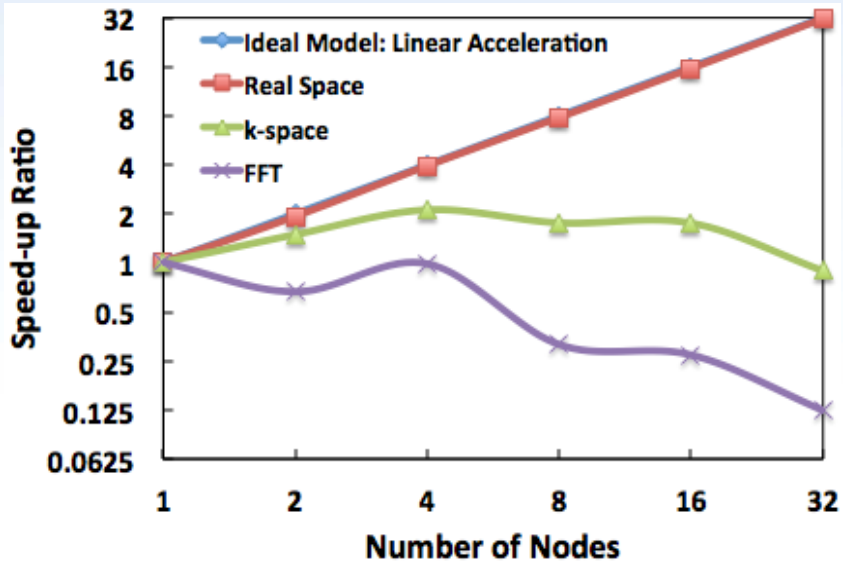
Parallel Scaling Challenges

Ranger (TACC)



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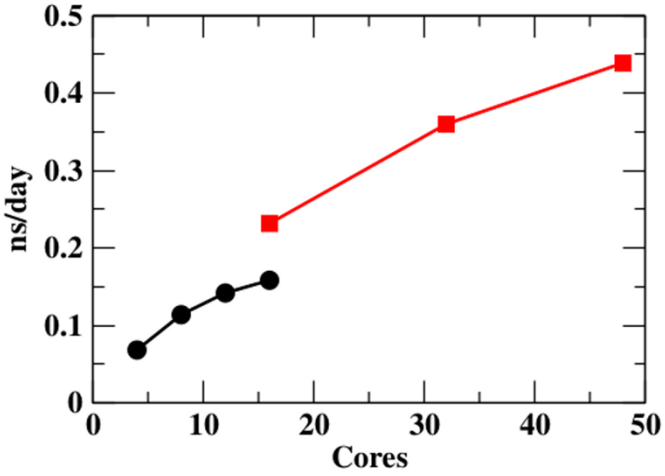
- Real-space interactions scale near perfectly (work is local to processor).
- Parallel performance degradation at high processor counts largely because of 3D FFTs (many tens of FFTs per time step).
- Critical to multistate algorithms, which evaluate several 3D FFTs per matrix element.
- Without affecting accuracy, a more efficient parallelization strategy is required.

Choosing a New Code

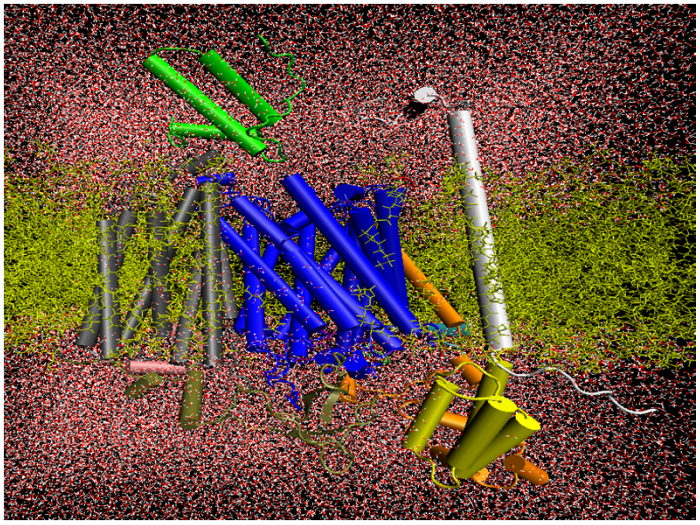
- Old Code: Reactive MD method implemented in DL_POLY code (DL_EVB)
  - Slow serial and parallel execution
  - Very easy to modify and extend
- New Code requirements
  - Reasonably fast
  - Easily modifiable and extensible by graduate students and postdocs
  - Suitable for accurate all-atom biomolecular simulation
- Benchmarked and compared codes
  - Gromacs and NAMD very fast, but harder to extend
  - LAMMPS ~2x slower, but simple to modify and extend due to modular design (uses C++ for high-level organization, plain C for low level stuff)
  - Ease of use and maintainability outweighed performance difference

Implementing Reactive MD in LAMMPS

- RAPTOR (Rapid Approach for Proton Transport and Other Reactions)
- Multistate algorithm is written as “fancy” potential and interfaced with LAMMPS through the “fix” mechanism.
- Immediately observed improvements in parallel scaling efficiency, but additional work was required.



Ranger (TACC): 512 Waters + Proton
for **DL_EVB (black)** and **RAPTOR (red)**



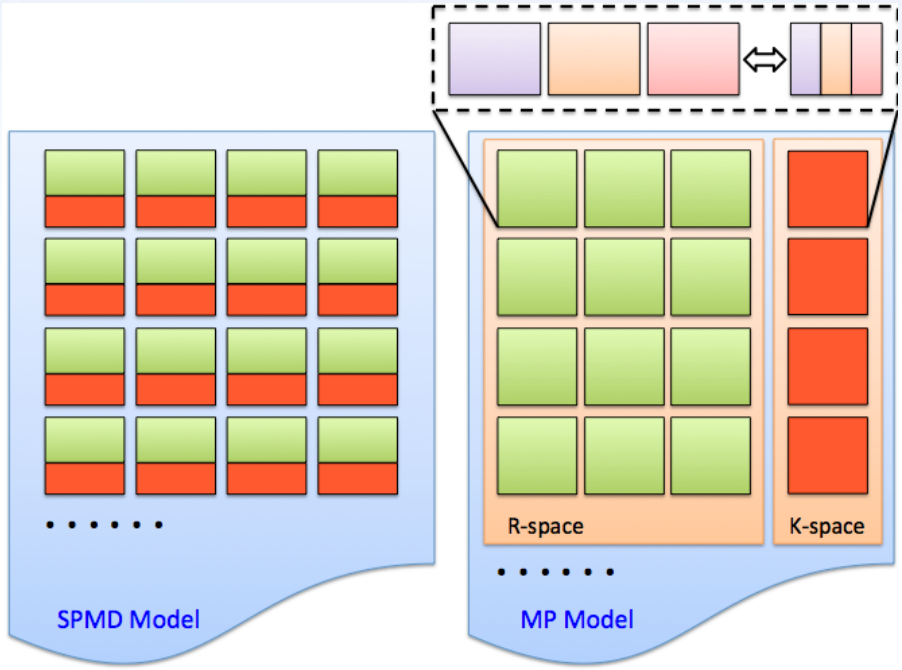
Cytochrome c Oxidase (159K atoms)

Improving Parallel Performance: Hybrid Strategy

- Tested new hybrid OpenMP/MPI LAMMPS developed by Axel Kohlmeyer
- Minimize MPI processes involved in all-to-all communication
- Added capability of using **single precision FFT** in LAMMPS to reduce required communication bandwidth
- Observed good speedup on Kraken

Multiple Program Strategy (R- and K-space)

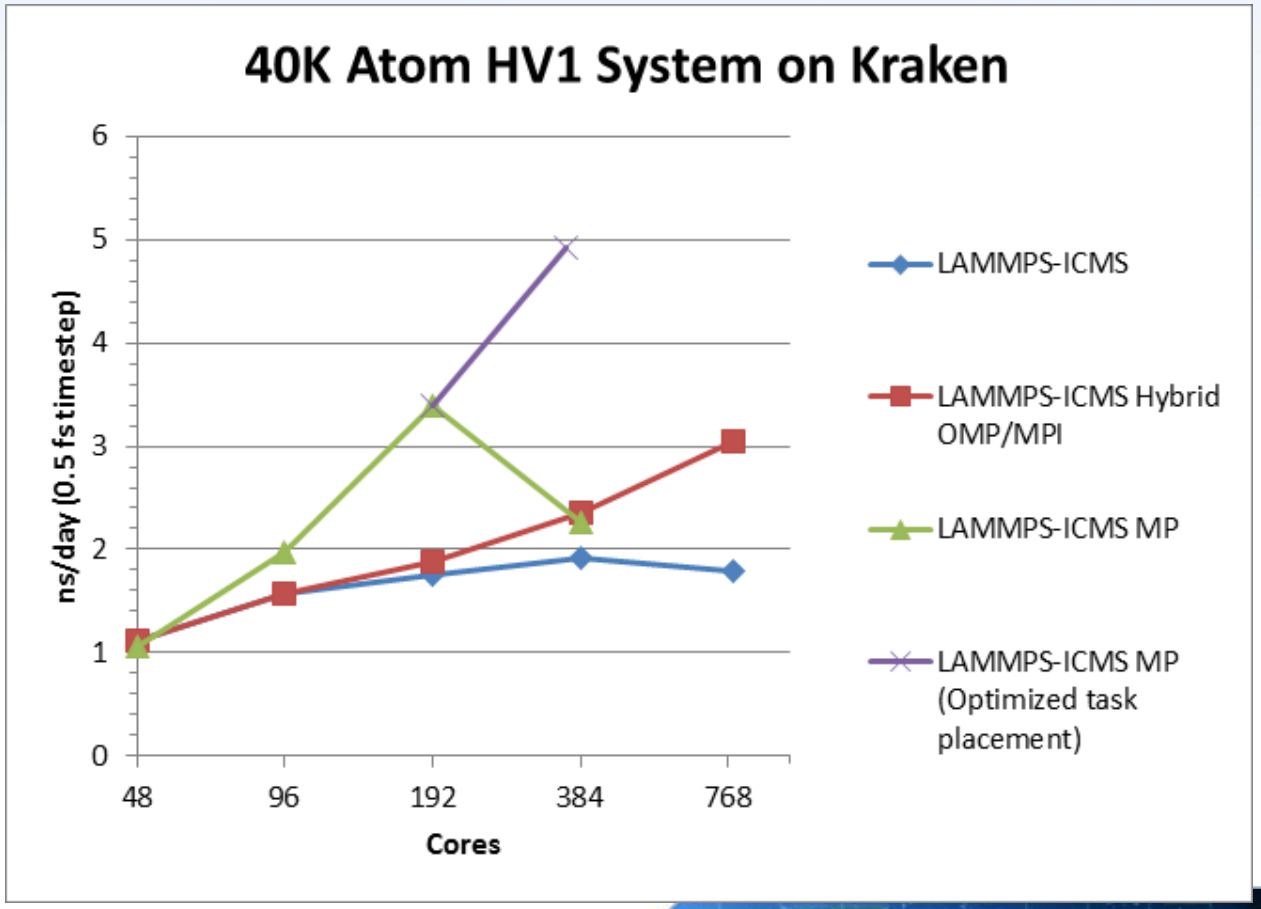
- Used by Gromacs and NAMD
- Divide processors into (at least) two separate partitions.
- 1st partition, usually larger, handles real-space forces, equations of motion integration, I/O, etc…
- 2nd partition handles only 3D FFTs
- Reduced communication and simultaneous evaluation lead to sizeable improvements in performance.



Implemented as "run_style verlet/split" in LAMMPS

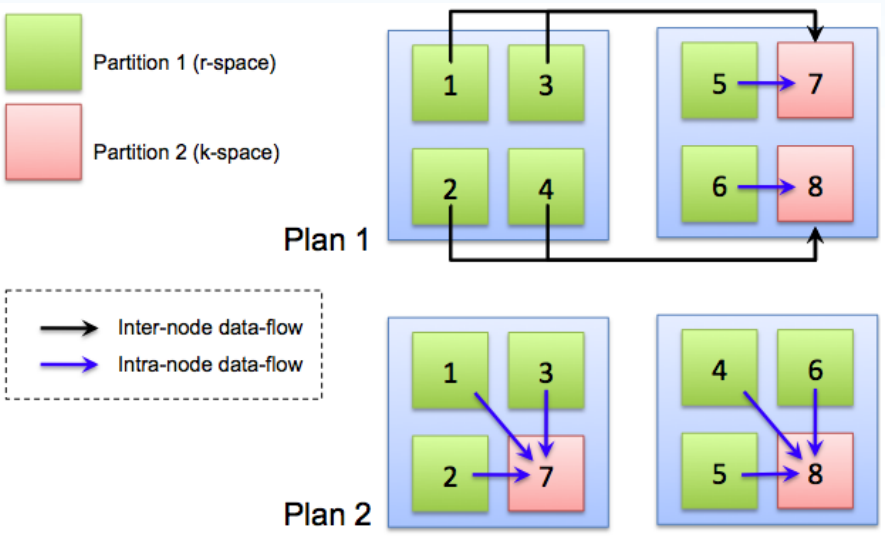
Multiple Program vs. Hybrid Strategy

- Multiple Program wins out – with proper rank placement



Multiple Program Strategy (R- and K-space)

- At higher processors counts, important to keep MPI ranks within comm. block proximal to each other on physical machine.
- Default assignment of MPI rank order is suitable for small core counts.
- Reordering typically becomes important beyond several nodes.
- Major Breakthrough: integration into main LAMMPS distribution



LAMMPS mechanism for MPI rank reordering: "-reorder nth 4"

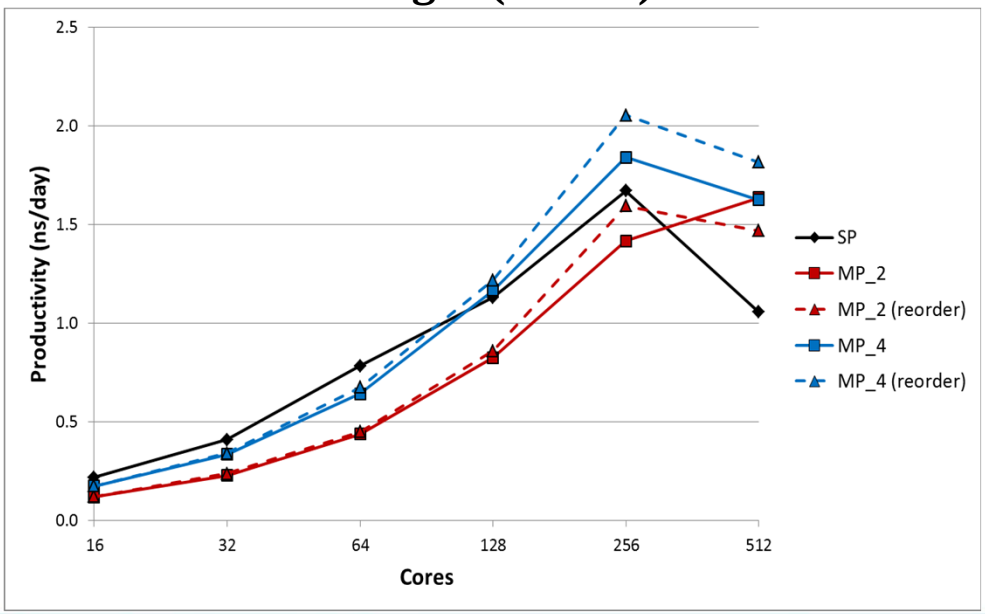
Project challenges

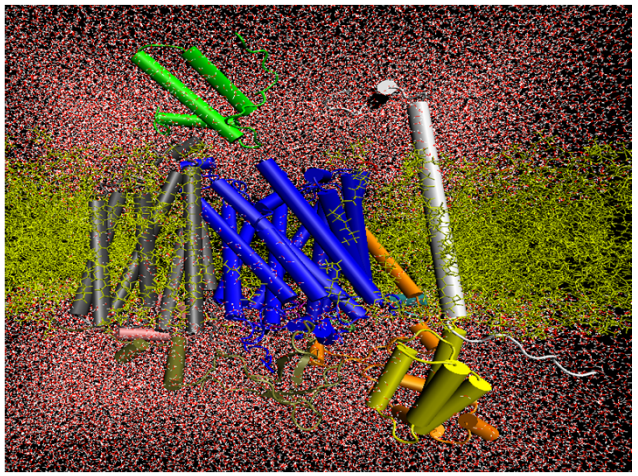
- Multi-year ASRT project challenges
  - Sporadic work due to finely divided time commitments
  - Restart overhead
  - Keeping track of project progress, ideas, code versions, benchmark parameters, etc.
  - Eventually used Google docs to standardize data sharing, keep track of results
- Machine-specific issues
  - Compilers (compiler and machine-specific bugs)
  - Performance tools (work with some compilers, not others)
  - Reproducible and self-consistent benchmarks (using same set of nodes for a given set of benchmarks)

Multiple Program Scaling- LAMMPS

- Benchmark: 159K atom CcO system
- Benefits of MP parallelization at 128 nodes and beyond.
- A 3:1 MP ratio was found to be optimal, with larger ratios better at larger processor counts.
- Additional speedups observed when MP is combined with OpenMP threads.

Ranger (TACC)

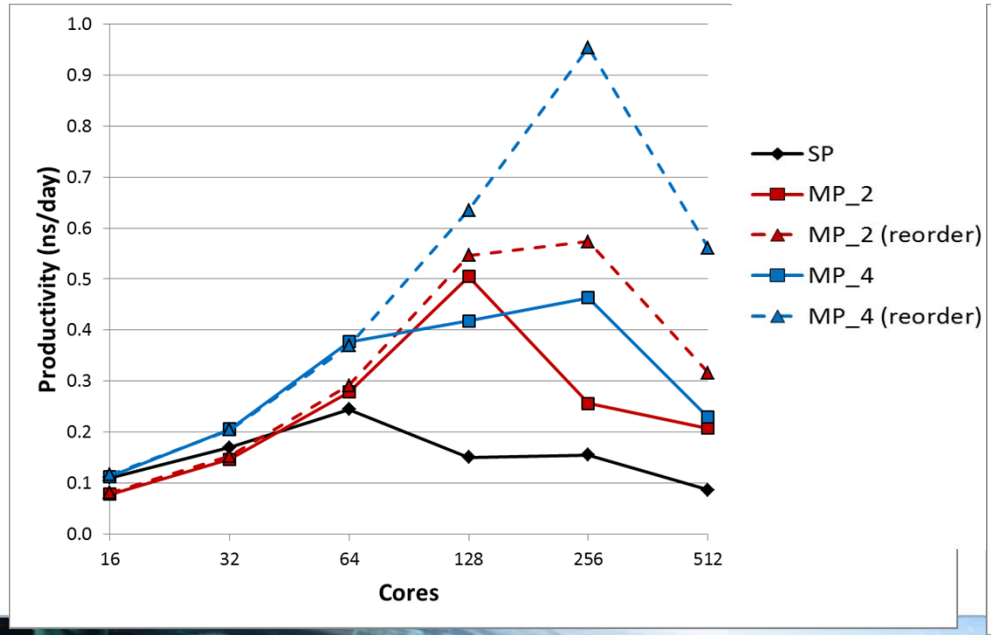




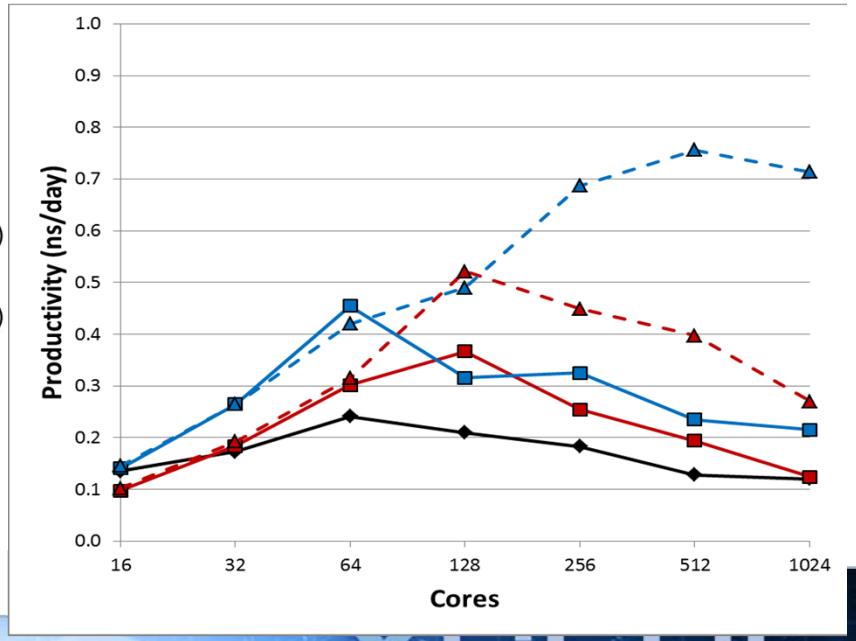
Multiple Program Scaling- RAPTOR

- Benchmark: 159K atom CcO system
- Improvements from MP observed by 32 cores.
- Reactive simulations are only **~2x** slower than nonreactive simulations!!
- Scaling analysis identifies **real-space partition waiting for k-space partition** to finish.
- Total speedup: 3-4x faster than Single Program RAPTOR

Ranger (TACC)



Kraken (NICS)



Key highlights for final project year

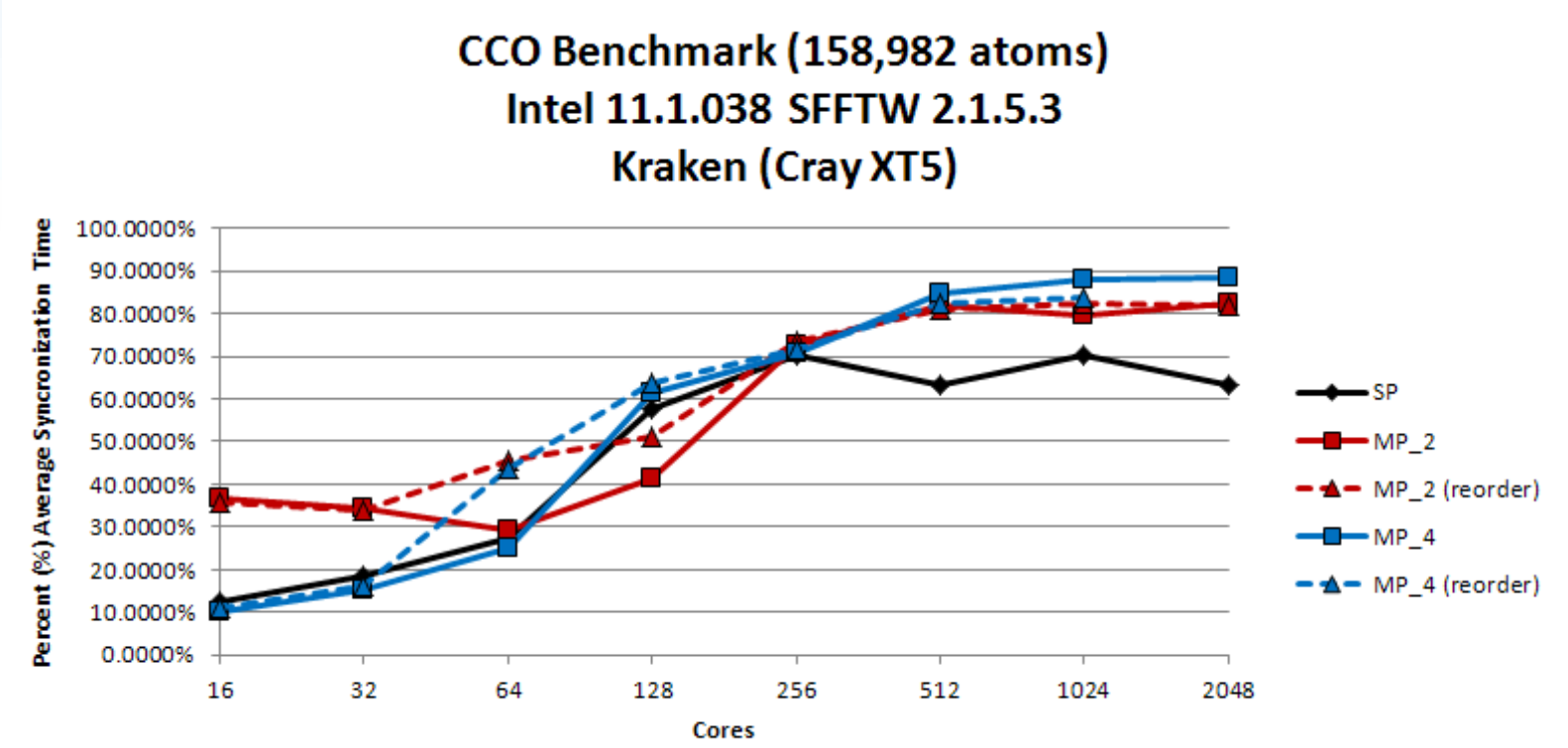
- Improved scaling of the general LAMMPS MD code
- Incorporated improvements into the main LAMMPS code base, benefiting the world-wide LAMMPS community. (http://lammps.sandia.gov/)
- For the reactive LAMMPS code (Raptor), increased the accessible simulation time by **4x (target was 2x)**, while maintaining parallel efficiency over 50%.
- Optimized and benchmarked the code on two XSEDE platforms: Kraken and Ranger.
- Results published in XSEDE12 paper: http://dl.acm.org/citation.cfm?id=2335833
- Overall improvement over previous reactive code (DL_EVB) is **20-30x**

Future Directions…

- Finish updating support for OpenMP in RAPTOR with MP.
- Approximate methods for electrostatics have been developed to greatly reduce the number of 3D-FFTs in multistate algorithms.
- Generalize MP algorithm in RAPTOR to arbitrary number of partitions for single and multiple reactive species. Parallelize over states.
- Address load balancing between partitions (parallelization over independent states may help overlap computation and communication).
- Further optimize electrostatics and FFTs

Load Imbalance

- Used the fpmpi lightweight profiling tool to obtain information about RAPTOR runs.
- MPI Synchronization time become significant portion of run time.



Source of Synchronization Time

- 64 cores single partition
  - Avg. MPI Sync Time = 56.69 s (206.44 s Wall Clock)
    - Avg. MPI_Wait + MPI_Waitany = 49.56 s
    - Avg. Collective Sync = 3.10 s
- 64 cores two partitions (32:32 cores)
  - Avg. MPI Sync Time = 86.84 s (191.19 s Wall Clock)
    - Avg. MPI_Wait + MPI_Waitany = 23.05 s
    - Avg. Collective Sync = 3.05 s
    - Avg. MPI_Bcast = 58.71 s
      - Tentatively attributed to bcast which transfers data from k-space to r-space partitions.