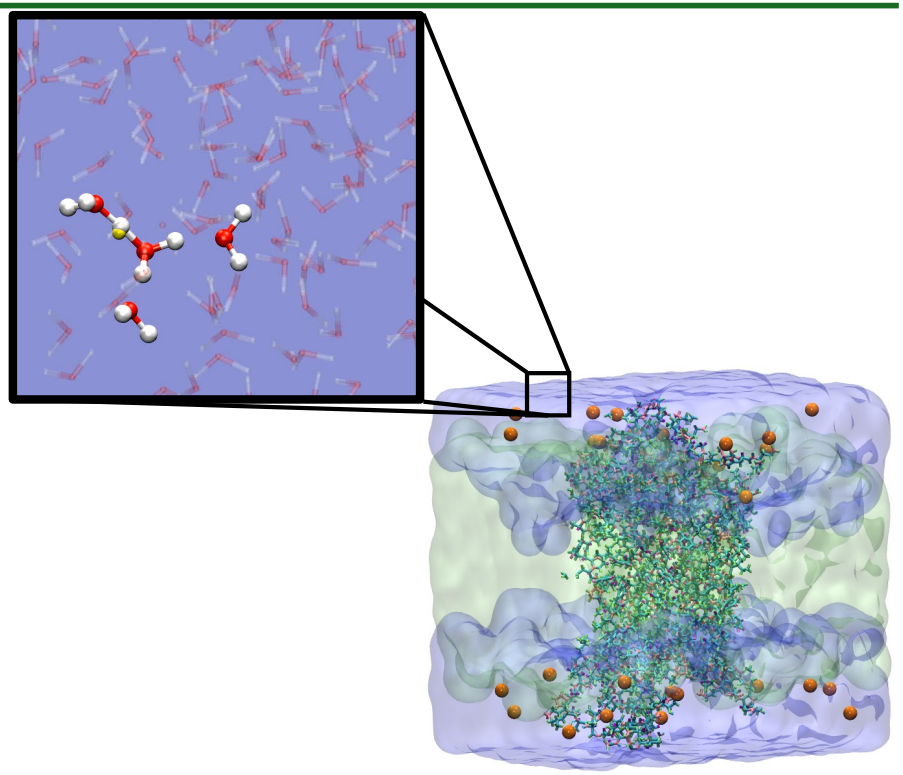
Continued Effort on Porting LAMMPS to Aurora

The Science

- Molecular Dynamics (MD) is awesome
- LAMMPS is extremely general and extensible software for large-scale molecular simulations (MD and beyond).
- Forcefields describe how particles interact:
    - Bonded interactions, dispersion, electrostatics (short + long ranged), granular, nonreactive vs. reactive
- LAMMPS on Aurora supported via two routes
    - Kokkos package: goal of being gpu-resident
        - Many capabilities still need to be ported
    - GPU package: only pair calculation off-loaded
        - Relies heavily on CPU parallelization

The Challenge

- A large number of different forcefield models and capabilities need to be evaluated for functionality, correctness, and performance.
- Aurora will be available to users soon and need to ensure key capabilities in LAMMPS are supported for users to achieve their science goals
- Support for long-range KSPACE electrostatics with Kokkos/SYCL was still missing.



Solvated proton in water and rhodopsin protein embedded in membrane (Image credit: Christopher Knight (ANL)).

Relevant publication(s) on science background: A.P. Thompson, et.al., *Comput. Physics. Commun.*, **271**, 108171 (2022).

https://www.lammps.org/
https://github.com/lammps/lammps

Awesome CPS logo created with AI image generator

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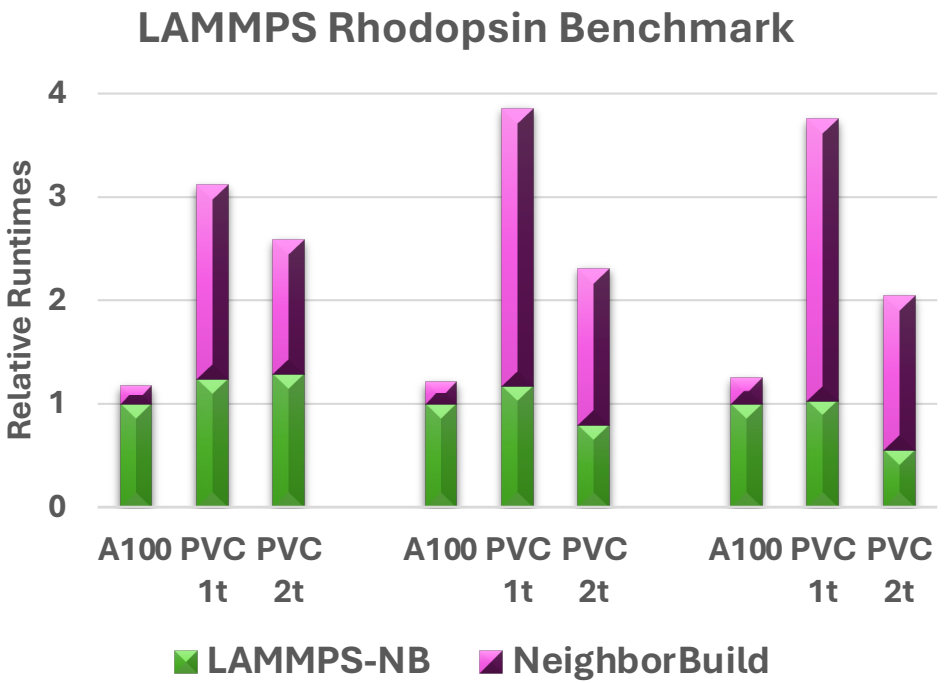
The Accomplishment

- Added support for offloading 1D FFTs via oneMKL when using the SYCL backend of Kokkos, thus enabling support for multiple capabilities in LAMMPS
  - Long-range electrostatic solvers
  - 17 additional pair potentials to utilize GPUs on Aurora
  - Initial support for other packages: ELECTRODE, DIELECTRIC, and AMOEBA (more testing needed)
- Competitive performance achieved with Kokkos??
  - Issue with NeighborBuild needs resolution
  - Waiting on new Intel Compiler drop to evaluate how broadly beneficial some optimizations are for indexing into multi-dimensional Kokkos views.
- CMake build issues for oneAPI and Kokkos/SYCL were resolved

The Impact

- Users getting access to Aurora in CY25 more likely to have success running their LAMMPS simulations
  - This directly supports one 2024 Aurora INCITE allocation.
- The Makefiles and CMake scripts provided also helps users with building LAMMPS on local Intel GPU resources.
- This also potentially helps with ongoing INCITE review and understanding the readiness of LAMMPS for specific workloads.



Relative runtimes of the rhodopsin benchmark on an NVIDIA A100 and Intel PVC GPU (1- and 2-tiles). Runtimes are scaled relative to A100 runtime with the NeighborBuild (NB) time separated. (Image credit: Christopher Knight (ANL))

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Publication/PR for this work: 9/3/24
https://github.com/lammps/lammps/pull/4313

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