# AMPI for LAMMPS USER-MESO

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Abstract:

The particle-based nano- to micro-scale fluid flow and transport models and high-performance computing (HPC) techniques are deployed to study source rocks such as shale at Idaho National Laboratory (INL). The dynamic processes of fluid flow are usually inhomogeneous in the sense that the distribution of particles as well as the computation of interparticle potentials can exhibit highly spatial and temporal variabilities. On HPC clusters, those types of inhomogeneity usually lead to severe load imbalance issue across processors and consequently poor scalability in simulations of those processes, and therefore making it extremely difficult for most of the current codes to reach the required ranges of spatial and temporal scales for simulations.

The core capability of Charm++: automatic load balancing based on over-decomposition and smart rank scheduling, is especially attractive to the particle flow and transport models in general. However, a “good” Charm++ implementation of those models is not trivial, especially when various engineered processes are considered in programming, and when sophisticated boundary conditions need to be implemented by strictly following the Charm++ paradigm.

In this work, we present the latest progress in the implementation of Adaptive Message Passing Interface (AMPI) for the LAMMPS based USER-MESO particle flow simulation package. First, the mesoscale particle model implemented in LAMMPS USER-MESO, dissipative particle dynamics (DPD), will be briefly introduced and examples of the scientific and engineering applications of DPD at INL will be overviewed. The existing load imbalance problem in the simulation of an engineered shale oil recovery process by injecting flow in high-resolution realistic nanoporous shale pore networks will be highlighted. Then, the computing performance will be carefully evaluated for the fluid flow simulation for runs with and without AMPI support. Finally, we will demonstrate the possibility of cooperative work of AMPI with the native load balancer in LAMMPS, recursive coordinate bi-sectioning (RCB).