A Performance Portable Discrete Element Sea Ice Model

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A new sea ice model, the Discrete Element Model for Sea Ice (DEMSI), is under development for use in E3SM. DEMSI treats collections of ice floes as Lagrangian particles that interact through contact forces and their trajectories are determined by directly integrating the equations of motion. In contrast to standard continuum models of the sea ice cover, this method enables the capture of the anisotropic sea ice deformation and fracture in response to ocean and atmospheric forcing. DEMSI utilizes the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for the dynamical core, which provides a high-performance base and enables the use of the Kokkos programming model for performance portability. We have implemented a Kokkos-enabled particle contact force model for sea ice that includes both bonded and unbonded interactions. We will provide an overview of ongoing efforts to validate the contact model using simple mechanical tests and experimental data in the literature while also highlighting the scalability and performance of the algorithm. The integration of a Lagrangian particle algorithm into a coupled Earth system model with traditional Eulerian PDE-based ocean and atmosphere codes requires a high fidelity, conservative, interpolation scheme for proper particle-to-grid coupling. In that regard, we also outline a moving least squares method that interpolates particle data to the Eulerian grid following an optimization-based scheme that enforces conservation and ensures bounds preservation.