DEMSI
Discrete Element Model for Sea Ice

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A Performance Portable Discrete Element Sea Ice Model



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OVERVIEW

Our objective in DEMSI is to develop a computationally efficient, performance portable DEM sea ice model for Earth system modeling

- This talk is a follow-on to plenary talk on DEMSI given by Adrian Turner
- We will focus on highlights from the ASCR-funded work including
  - Particle to grid interpolation for ocean/atmosphere coupling
  - Particle to particle remap
  - Preliminary performance
  - Contact model calibration and validation

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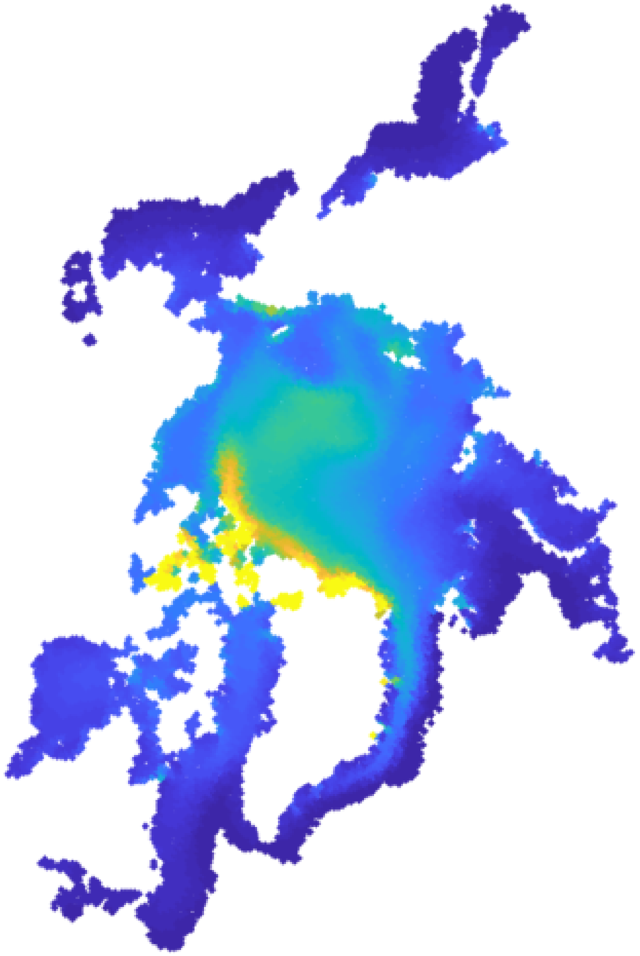


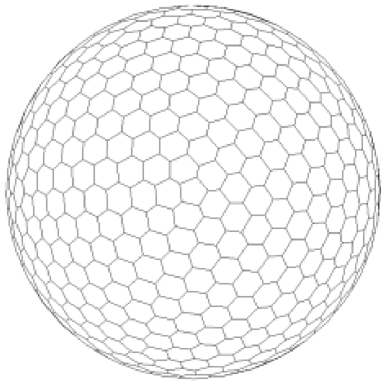
OCEAN/ATMOSPHERE COUPLING

- Incorporating Lagrangian sea ice model in E3SM requires particle to grid remapping capability
  - Need to transfer fluxes between ice/ocean/atmosphere
  - Requires conservation and bounds preservation
- Implemented second-order moving least squares-based method with bounds preservation

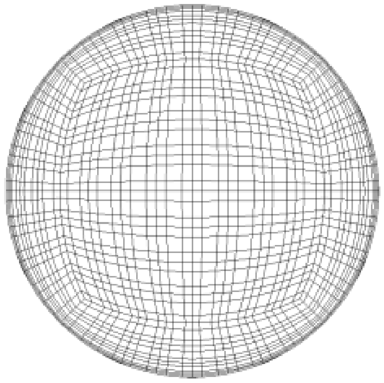
$$f(x) = \sum_{p \in N_x} \psi_p(x) f_p \qquad \psi_p = b M^{-1} b^T w_p(x)$$

$$M = \sum_{p \in N_x} b b^T w_p(x) \qquad b^T = [1 \quad (x - x_p) \quad (y - y_p)]$$

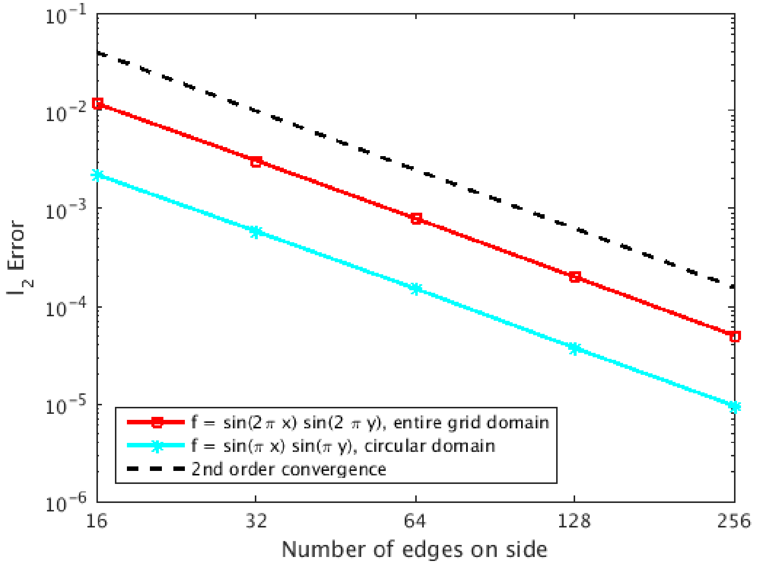
MPAS-O Grid



EAM Grid



Convergence plots for second-order MLS interpolation



Next Steps:

- Extend remapping capability to MPAS-O and EAM grids
- Opportunities to collaborate with CANGA project

PARTICLE-TO-PARTICLE REMAPPING

- Working with LANL on high-order particle-to-particle remap implementation
  - To manage large deformations,
  - To add new particles due to thermodynamic growth.
- Requires accuracy, bounds preservation, and conservation
- Challenges
  - Gaps and overlaps for particle effective areas
  - Relationships between tracers

Conserved Quantities

Total ice area: $A_{ice} = \sum_p c_p A_p = \sum_p \sum_i a_{ip} A_p$

Total ice volume: $V_{ice} = \sum_p c_p h_p A_p = \sum_p \sum_i v_{ip} A_p$

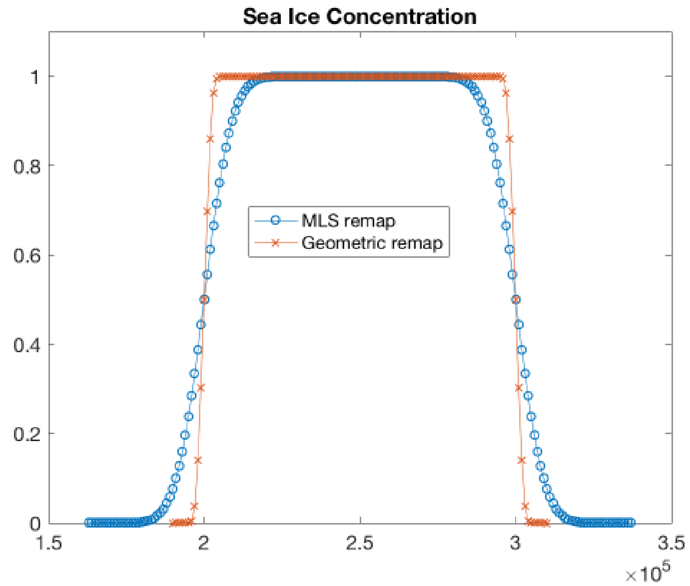
$$0 \leq h_p \leq \infty \qquad 0 \leq c_p \leq 1$$

$$h_p = v_p / c_p$$

Two methods:

- Geometric remap with flux-based optimization for property preservation.
- Moving least squares remap with mass-based optimization for property preservation.

Investigating both flux-based and MLS-based remap options using simple test cases for verification

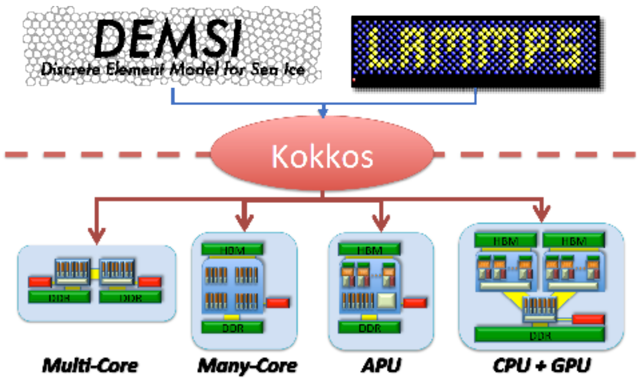


Next Steps:

- Comparison of efficiency and accuracy for remap methods.
- Remap for bonds between particles.

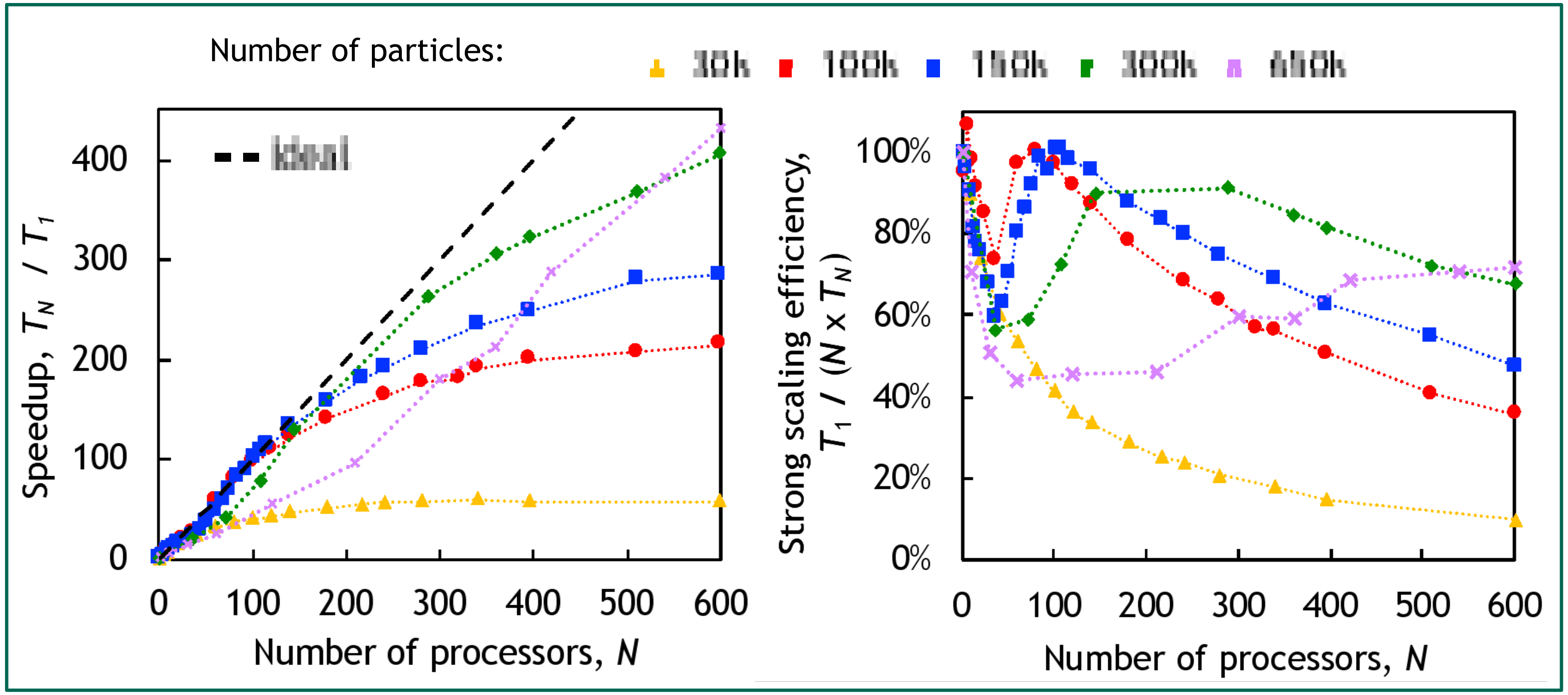
DEMSI PRELIMINARY PERFORMANCE

- Contact model implemented with LAMMPS (https://lammps.sandia.gov)
  - Computationally efficient providing high-performance baseline
- Using Kokkos for performance portability
- Performance plots for uniform stress test case with varying particle count

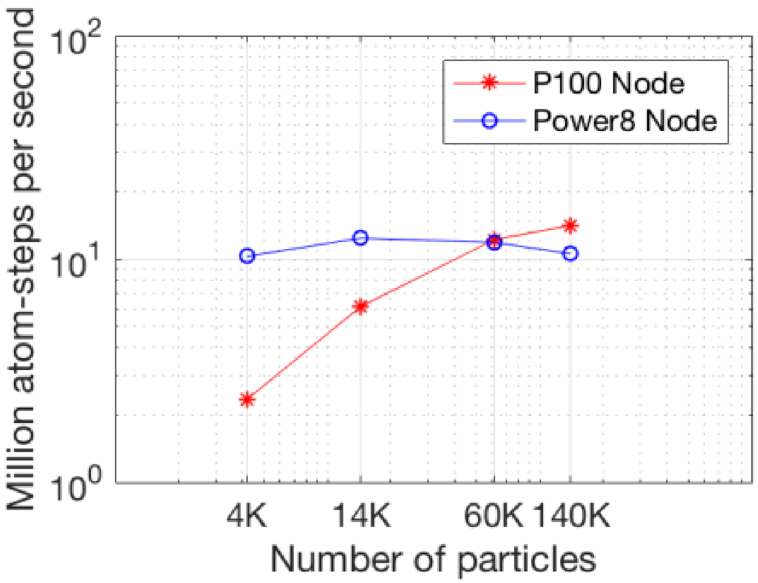


https://github.com/kokkos

Strong scaling on CPU



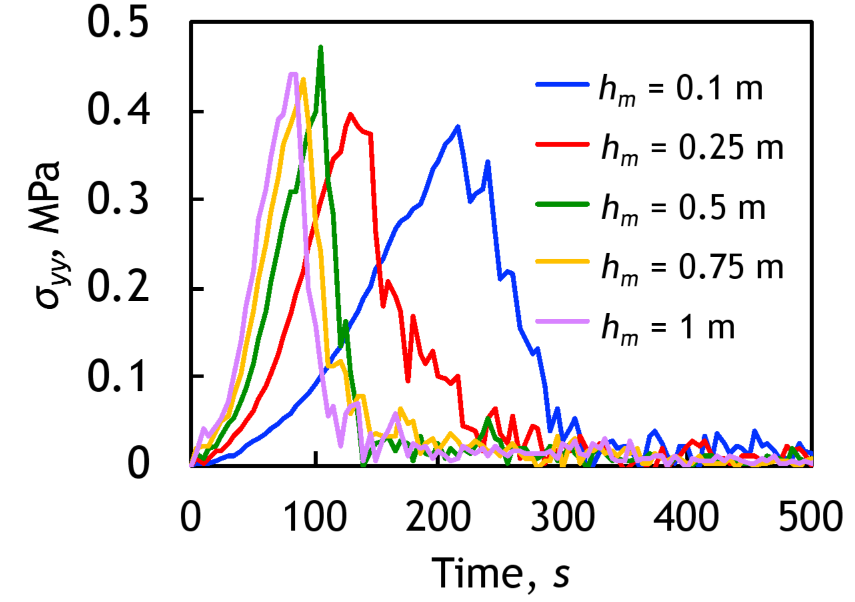
Performance on Nvidia Tesla P100 GPU node versus Power8 node with eight Garrison dual socket cores

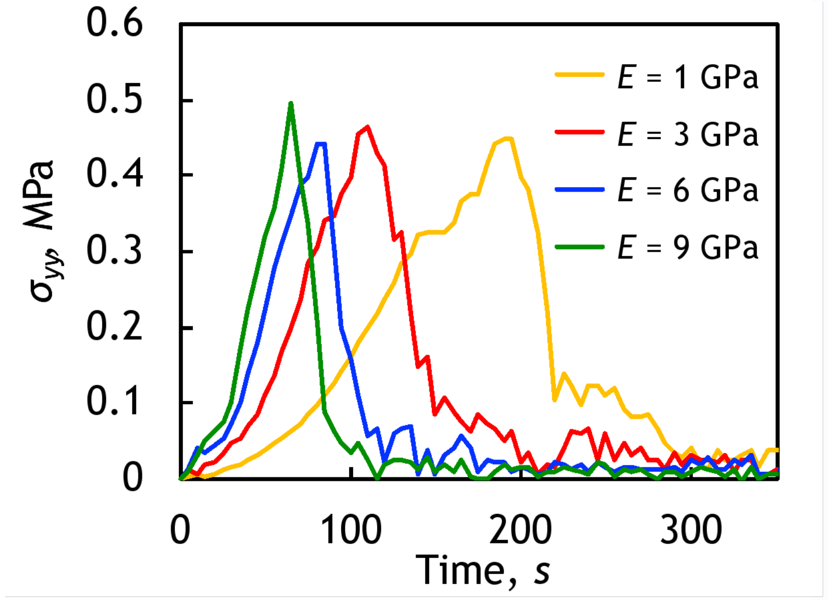


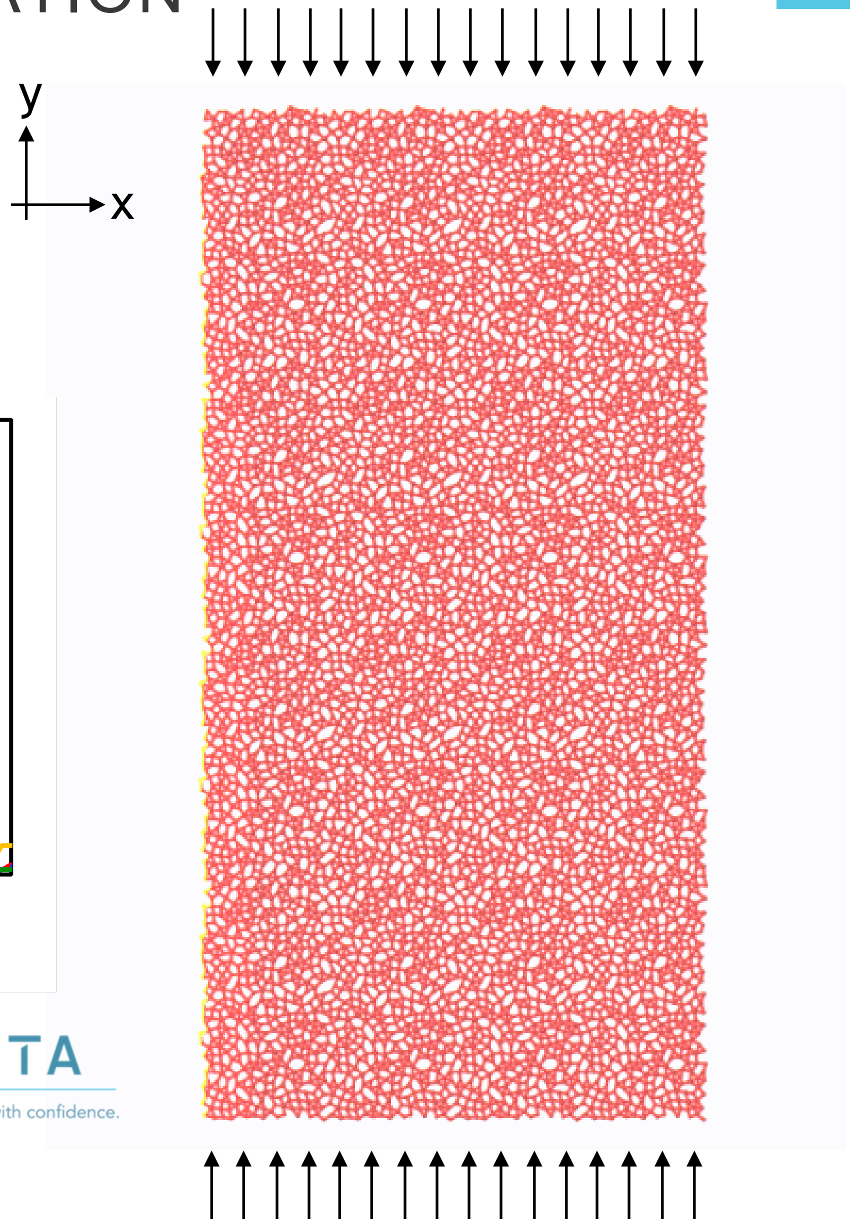
- ***Next Steps***: Performance for Arctic basin test case and code optimization.

CONTACT MODEL CALIBRATION AND VALIDATION

- Performing simple mechanical tests of sea ice contact model
  - Contact model parameter study using uniaxial **compression**
  - Brittle-like failure as E and h_m increase
  - Consistent with results in the literature (Herman *GMD* 2016)







<u>Next Steps:</u>

- Parameter sensitivity and calibration with DAKOTA
- Comparison with experimental data and continuum sea ice models
- Explore data-driven (machine learning) contact model

DAKOTA
Explore and predict with confidence.