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Title: Discrete Element Model for Sea Ice: 2020 ESMD-E3SM PI Meeting

Author(s): Turner, Adrian Keith

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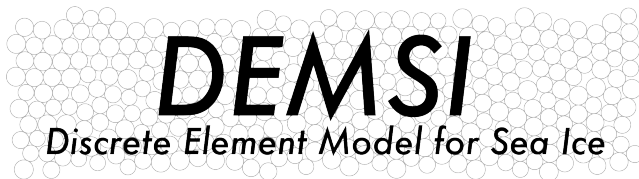
Discrete Element Model for Sea Ice

2020 ESMD-E3SM PI Meeting

The DEMSI Team

LANL, SNL

28th October 2020



- **Los Alamos National Laboratory**

- Adrian Turner (BER PI)
- Andrew Roberts
- Steven Brus



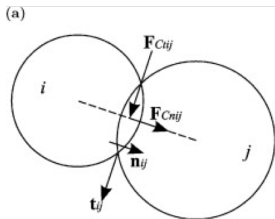
- **Sandia National Laboratories**

- Kara Peterson (ASCR PI)
- Dan Bolintineanu
- Svetoslav Nikolov
- Joel Clemmer



Discrete Element Model for Sea Ice (DEMSI)

- **Develop a discrete element method sea ice model as new component of E3SM**
- Particle method with discrete elements representing regions of sea-ice
 - Explicitly calculate forces between elements
 - Integrate equation of motion for each element
- Collaboration between LANL (BER) and SNL (ASCR)
 - Phase 1: Developing basic model (just finished)
 - Phase 2: Coupling into E3SM



Potential advantages:

- Performance:

- MPAS-Seaice is already run at the limit of strong scaling in E3SM
- LANL projects to port MPAS-Seaice to GPUs were not hugely successful
- Two essential performance limitations for current DOE sea-ice models:
- Particle methods have been shown to run effectively on GPUs

- Dynamics fidelity:

- Current E3SM sea-ice model uses a viscous-plastic-elastic material
- Assumes grid cells are large enough that there is an isotropic distribution in each of linear openings (“leads”) in the ice pack – $\sim 100\text{km}$
- Some observations suggest viscous-plastic models perform poorly for resolutions $< \sim 10\text{km}$
- A discrete element method allows explicit and complex force law – capture anisotropic, heterogeneous and intermittent nature of sea ice deformation

Project Overview

- **DEMSI:**

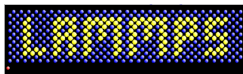
- Circular elements for computational efficiency
- Each element represents a region of sea ice, and has its own ice thickness distribution (initial resolution $>$ floe size)

- **Dynamics:** Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

- Particle based molecular dynamics code
- Built in support for DEM methods including history dependent contact models
- Computationally efficient with massive parallelization

- **Thermodynamics:** CICE consortium Icepack library

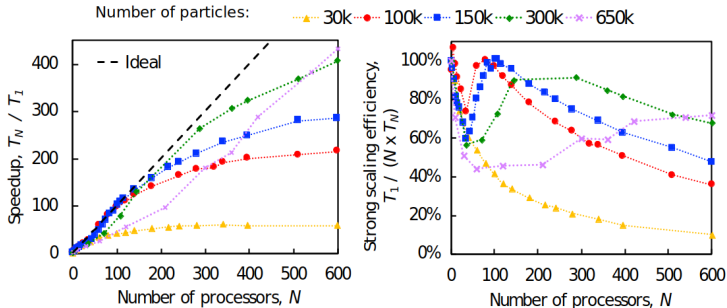
- State-of-the-art sea-ice thermodynamics package
- Vertical thermodynamics, salinity, shortwave radiation, snow, melt ponds, ice thickness distribution, BGC



- **Computational performance**
 - How to make the model fast enough for global climate applications?
- **Contact model**
 - How should elements interact to represent sea ice physics?
- **Coupling**
 - How to couple particles to Eulerian mesh conservatively?
- **Ridging**
 - Convergence of sea ice converts area to thickness – how to manage element distortion?

Companion talk

- Kara Peterson will present more details on the ASCR side of project
 - GMLS particle to grid interpolation for ocean/atmosphere coupling
 - GMLS Particle to particle remapping
 - Performance – Kokkos performance on GPUs
 - Contact model calibration and validation
- Infrastructure + NGD Software and Algorithms Session - **Tomorrow, Thursday 29th October 2020, 11:10am**

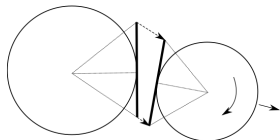


Contact Model

- Initial implementation based on Mark Hopkins model - modified for circular elements
- Elements can be bonded (frozen) or unbonded (fracture)

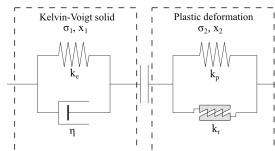
Bonded elements

- Linear bonds between elements with viscous-elastic “glue” at each point
- Mohr-Coulomb fracture law



Unbonded elements

- No strength in tension, Compression represents ridge formation
- Normal friction force term



Contact model

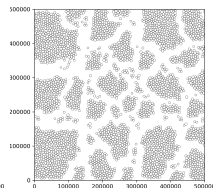
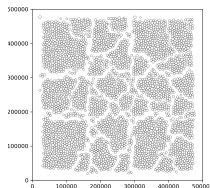
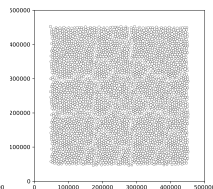
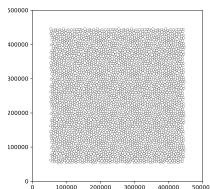
- Numerous test cases developed to validate the various aspects of the model
- Mechanical tests to better validate the contact model presented *tomorrow*
- Future work will use machine learning to develop better contact model
 - Observations
 - High resolution process simulations



Two particle fracture



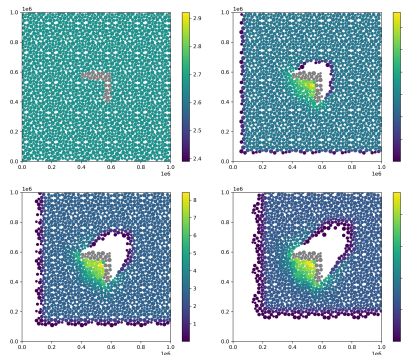
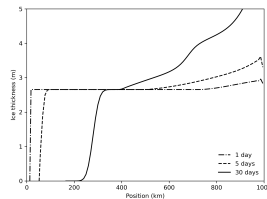
Cantilever



Uniform stress

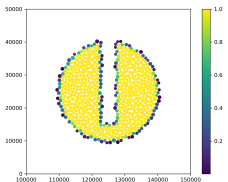
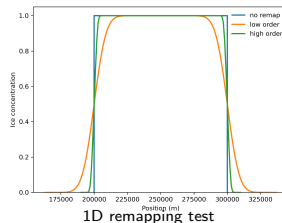
Ridging

- Convergence of sea ice generates pressure ridges - conversion of ice area into thickness
- Developed a ridging methodology for a discrete element model
 - Above threshold elastic behaviour gives way to normal friction (plastic deformation) between elements
 - Based on simulations of individual ridge by Hopkins
 - Calculated convergence moves ice from thin thickness categories to thicker ones

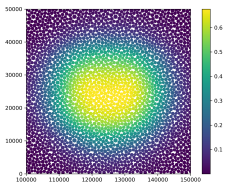


Remapping

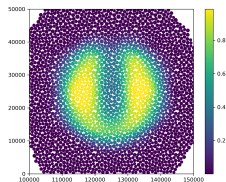
- Ridging causes shrinking of elements – element size controls allowable time step
- Need to ameliorate this effect
- Implemented global remapping of distorted particle distribution back to a “good” initial distribution
 - Simple geometric overlap – Higher order to reduce numerical diffusion
 - Advanced GMLS method – *Tomorrow*



No remapping



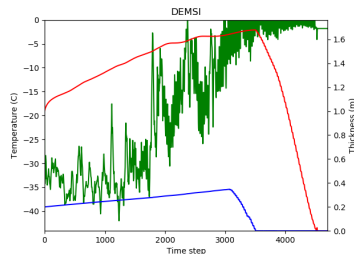
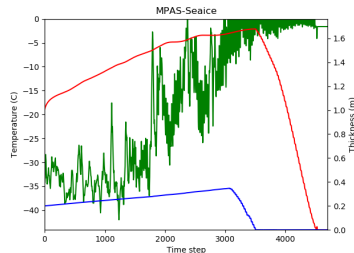
Low order



Higher order

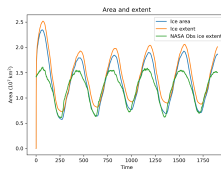
Column physics

- CICE consortium Icepack column physics library fully integrated
- BFB for column test case
- Some complexity for coupling between C++ and Fortran

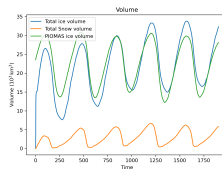


Basin scale simulations

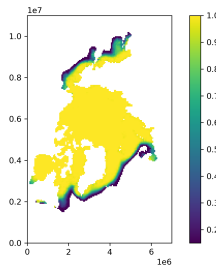
- All of above combined into Arctic basin simulations
- Broadly similar physics level to MPAS-Seaice - no fracturing yet
- Preliminary results promising
- Need to carefully assess dynamics
- CompyMcNodeFace proving vital for this work



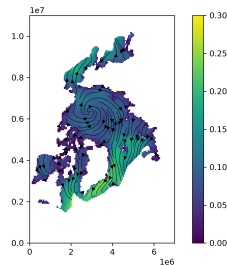
Ice Extent



Ice volume



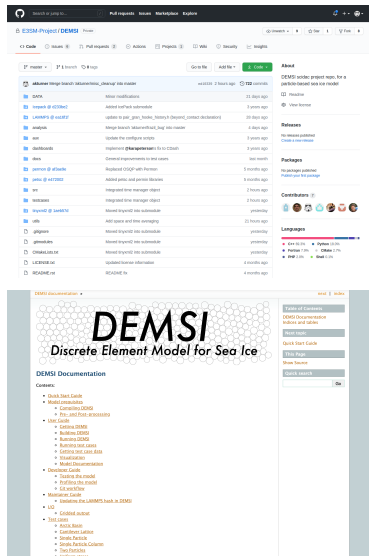
Ice concentration



Ice velocity

DEMSI Workflow

- Project repository built around ease of use and collaboration
- Contains more than source code:
 - Test cases
 - Source code
 - CMake build system
 - CTest testing system - unit/test case regression
 - Documentation (Sphinx/doxygen)
 - Analysis code
 - Visualization
 - Data download scripts



Future work includes:

- Improved contact model using machine learning
- Further improvements to performance in both LAMMPS (kokkos) and DEMSI
- Enhanced coupling improved preservation physical bounds
- Coupling DEMSI into E3SM
- Coupled simulations
- Improved metrics for model assessment