Discrete Element Model for Sea Ice

2020 ESMD-E3SM PI Meeting

The DEMSI Team

LANL, SNL

28th October 2020

DEMSI Team

- **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

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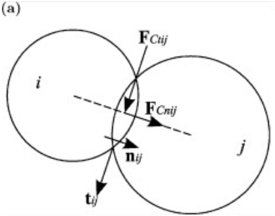
Sandia National Laboratories

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$100km
  - Some observations suggest viscous-plastic models perform poorly for resolutions $< \sim$10km
  - A discrete element method allows explicit and complex force law – capture anisotropic, heterogeneous and intermittent nature of sea ice deformation

Project Overview

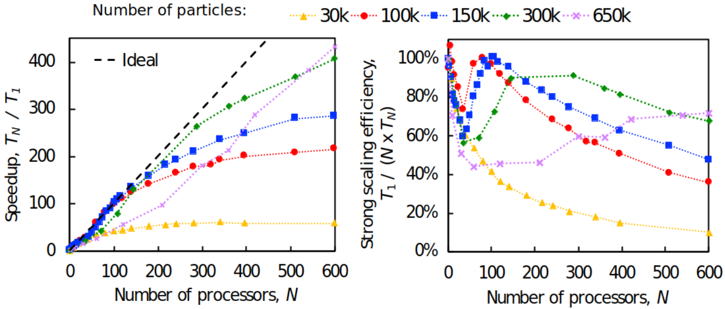
- **DEMSI**:
  - Circular elements for computational efficiency
  - Each element represents a region of sea ice, and has its own ice thickness distribution (initial resolution $>$ floe size)
- **Dynamics**: Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
  - Particle based molecular 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

Principle challenges

- **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**

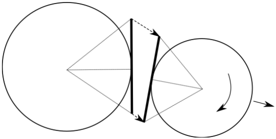


Contact Model

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

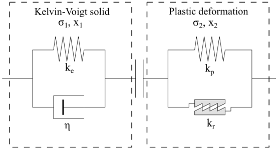
Bonded elements

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



Unbonded elements

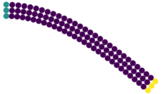
- No strength in tension, Compression represents ridge formation
- Normal friction force term



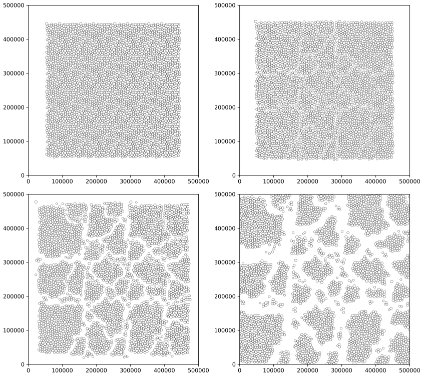
Contact model

- 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



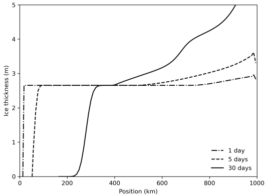
Cantilever

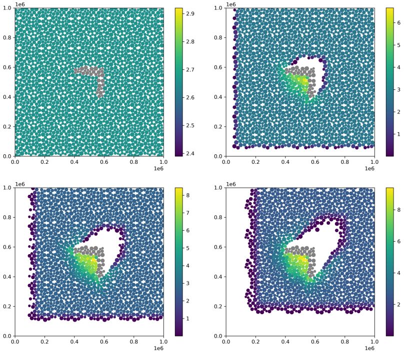


Uniform stress

Ridging

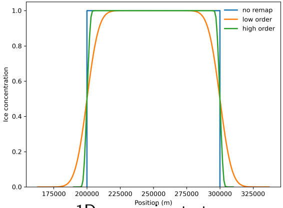
- Convergence of sea ice generates pressure ridges - conversion of ice area into thickness
- Developed a ridging methodology for a discrete element model
    - Above threshold elastic behaviour gives way to normal friction (plastic deformation) between elements
    - Based on simulations of individual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



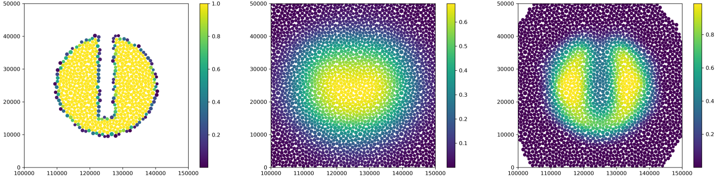


Remapping

- 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*



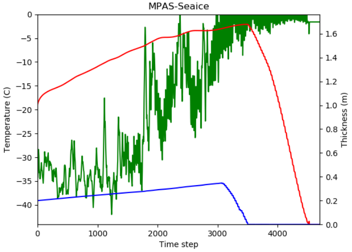
1D remapping test

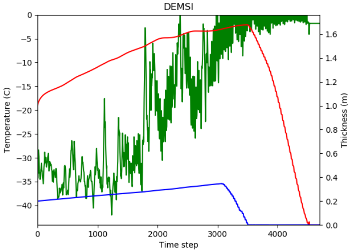


No remapping   Low order   Higher order

Column physics

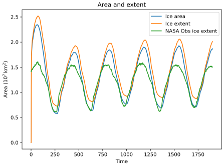
- CICE consortium Icepack column physics library fully integrated
- BFB for column test case
- Some complexity for coupling between C++ and Fortran



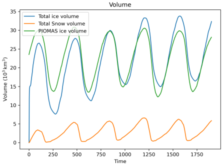


Basin scale simulations

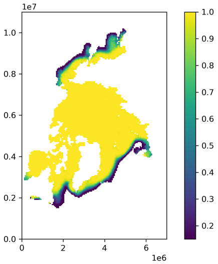
- All of above combined into Arctic basin simulations
- Broadly similar physics level to MPAS-Seaice - no fracturing yet
- Preliminary results promising
- Need to carefully assess dynamics
- CompyMcNodeFace proving vital for this work



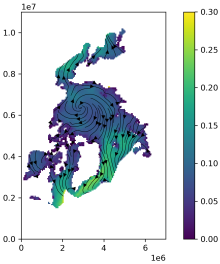
Ice Extent



Ice volume



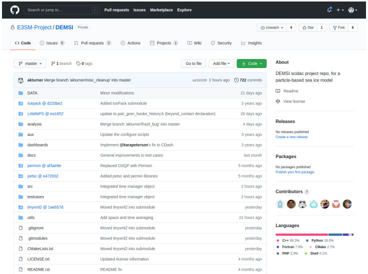
Ice concentration

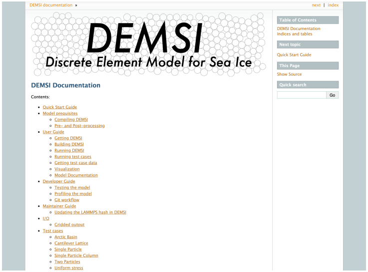


Ice velocity

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

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