Discrete Element Model for Sea Ice

E3SM all hands

The DEMSI Team

LANL, SNL

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DEMSI Team

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- **Naval Postgraduate School**
  - Travis Davis

Discrete Element Model for Sea Ice (DEMSI)

- **Develop a discrete element method sea ice model suitable for global climate applications**
  - Improved sea ice dynamics fidelity
  - Improved performance on future DOE heterogeneous computing architectures
- Particle method with discrete elements representing regions of sea-ice
  - Explicitly calculate forces between elements
  - Integrate equation of motion for each element

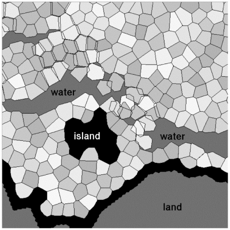


Figure: Hopkins (2006)

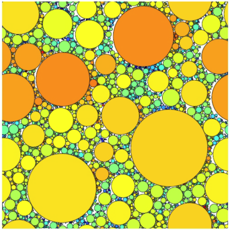


Figure: Herman (2012)

SciDAC

- Part of DOE Scientific Discovery through Advanced Computing(SciDAC) funding call
  - Combines researchers from Advanced Scientific Computing Research (ASCR) and Earth System Modeling (ESM)
  - 2 major projects and 6 pilot projects (high risk, high reward)
  - DEMSI: $3million over 2.5 years, with possibility of continuance for further 2.5 years
  - Develop new components for DOE Energy Exascale Earth System Model (E3SM)

Scientific Goals

- Current models of sea ice generally treat it as a viscous-plastic material
  - Assumes grid cells are large enough that there is an isotropic distribution in each of linear openings (leads) in the ice pack
  - Developed when grid cell size was $\sim$100km
  - Models now use much higher resolution – e.g. $\sim$6km cells for E3SM/MPAS-Seaice
- Observations suggest viscous-plastic models poor for resolutions $< \sim$10km
  - Spatial/temporal deformation scaling, dispersion of buoys
- A discrete element method allows explicit and complex force law Hope to capture anisotropic, heterogeneous and intermittent nature of sea ice deformation
  - Capture explicitly fracture and break up of pack

Project Overview

- **DEMSI**:
  - Circular elements to start (speed)
  - 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

DEMSI Discrete Element Model for Sea Ice

LAMMPS

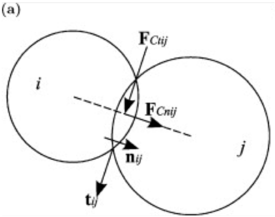
CICE Consortium

Principle challenges

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

Contact Model

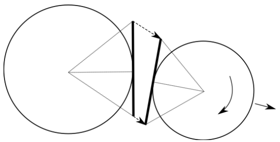
- Determines normal and tangential forces between elements
- These forces (as well as body forces) are integrated to determine velocity – velocity Verlet solver
- For sea ice we consider two situations:
  - Elements are bonded together
  - Elements are not bonded together
- Our initial implementation adapts the work of Hopkins for circular elements

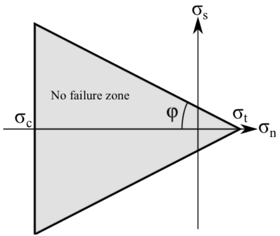


Interacting elements in DEM

Contact Model: Bonded elements

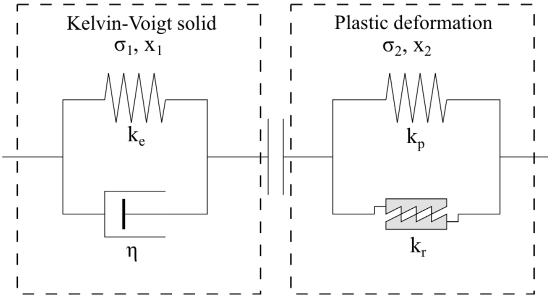
- Bonded elements have linear bonds between them
- Each point on bond has viscous-elastic glue
- Relative motion of elements places each point on bond under normal and tangential displacement
  - Elastic and damping forces at each point
  - Mohr-Coulomb fracture law
  - Cracks propagate from bonds ends inwards





Contact Model: Unbonded elements

- Unbonded elements have no strength in tension
- On compression elements must represent ridge formation
  - Element area is converted to thickness
- Initially based on Hopkins ridge model normal friction force term independent of relative element velocity



Contact Model Validation

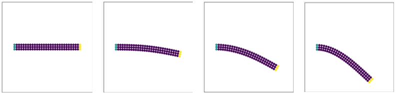


Figure: Cantilever test case

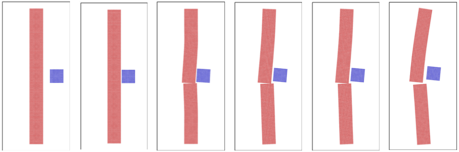


Figure: Impact test case

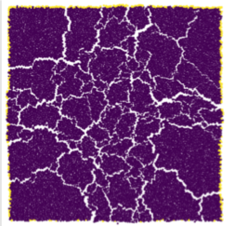


Figure: Uniform stress test case

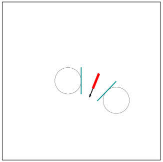
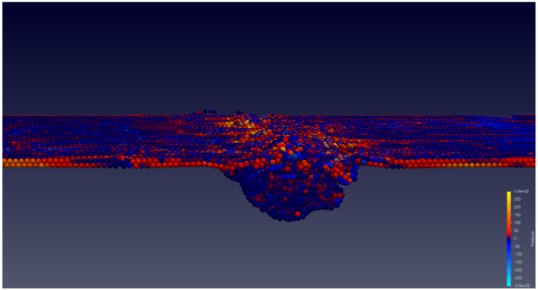


Figure: Two particle test case

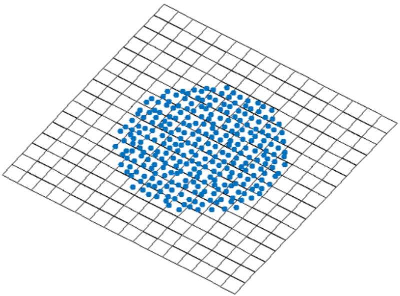
Improved contact model

- Performing high resolution floe-resolving simulations
  - Results will be averaged to derive contact model for lower-resolution
- Simulations of individual floes with LAMMPS to determine ridge formation force



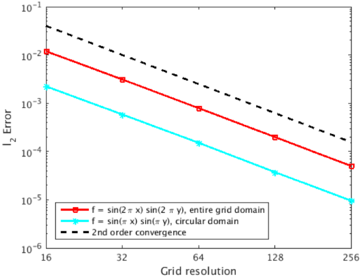
Coupling to Atmosphere/Ocean

- DEMSI requires an method for interpolation between Lagrangian particles and Eulerian grids
- Have developed a MLS method for interpolating particle data to a fixed structured grid within DEMSI
- Next steps – Implementing optimization-based strategy to ensure property preservation

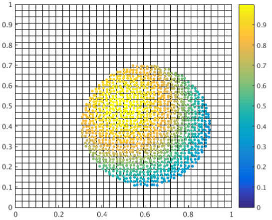


Schematic showing elements on Eulerian grid

Second-order convergence

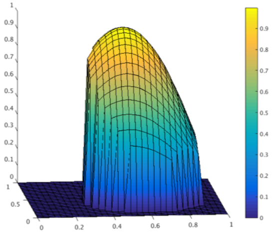


Particle Distribution and Values



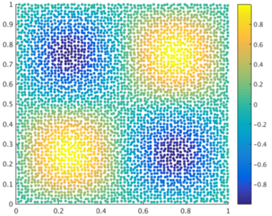
$$f = \sin(\pi x)\sin(\pi y)$$

Interpolated Grid Values (32x32 cells)

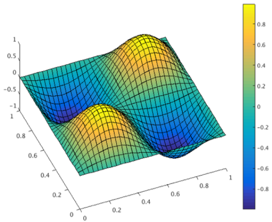


$$f = \sin(\pi x)\sin(\pi y)$$

- Approximately 4 particles-per-cell, particle resolution increases with grid resolution
- Particles initialized with random perturbation from structured arrangement
- Error in grid solution compared to exact solution, computed for interior nodes



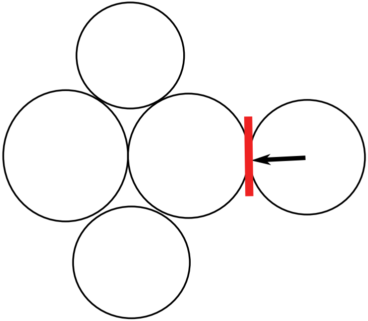
$$f = \sin(2\pi x)\sin(2\pi y)$$



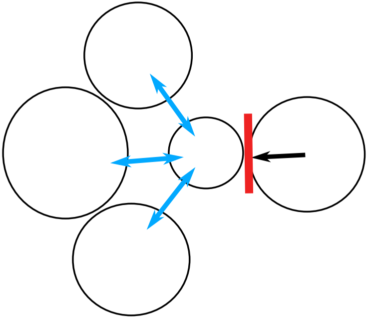
$$f = \sin(2\pi x)\sin(2\pi y)$$

Element creation and destruction

- Convergence of sea ice results in the formation of a pressure ridge – Sea ice build up on Canadian Archipelago
  - Sea ice area is converted to sea ice thickness while mass is conserved
  - Model elements will decrease in area during simulation
  - Decreases time step, add artificial strain



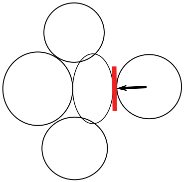
Convergence and ridge formation of two elements in pack



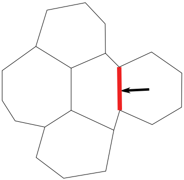
Shrinking of element adds strain to the pack

Element creation and destruction

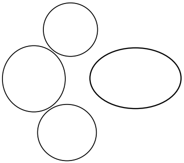
- Possible solutions – Ellipses, Polygons, Merging, Remapping, Transference



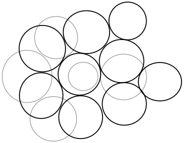
Use elliptical elements



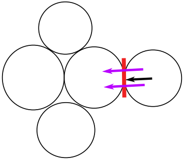
Use polygonal elements



Merge elements that get too small

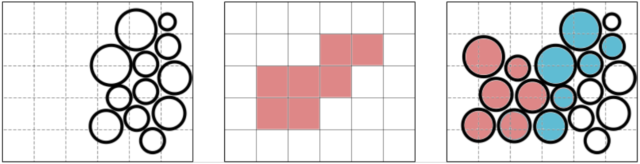


Periodically remap elements back to initial distribution



Keep elements same size and transfer mass between them

Frazil formation

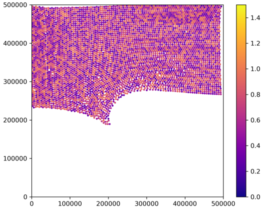


(*left*): Elements before frazil formation. (*center*): Frazil formation on Eulerian mesh. (*right*): Elements after frazil added. (*red*): New elements. (*blue*): Existing elements with frazil added.

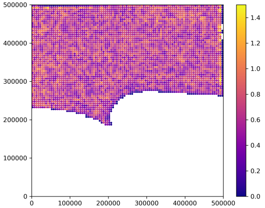
- Another significant challenge is addition of ice from frazil formation
- Take frazil from underlying Eulerian mesh
  - Add to existing elements
  - Create new elements
- Challenge is how to create the new elements with a tightly packed distribution

Geometrical remapping

- Deformation of elements during ridging slows time step, results in artificial strain
- Investigating a global remapping back to an initial "good" element distribution
- Geometric version implemented and tested
- Later will use the coupling system



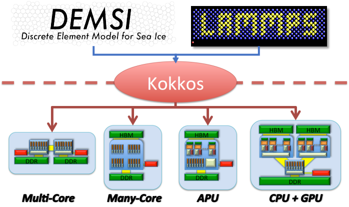
Particle distribution before remapping



Particle distribution after remapping

Computational Performance

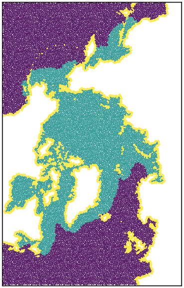
- Global climate simulations will be computationally expensive
- DOE next generation computers will have heterogenous architectures
  - Oakridge Summit: IBM's POWER9 CPUs and Nvidia Volta GPUs
  - NERSC Perlmutter: both CPU-only and GPU-accelerated nodes
- Modifying LAMMPS DEM to use Kokkos programming model
  - Allows good performance on CPU and GPU
- Will also investigate if elastic modulus can be reduced without affecting simulation fidelity
  - Will allow longer timesteps



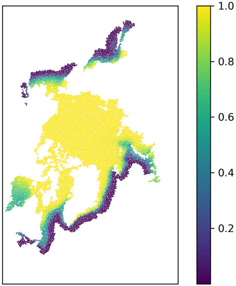
https://github.com/kokkos

Realistic simulations

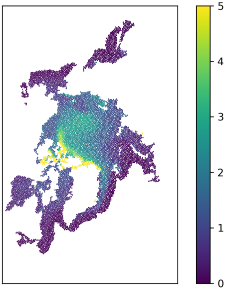
- Work has begun to perform Arctic basin scale simulations
- Particle distribution initialization, forcing, domain
- Currently integrating previous work



Element type

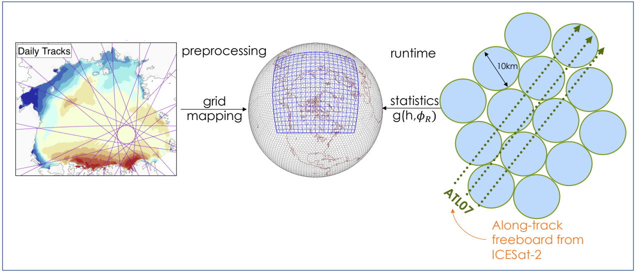


Ice fraction



Ice thickness

Metrics for assessing model fidelity



- ICESat-2 emulator
- Spatial and temporal deformation scaling
- Buoy dispersion analysis - easier for particle method!
- Other standard sea-ice metrics

Future work

- Currently writing renewal proposal for phase 2
- **Phase 2 goal**: couple DEMSI into E3SM and perform coupled simulations
  - Considerations to conservative coupling with rest of model, coastline
  - Machine learning techniques to determine suitable contact model
  - Improved performance on GPUs
- Also explore performance advantage of DEMSI with large numbers of tracers
  - No explicit transport scheme needed
- DEMSI likely to be publicly available through *github* eventually
  - Includes code, pre/post-processing, documentation, testing, test cases