DEMSI: Discrete Element Model for Sea Ice

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Overview

The DEMSI project aims to build a sea-ice model based on the Discrete Element Method (DEM) suitable for inclusion in E3SM. A DEM model has two main advantages over existing model:

- DEM models have the potential to better utilize the new heterogeneous computing architectures being built by the Department of Energy.
- DEM models allow an explicit representation of dynamical processes, and better represent of sea-ice dynamics including spatial/temporal scaling, dispersion, intermittency, heterogeneity, and anisotropy of sea-ice dynamics.

DEMSI leverages two existing libraries:

- The **Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)** developed at Sandia National Laboratories [1]. This forms the dynamical core of DEMSI and includes DEM methods with history dependent contact models and is computationally efficient with massive parallelization
- The **CICE Consortium Icepack** library [2, 3, 4]. This provides state of the art sea-ice thermodynamics, biogeochemistry and mechanical redistribution capabilities.

Challenges

Developing a DEM sea-ice model suitable for inclusion in E3SM has four main challenges:

- **Performance:** Allow sufficient performance for global climate applications
- **Contact model:** Development of an element contact model suitable for sea-ice
- **Coupling:** Development of an efficient methodology to couple conservatively between model elements and other Eulerian components in the coupled system.
- **Deformation:** Account for sea-ice deformation during ice ridging
- **Creation of new elements:** How to maintain a compact pack
- **Model analysis:** How to validate the model dynamics

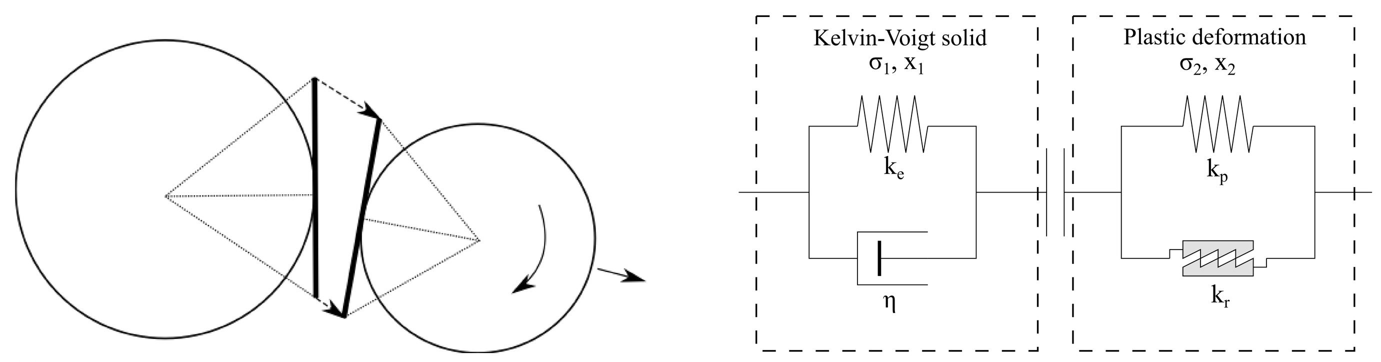
Contact Model

The element contact model determines the forces between elements in close proximity. An advantage over previous methods is the ability to explicitly represent physical processes. Initially we represent two main processes:

- Fracturing of bonded elements
- Ridge formation during ridging

We have implemented the sea-ice contact model developed by Mark Hopkins [6]. A significant challenge of the project is to determine an appropriate contact model for sea ice. To do this we plan to perform simulations of individual ridges, high resolution floe resolving simulations, and regional simulations.

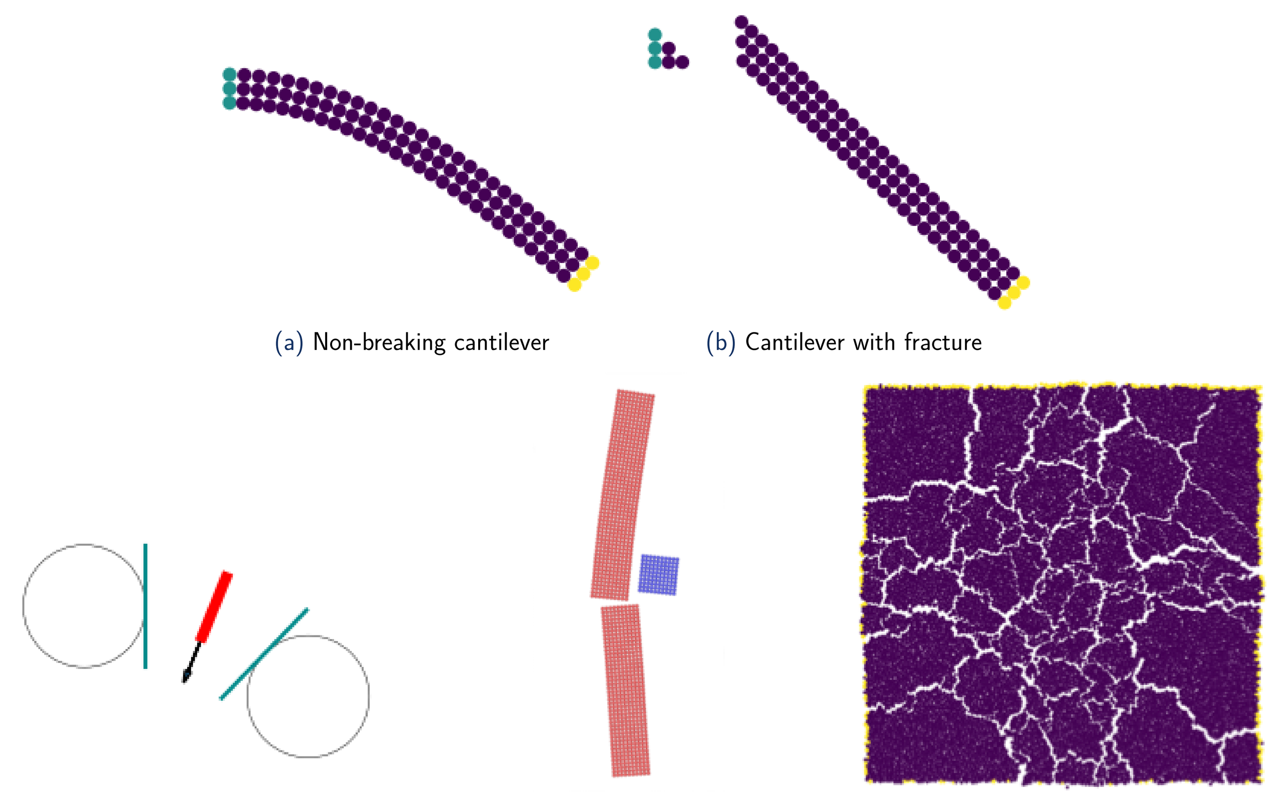
Two contact modes have been implemented: bonded and un-bonded contacts. Bonded contacts represent a frozen pack and can undergo fracture with an applied external stress. Un-bonded contacts undergo plastic deformation on onvergence representing ridge formation.



(a) Bond between two bonded elements (heavy black line) undergoing deformation.

(b) Representation of the un-bonded contact model with plastic deformation representing ridging.

The history dependence and possibility of strength in tension needed for the contact model have required special treatment in LAMMPS. The Hopkins contact model is being validated with a series of test cases



(a) Non-breaking cantilever (b) Cantilever with fracture

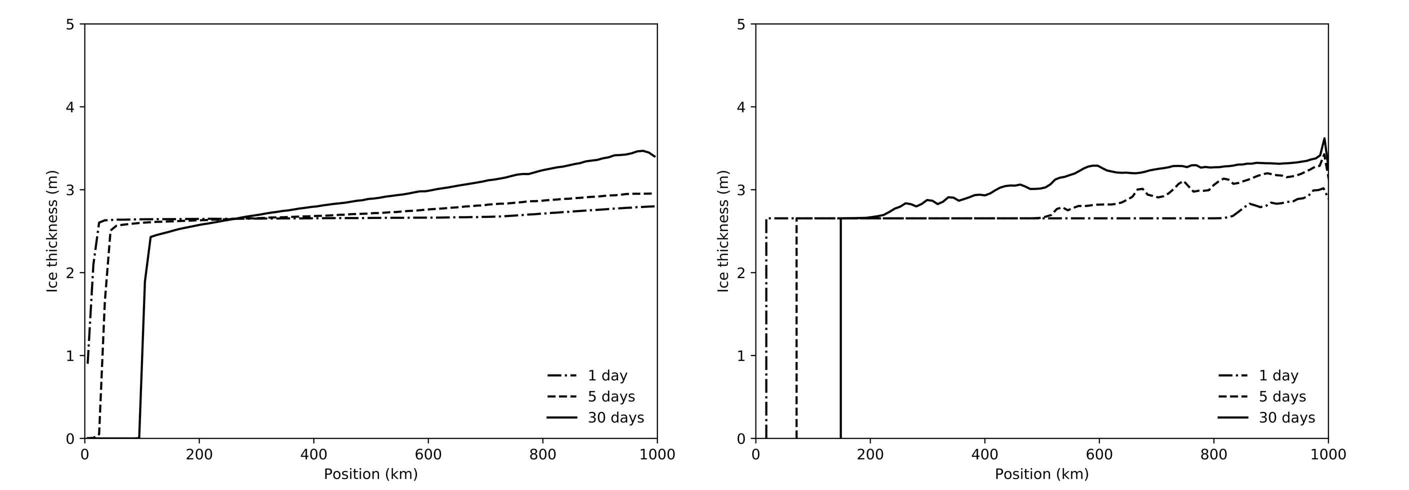
(c) Two particle fracture (d) Impact (e) Uniform stress

Figure 3: Test cases for contact model

We are investigating the use of high resolution floe resolving simulations to better determine the appropriate contact model at global climate resolutions.

Deformation

Convergence of sea ice results in the formation of a pressure ridge – sea ice area is converted to sea ice thickness while mass is conserved. Ridging presents several unique challenges for a DEM sea ice model. Firstly, the contact model between elements needs a representation of the ridging process (see previous section). Secondly, elements undergoing ridging must decrease their size as sea-ice area is converted into thickness. During this process the elements can either shrink equally in all directions or preferentially in the direction of convergence, in which case the element shape changes from a disk to an ellipse. Finally, sea-ice must be moved from thinner thickness categories to thicker thickness categories. In the figure below we present a comparison one dimensional simulation between ridging in MPAS-Seaice and DEMSI. In this simulation sea ice blown by constant winds against a fixed barrier on the right hand side of the domain where ridging causes the ice to thicken.



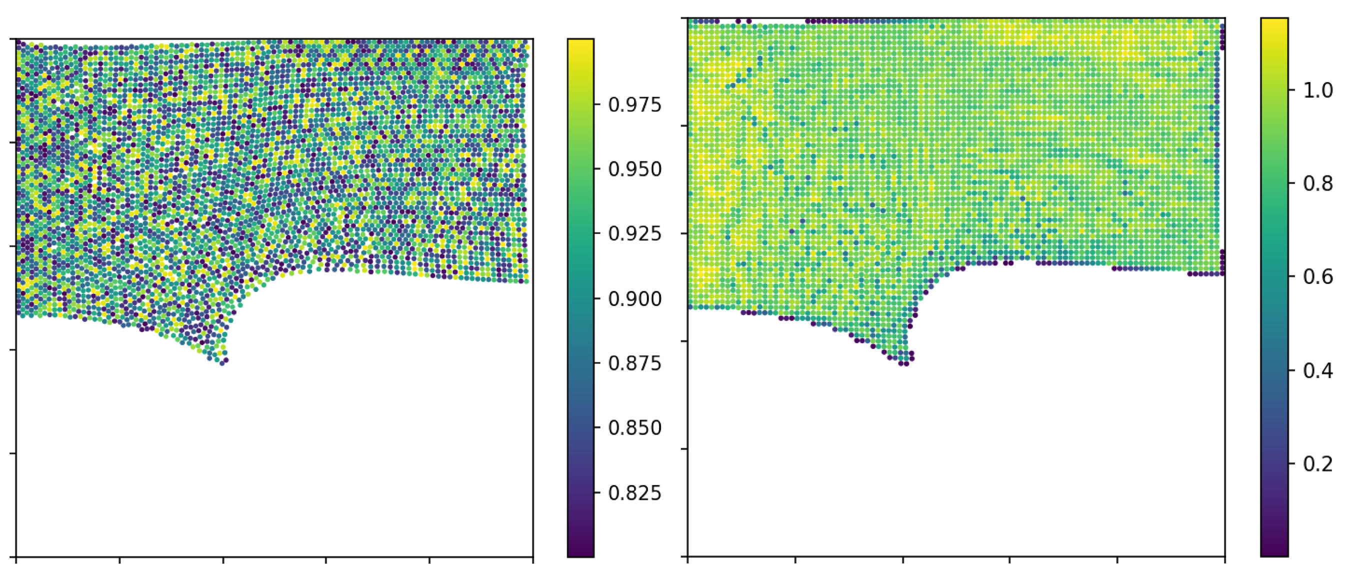
(a) 1D ridging simulation with MPAS-Seaice

(b) 1D ridging simulation with DEMSI

In DEMSI model simulations this is problematic for two main reasons:

- As elements get smaller, the maximum allowable time step decreases slowing the model
- Decreasing element size could add an artificial strain in the pack

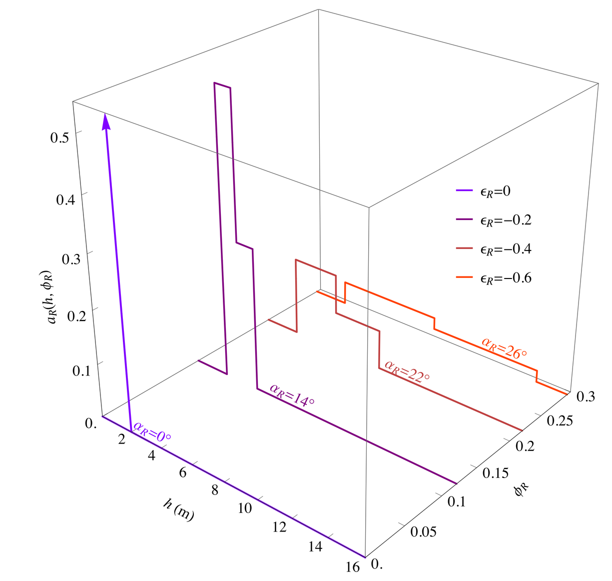
The solution to this problem that we are implementing is to perform a periodic global remapping of the element distribution back to a the initial particle distribution. Initially we will use a geometric implementation but plan to eventually utilize the coupling infrastructure. For the geometric implementation circular elements are represented as regular many-sided polygons, while a radical Voronoi tessellation is made of the initial distribution. Remapping is performed by finding the intersection area of the tessellation and regular polygons.



(a) Particle distribution before remapping

(b) Particle distribution after remapping

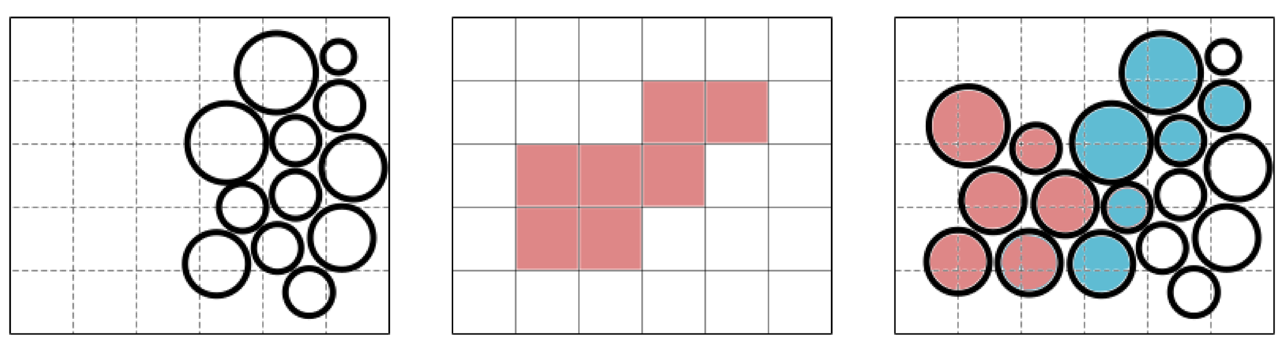
We will also include recent work to develop a new variational based ice morphology scheme[7] to improve the representation of ridging in the model.



Bi-variate ice thickness distribution considering ridge porosity as well as ice thickness[7].

Frazil formation

Another significant challenge is addition of ice from frazil formation. Cooling of the underlying ocean results in the formation of frazil ice which must be added to the sea-ice model. For a DEM sea-ice model this requires the addition of new elements to the pack. However, these new elements cannot overlap existing elements otherwise the large unphysical contact forces will be generated. The new elements must also form a tight pack.



(*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.

We are investigating several methods to do this including using a combination of Lloyd's Voronoi tessellation generating algorithm and a largest inscribed circle algorithm so generate tightly fitting new pack elements.

DEMSI Data Fusion

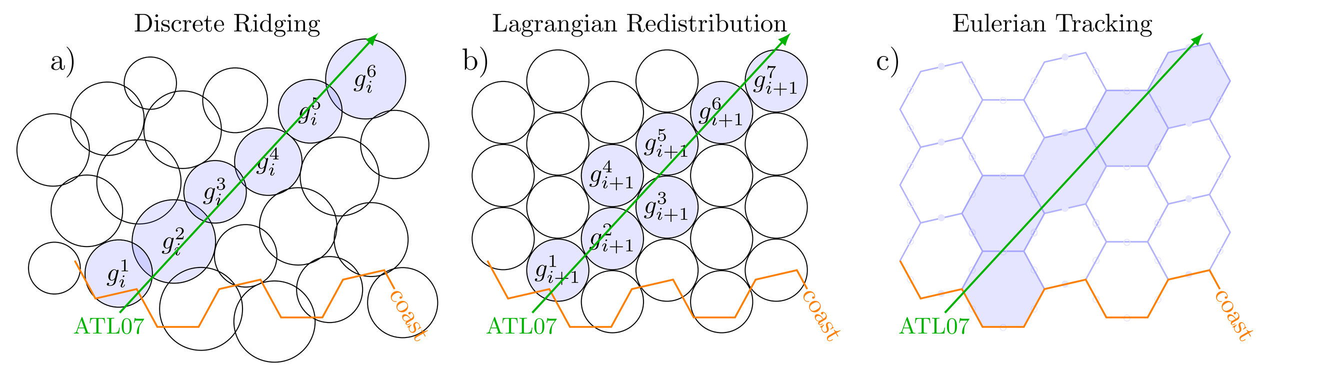
New data fusion techniques are being developed to evaluate DEMSI and to advance quantifying sea ice model skill and bias.

DEMSI diagnostic		Final Phase 1 Evaluation method and dataset	Duration
Concentration/extent	E	NOAA Climate Data Record	1979-
Drift & deformation	E	Polar Pathfinder Drift	1978-2015
	L	International Arctic Buoy Program	1980-
	L	RADARSAT-1 Arctic Ocean deformation	1997-2008
	L	Envisat Arctic Ocean deformation	2008-2012
Freeboard	S	ICESat	2003-2008
	S	ICESat-2	2018-
Draft	E	U.S. Navy and Royal Navy	1960-2005
Ice age	E	Arctic sea-ice age	1978-2015
Mass balance	L	IMB buoys	1993-2017
Ice-ocean flux	L	Ocean Flux Buoys	2002-2017
Ice-atmosphere flux	L	SHEBA flux tower data	1997-1998

Core observations being used to evaluate DEMSI (upper tier) and its coupling (lower tier) using: E - Eulerian mapping; L - Lagrangian observation emulator; and S - Satellite altimetric emulators.

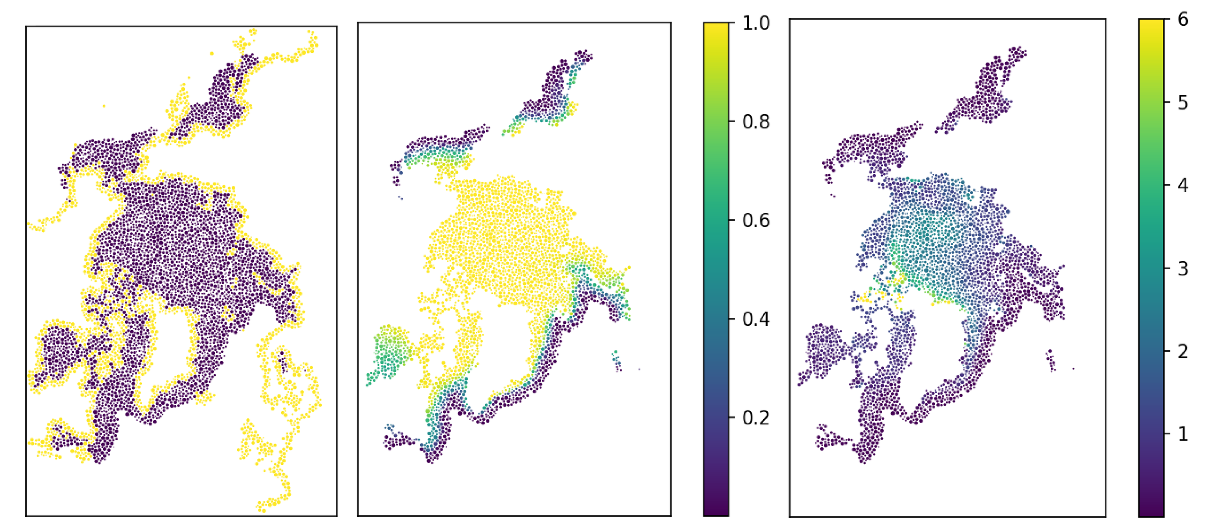
This project is contributing to the development of POLeSTAr Polar System Analysis

Satellite emulators are a key component of our methodology, 'flying' virtual ICESat and ICESat-2 above the model mesh to evaluate DEMSI freeboard.



Arctic basin simulations

Next big step is running basin scale simulations. This will allow realistic performance benchmarking and validation of the contact model.



(a) Element type showing coastlines (b) Ice concentration (c) Ice thickness

Figure 6: Initial condition for future Arctic basin simulations

Performance and Coupling

Kara Peterson will present DEMSI progress on performance and coupling on Thursday.

Future work

- **Phase 1**: For the remainder of phase 1 of the project we will be putting everything together and performing and analyzing realistic simulations of Arctic sea ice.
- **Phase 2**: Phase 2 of the project focuses on coupling DEMSI into the E3SM model and performing coupled simulations. Also includes is:
  - Performance optimization of both the Kokkos LAMMPS and DEMSI parts of the code
  - Using machine learning to improve generate improved contact models
  - Implementing a remapping methodology that can accurately remap the sea-ice stress state

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