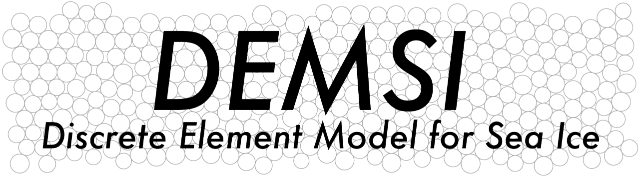
Discrete Element Model for Sea Ice

SciDAC PI Meeting 2019

The DEMSI Team

LANL, SNL, NPS

17th July 2019



DEMSI Team

- **Los Alamos National Laboratory**
  - Adrian Turner (BER PI)
  - Andrew Roberts
  - Min Wang
- **Sandia National Laboratories**
  - Kara Peterson (ASCR PI)
  - Dan Bolintineanu
  - *Dan Ibanez*
  - *Paul Kuberry*
- **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

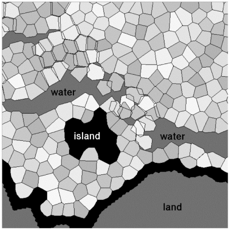


Figure: Hopkins (2006)

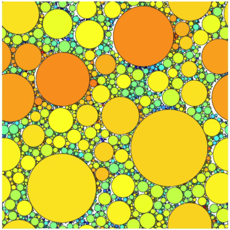


Figure: Herman (2012)

Scientific Goals

- Current models are poorly suited to future GPU architectures:
  - Stencil operators have small flop-memory rations – memory bandwidth/latency limited
  - Often at limit of strong scaling – Not enough work to exploit parallelism of GPU system
- 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
- 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

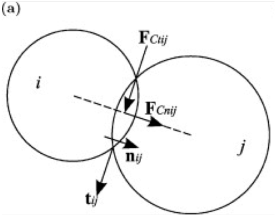
CICE
Consortium

Principle challenges

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

Contact Model

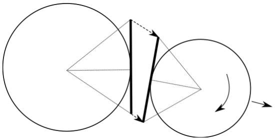
- Determines normal and tangential forces between elements
- These forces (as well as body forces) are integrated to determine velocity – velocity Verlet solver
- For sea ice we consider two situations:
  - Elements are bonded together
  - Elements are not bonded together
- Our initial implementation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

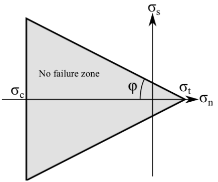


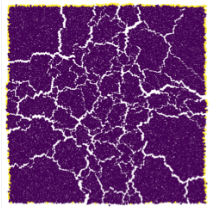
Interacting elements in DEM

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

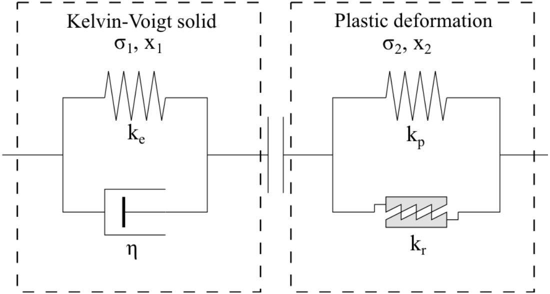






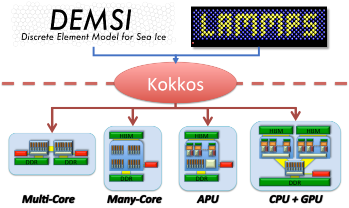
Contact Model: Unbonded elements

- 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



Computational Performance

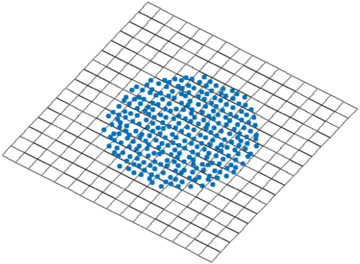
- Global climate simulations will be computationally expensive
- DOE next generation computers will have heterogenous architectures
  - Oakridge Summit: IBM's POWER9 CPUs and Nvidia Volta GPUs
  - NERSC Perlmutter: both CPU-only and GPU-accelerated nodes
- Modifying LAMMPS DEM to use Kokkos programming 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

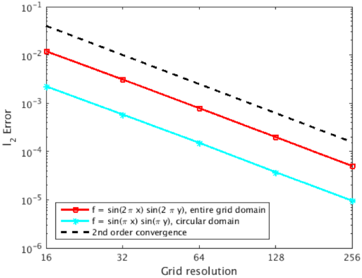
Coupling to Atmosphere/Ocean

- 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
    - Exploring possible use of Compadre toolkit

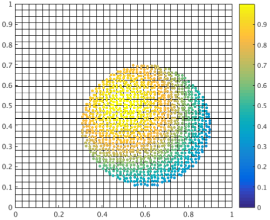


Schematic showing elements on Eulerian grid

Second-order convergence

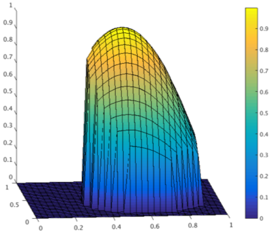


Particle Distribution and Values



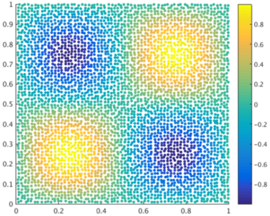
$$f = \sin(\pi x)\sin(\pi y)$$

Interpolated Grid Values (32x32 cells)

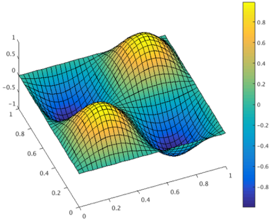


$$f = \sin(\pi x)\sin(\pi y)$$

- 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



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



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

Ridging in DEM models

- 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
- DEMSI ridging methodology:
  - Friction contact model allows element overlap
  - Elements are decreased in area representing ridging
  - Ice from thin elements is moved to thicker elements

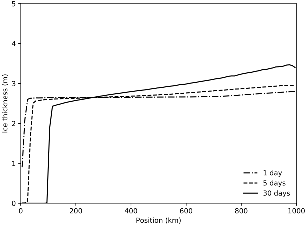


Figure: 1D ridging simulation with MPAS-Seaice. Rightwards wind causes ice pileup.

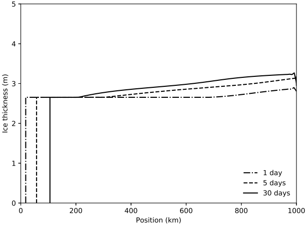
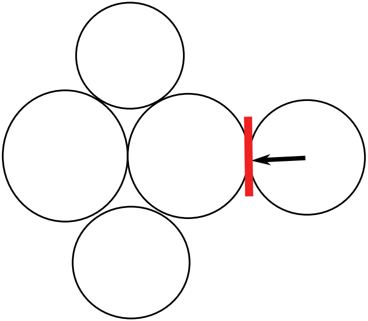


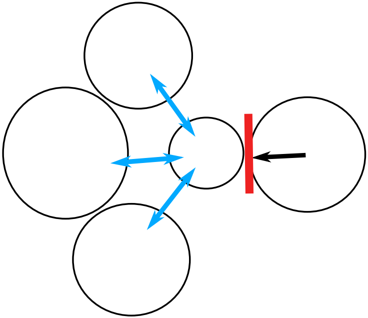
Figure: Implementation of the Hopkins ridging contact model with 5 category ice thickness distribution and column ridging method.

Element distortion from ridging

- Ridging results in model elements decreasing in area during simulation
- Decreases time step, add artificial strain



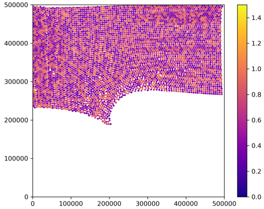
Convergence and ridge formation of two elements in pack



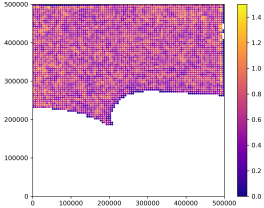
Shrinking of element adds strain to the pack

Geometrical remapping

- Investigating a global remapping back to an initial "good" element distribution
- Geometric version implemented and tested
- Later will use the coupling system
- Also investigating local remapping techniques

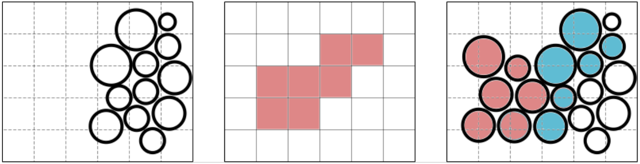


Particle distribution before remapping



Particle distribution after remapping

Frazil formation

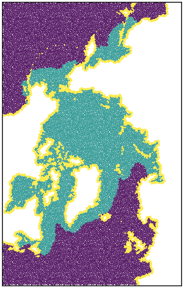


(*left*): Elements before frazil formation. (*center*): Frazil formation on Eulerian mesh. (*right*): Elements after frazil added. (*red*): New elements. (*blue*): Existing elements with frazil added.

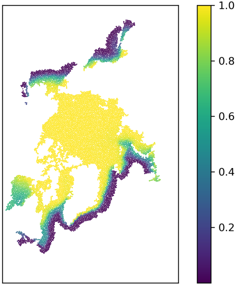
- Another significant challenge is addition of ice from frazil formation
- Take frazil from underlying Eulerian mesh
  - Add to existing elements
  - Create new elements
- Challenge is how to create the new elements with a tightly packed distribution

Realistic simulations

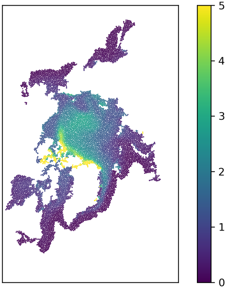
- Work has begun to perform Arctic basin scale simulations
- Particle distribution initialization, forcing, domain
- Currently integrating previous work



Element type



Ice fraction



Ice thickness

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

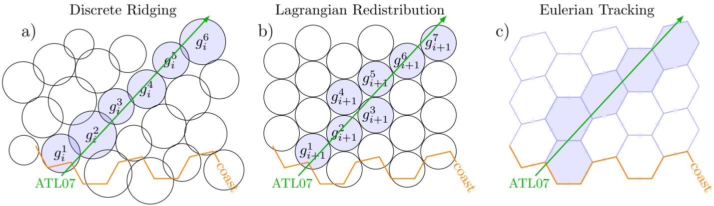
Core observations being used to evaluate DEMSI (upper tier) and its coupling (lower tier) using: E - Eulerian mapping; L - Lagrangian observation emulator; and S - Satellite altimetric emulators.

This project is contributing to the development of

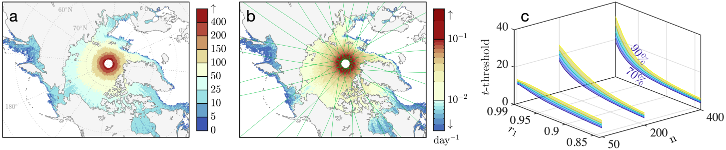
POLeSTAr
Polar System Analysis

DEMSI Data Fusion

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

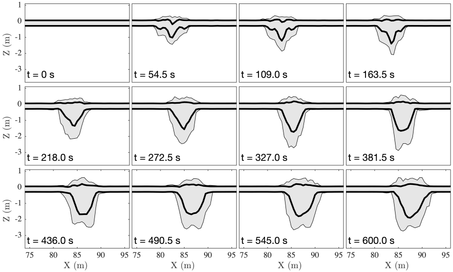


- We are optimizing the use of a finite number of satellite passes to generate continuous p-values for highly autocorrelated DEMSI output.

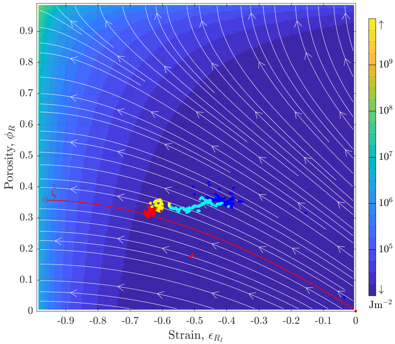


Masters Thesis - Travis Davis, Naval Postgraduate School

- Three dimensional finite element model of an individual ridge.



Cross sectional average of ridge evolution



- This research independently corroborates a new theoretical development to be used to simulate macro-porosity of the pack.

Future work

- **Phase 1**
    - Putting everything together and perform realistic Arctic basin scale simulations
- **Phase 2**
    - Coupling DEMSI into E3SM
    - Performance optimization
    - Machine learning to improve contact model
    - Stress state remapping
    - Analysis of coupled simulations