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DEMSI
Discrete Element Model for Sea Ice

Los Alamos NATIONAL LABORATORY EST. 1943

A Performance Portable Discrete Element Sea Ice Model for Earth System Modeling



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ESCO 2020

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SciDAC
Scientific Discovery through Advanced Computing

SEA ICE

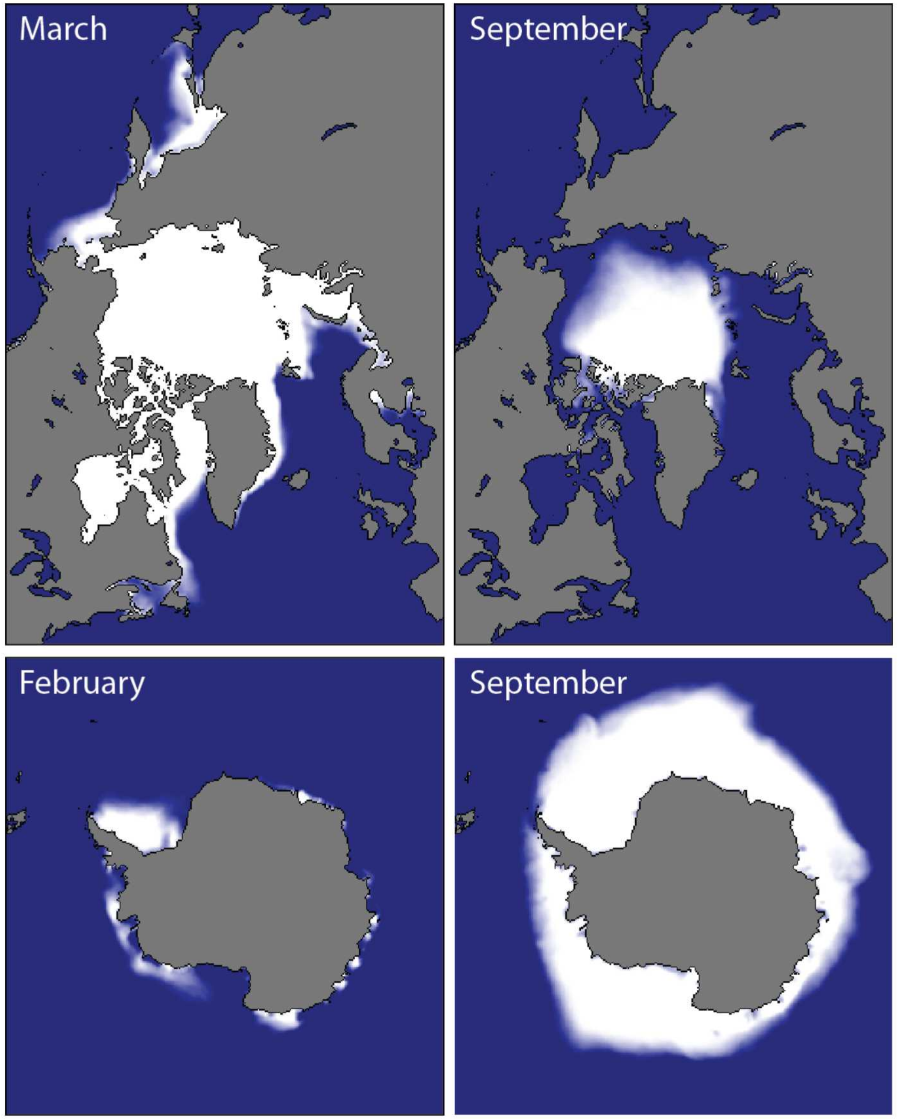
Importance in global climate:

- Reflects solar radiation
- Insulates ocean from atmosphere
- Influences ocean circulation

Physical processes:

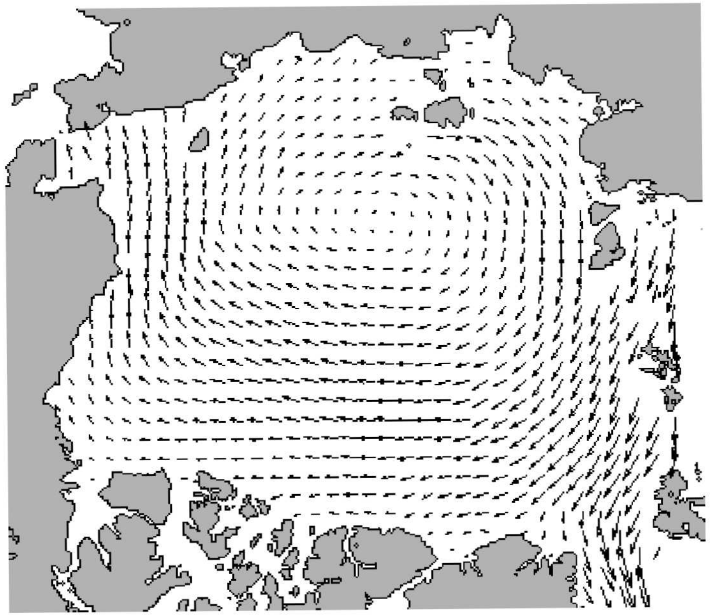
- Mechanical deformation due to surface winds and ocean currents
- Formation of leads (cracks) and pressure ridges
- Annual cycle of growth and melt due to radiative forcing

Climatology: 1981-2010 (nsidc.org)



SEA ICE GOVERNING EQUATIONS

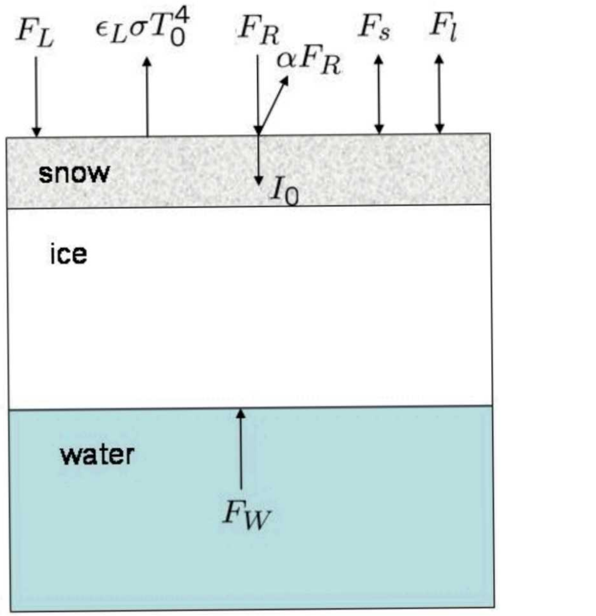
Dynamics



$$\rho h \frac{d\mathbf{v}}{dt} = \nabla \cdot (\sigma h) + \mathbf{t}_a + \mathbf{t}_o - \mathbf{f}_c - \rho \mathbf{g} \nabla H$$

2-D momentum equation for velocity

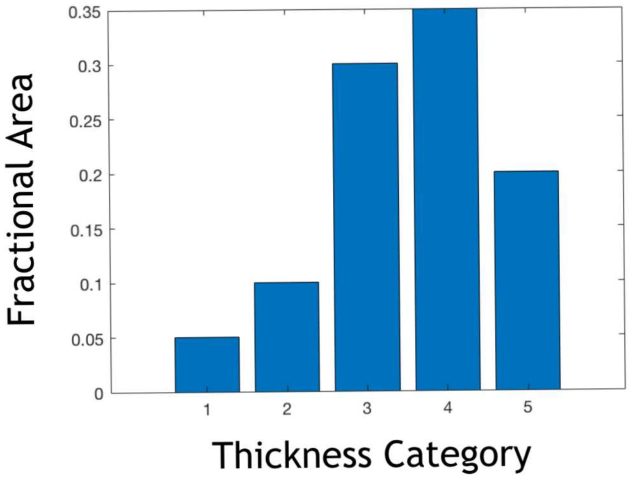
Thermodynamics



$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z} \right) + \kappa I_0 e^{-\kappa z}$$

Column (1-d) energy equation for temperature and thickness

Thickness Distribution



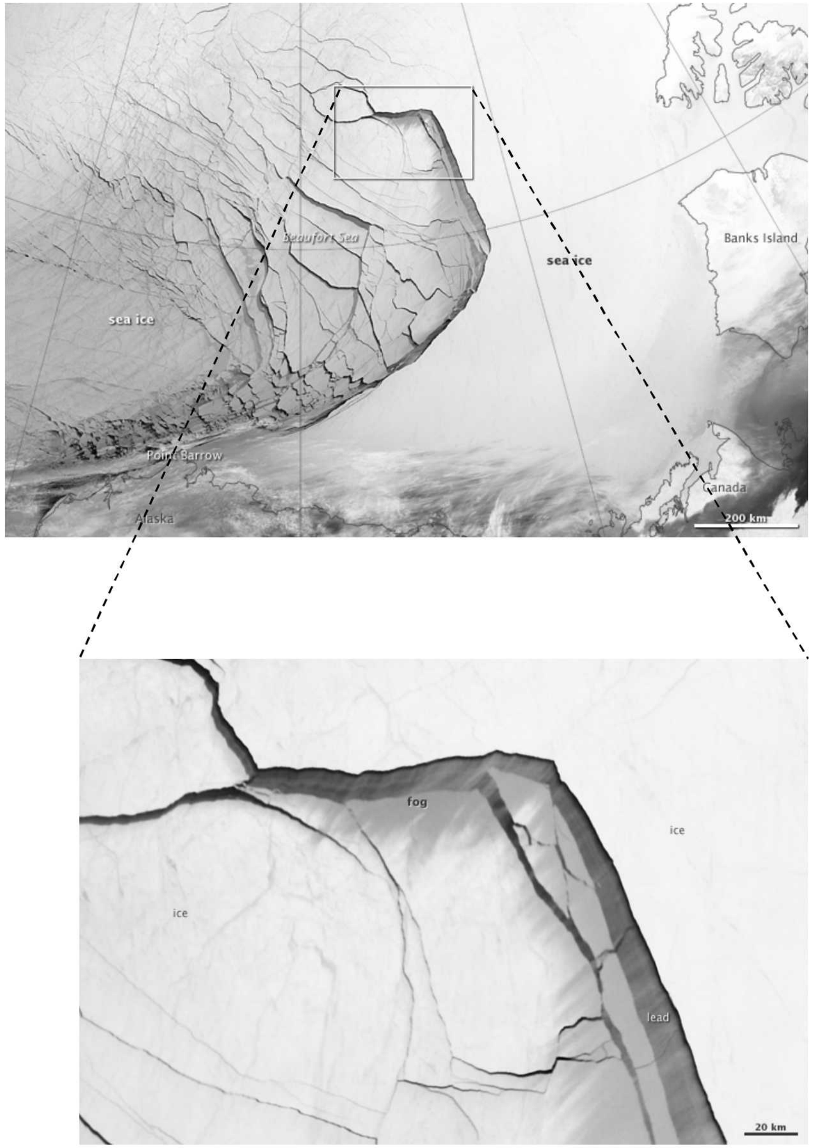
$$\frac{dg}{dt} + (\nabla \cdot \mathbf{v}) g + \frac{\partial (f g)}{\partial h} =$$

Connects horizontal dynamics to vertical thermodynamics

SEA ICE MODEL LIMITATIONS

Why a new sea ice model?

- Models now use much higher resolution – e.g. ~6 km cells for DOE Energy Exascale Earth System Model
- At high resolutions isotropic continuum models not good approximation of dynamics
- Need to run on advanced accelerated computing architectures being adopted by leadership computing facilities
- Particle methods offer potential for increased on node parallelism

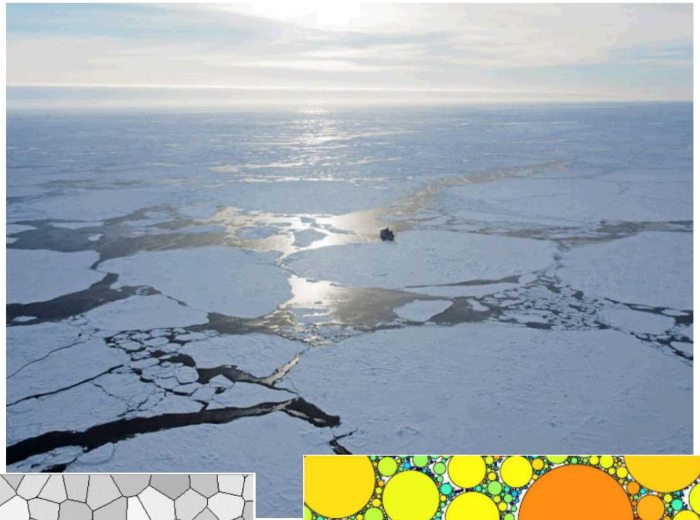


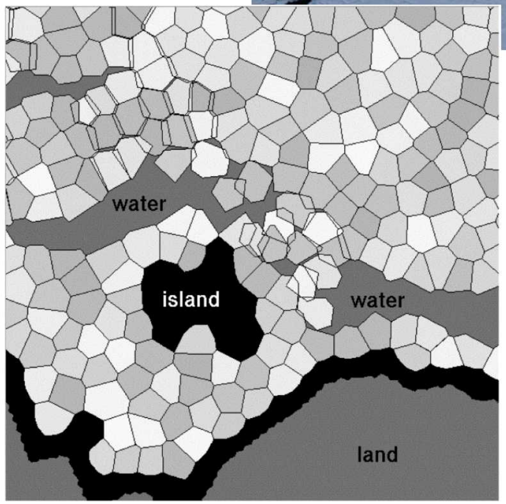
Visible Infrared Imaging Radiometer Suite (VIIRS) on Suomi NPP satellite earthobservatory.nasa.gov

DISCRETE ELEMENT MODEL FOR SEA ICE (DEMSI)

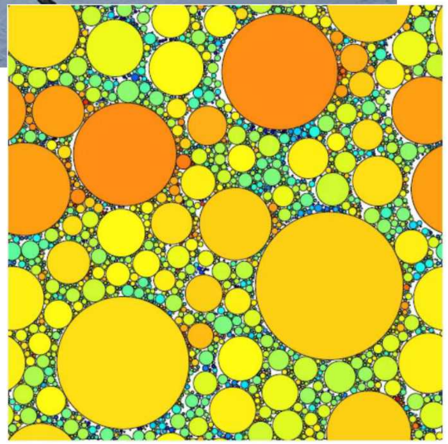
Our objective is to develop a computationally efficient, performance portable DEM sea ice model for Earth system modeling

- DEM for sea ice dynamics enables capture of
  - Anisotropic, heterogenous and intermittent nature of sea ice deformation
  - Explicit fracture and break-up of pack
- Previous DEM sea ice modeling efforts focused on regional scale, short-term simulations





Hopkins and Thorndike (2006)



Herman (2012)

DEMSI

- Replaces continuum dynamics with DEM, using circular elements for efficiency
- Each element represents a region of sea ice, and has its own ice thickness distribution
- Leverages the following libraries:

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

- Plimpton 1995, https://lammps.sandia.gov
- Particle based molecular dynamics code
- Includes support for DEM and history dependent contact models
- Computationally efficient with massive parallelization

Thermodynamics: CICE Consortium Icepack Library

- Hunke et al. 2018, https://github.com/CICE-Consortium/Icepack
- State-of-the-art sea-ice thermodynamics package
- Vertical thermodynamics, salinity, shortwave radiation, snow, melt ponds, ice thickness distribution, biogeochemistry

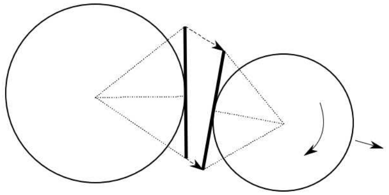
CHALLENGES

- Contact model
  - Must include bonds and fracture
  - Validated and accurate for sea ice
- Computational performance
  - Require performant code on heterogeneous architectures
  - Explicit DEM requires small time steps
- Coupling with gridded ocean/atmosphere
  - Need to transfer fluxes between ice/ocean/atmosphere
  - Requires conservation and bounds preservation
- Large deformations and new ice growth
  - Requires accurate, conservative remapping

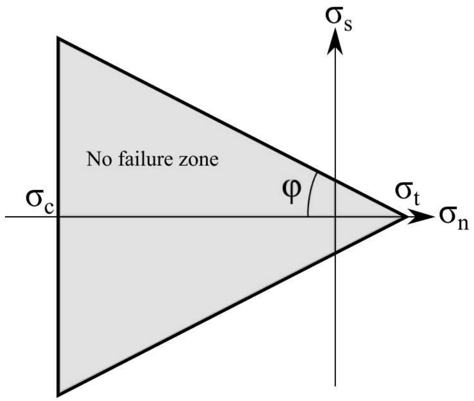
CONTACT MODEL

- Determines normal and tangential forces between elements
- These forces (as well as external forces) are integrated to determine velocity
- Initial implementation adapts the work of Hopkins 2004, Wilchinsky et al. 2010, to circular elements
- Includes both bonded and unbonded elements

- Each point on bond has viscous-elastic “glue”
- Mohr-Coulomb fracture law



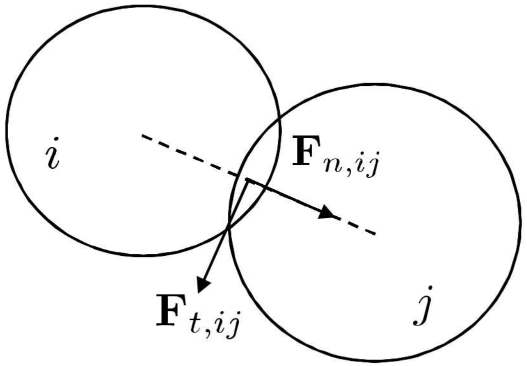
Two bonded elements in relative motion



Total force on particle i: $$\mathbf{F}_i = \sum_{j,j\neq i}^{N} (\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij}) + \mathbf{F}_{ext}(\mathbf{r}_i)$$

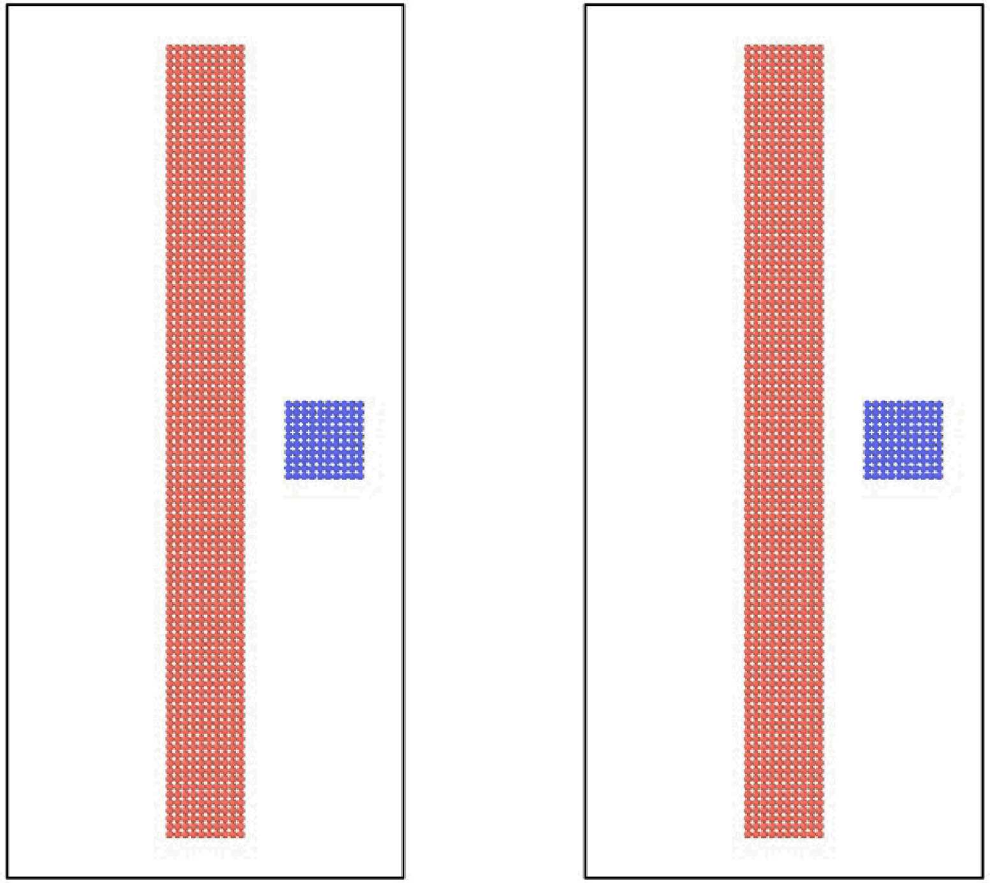
$$\mathbf{F}_{ext}(\mathbf{r}_i) = \rho_a C_a \|\mathbf{v}_a\| \mathbf{v}_a \pi R_i^2 + \rho_w C_w \|\mathbf{v}_w - \mathbf{v}_i\| (\mathbf{v}_w - \mathbf{v}_i) \pi R_i^2 - f_c m_i (\mathbf{k} \times \mathbf{v}_i) + f_c m_i (\mathbf{k} \times \mathbf{v}_w)$$

Wind drag — Ocean drag — Coriolis force — Surface tilt

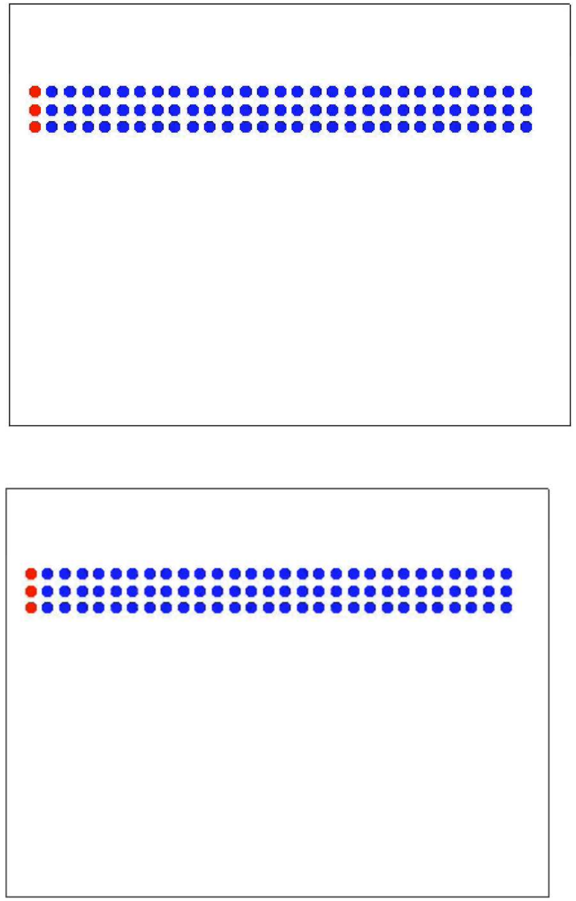


CONTACT MODEL TESTS

Impact



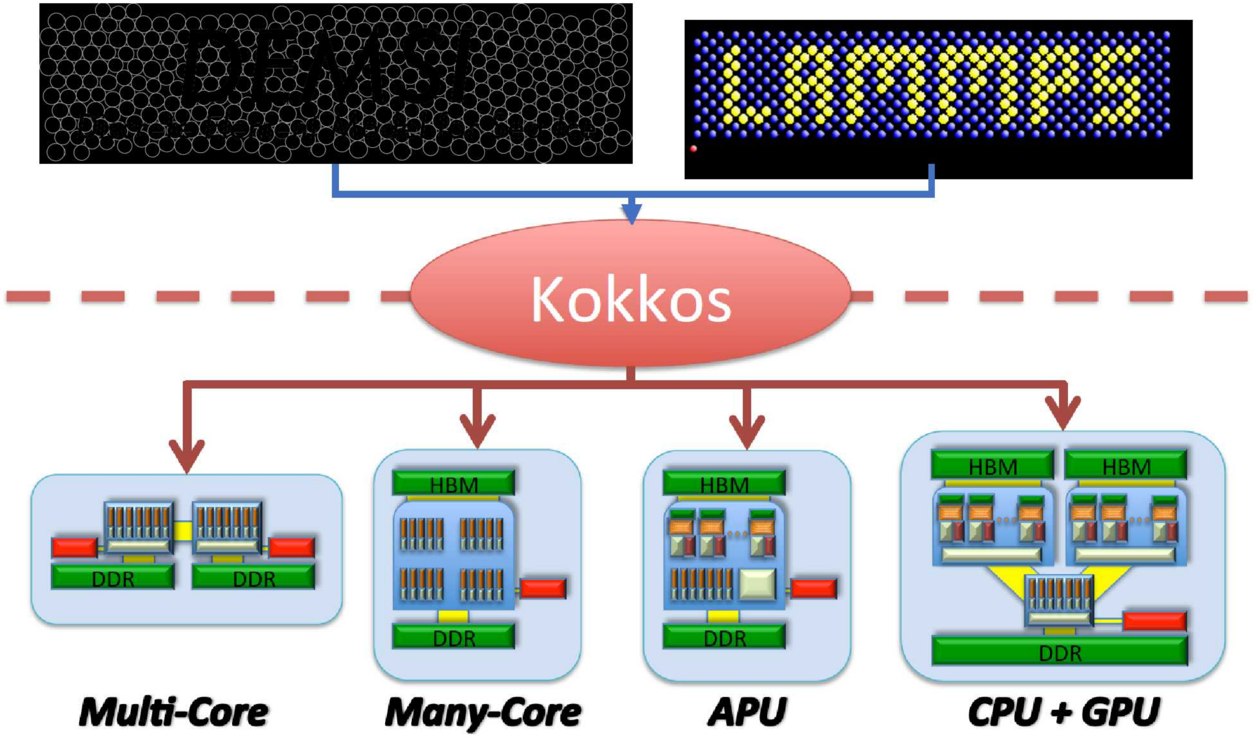
Cantilever Beam



DEMSI using Kokkos programming model for acceleration

- C++ library
- Shared-memory programming model
- Enables writing algorithms once for many architectures
- Uses multi-dimensional arrays with architecture-dependent layouts
- (Edwards et al. 2014)

- Contact model within LAMMPS as well as many functions within DEMSI have been converted to Kokkos

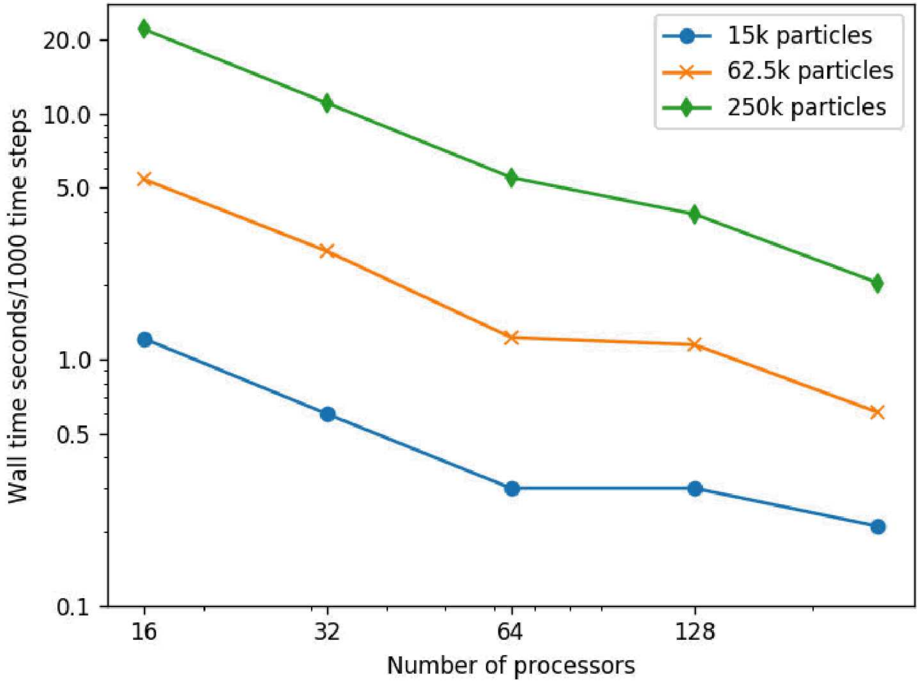


https://github.com/kokkos

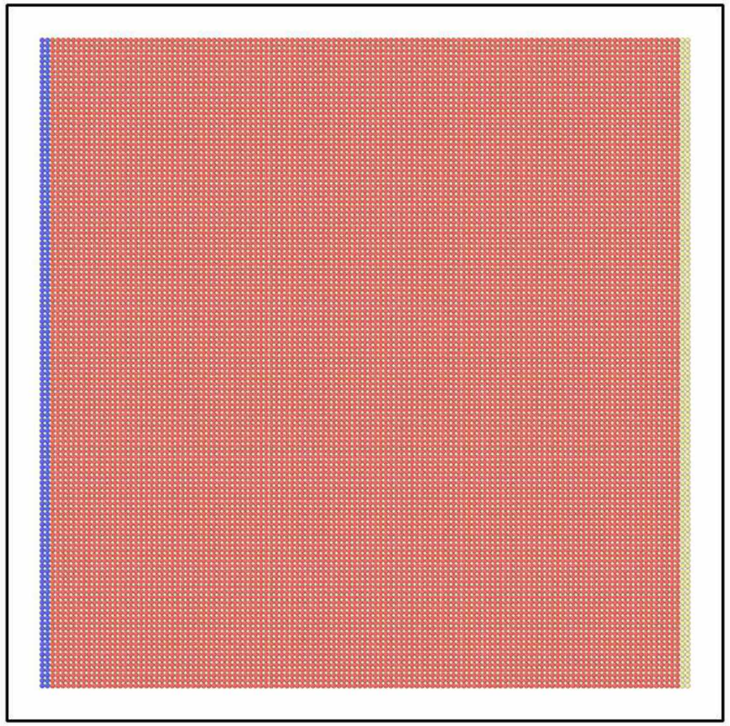
MPI PERFORMANCE

Preliminary performance benchmark – MPI only

- Simple shear + compression
- Lattice arrangement of monosized particles
- Opportunities for performance increase
    - Decrease stiffness for larger time step
    - Kokkos and GPUs

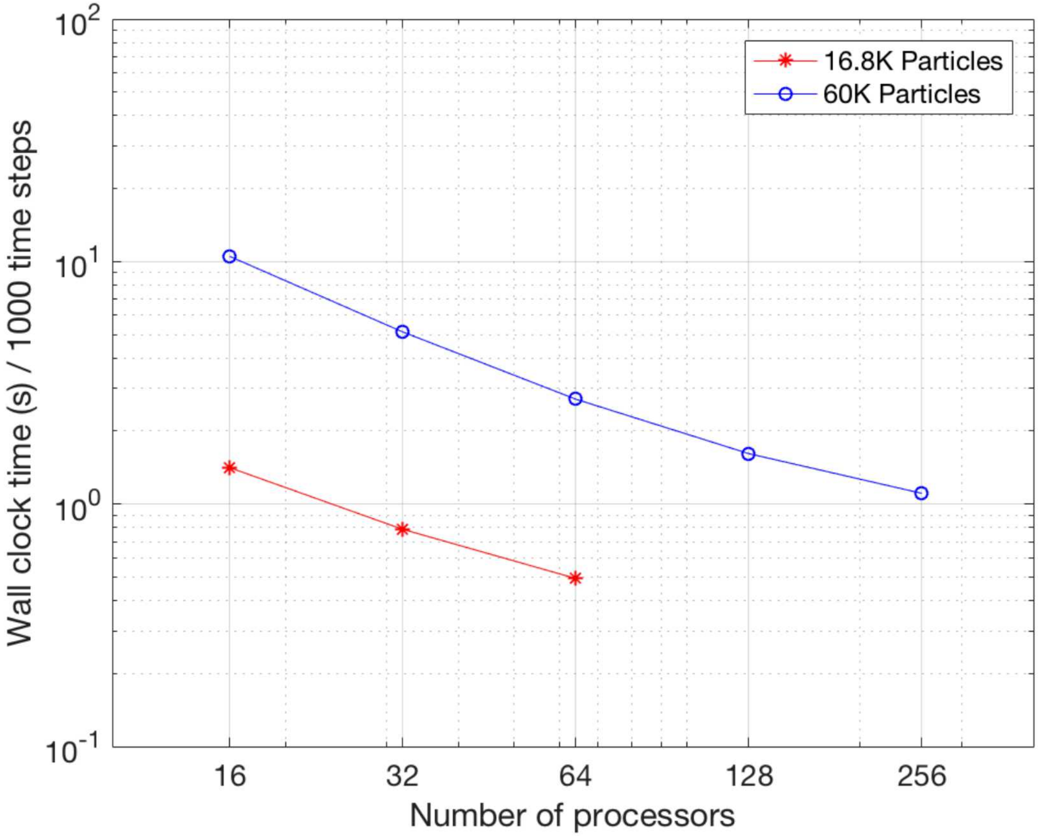


15K particles

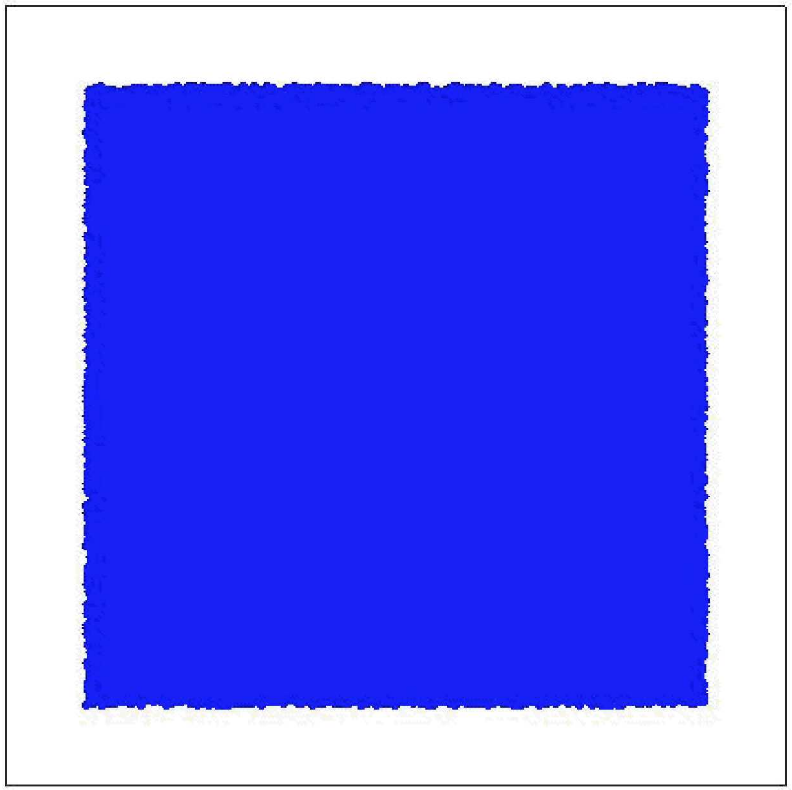


PERFORMANCE FOR KOKKOS CONTACT MODEL

- Uniform stress test case
- Polydisperse random packing of particles undergoes fracture
- Initial test for CPU-only scaling

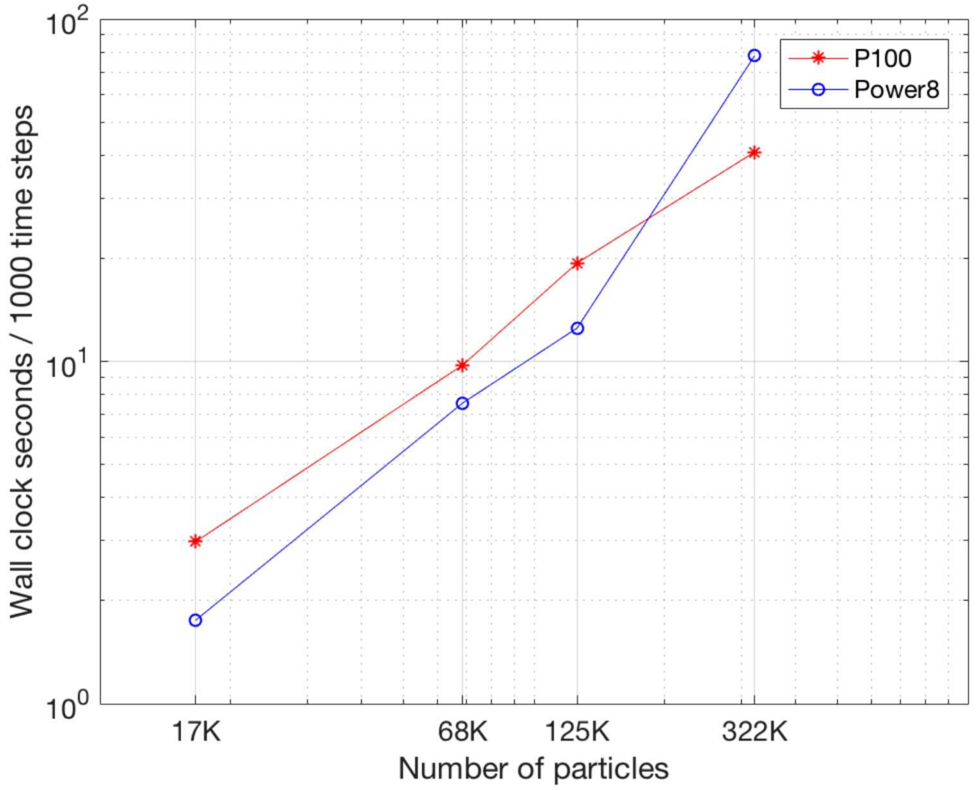


16.8 K Particles

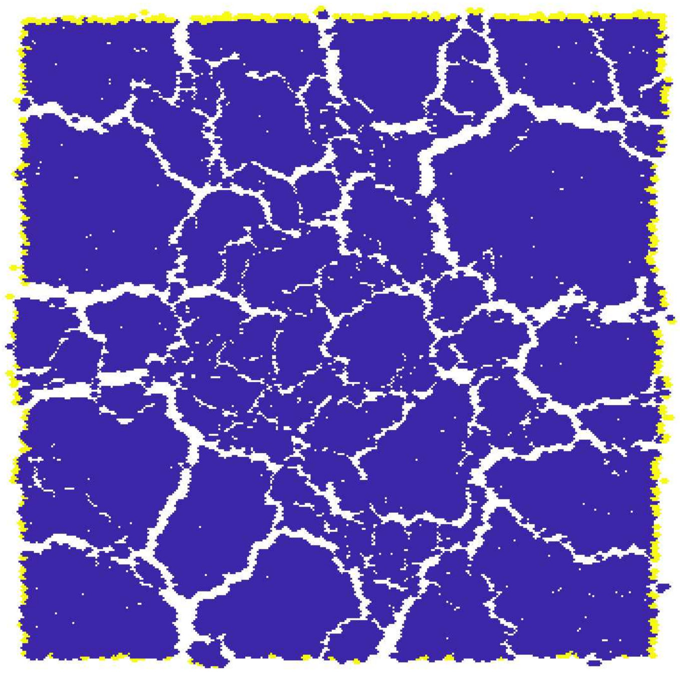


PERFORMANCE FOR KOKKOS CONTACT MODEL

- Tests on White, a Heterogeneous Advanced Architecture Platform at SNL
- Eight Garrison dual socket compute nodes and Nvidia Tesla P100 GPUs



Uniform Stress



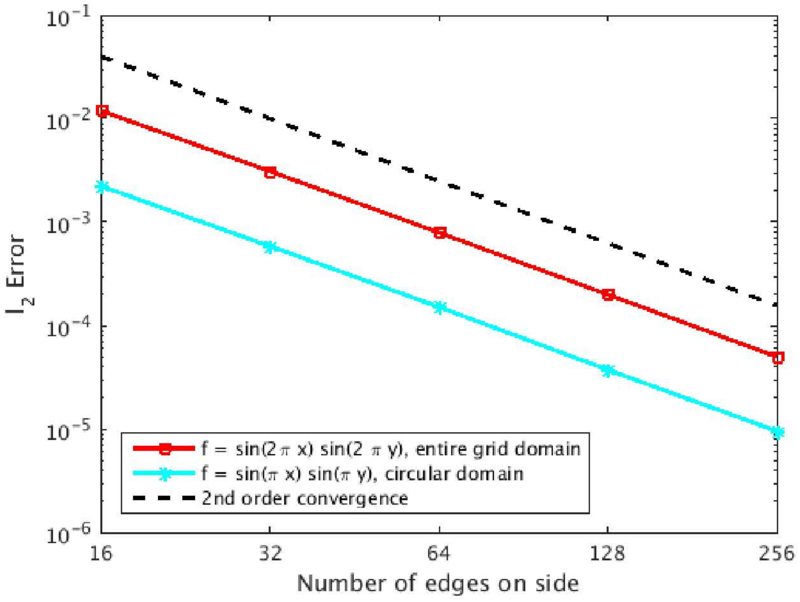
OCEAN/ATMOSPHERE COUPLING

Particle to grid:

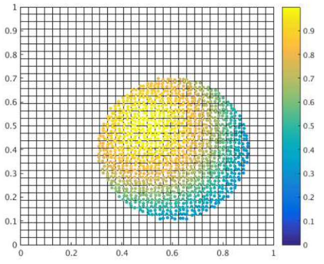
- Sea ice quantities mapped to ocean/atmosphere
- Second-order moving least squares-based method with limiting implemented

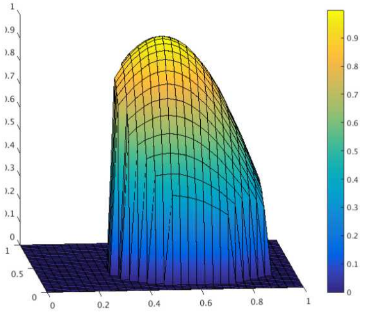
Grid to particle:

- Gridded ocean/atmosphere quantities to sea ice
- Bilinear remap implemented



- Approximately 4 particles-per-cell for all grid resolutions
- Particles initialized with random perturbation from structured arrangement





Given bilinear basis functions $\{N_i\}$, and a set of discrete elements indexed by e, a grid function indexed by nodes, i, can be written

$$f_i = \sum_e \psi_e f_e$$

where

$$\psi_e = bM^{-1}b^T N_i(x_e)$$

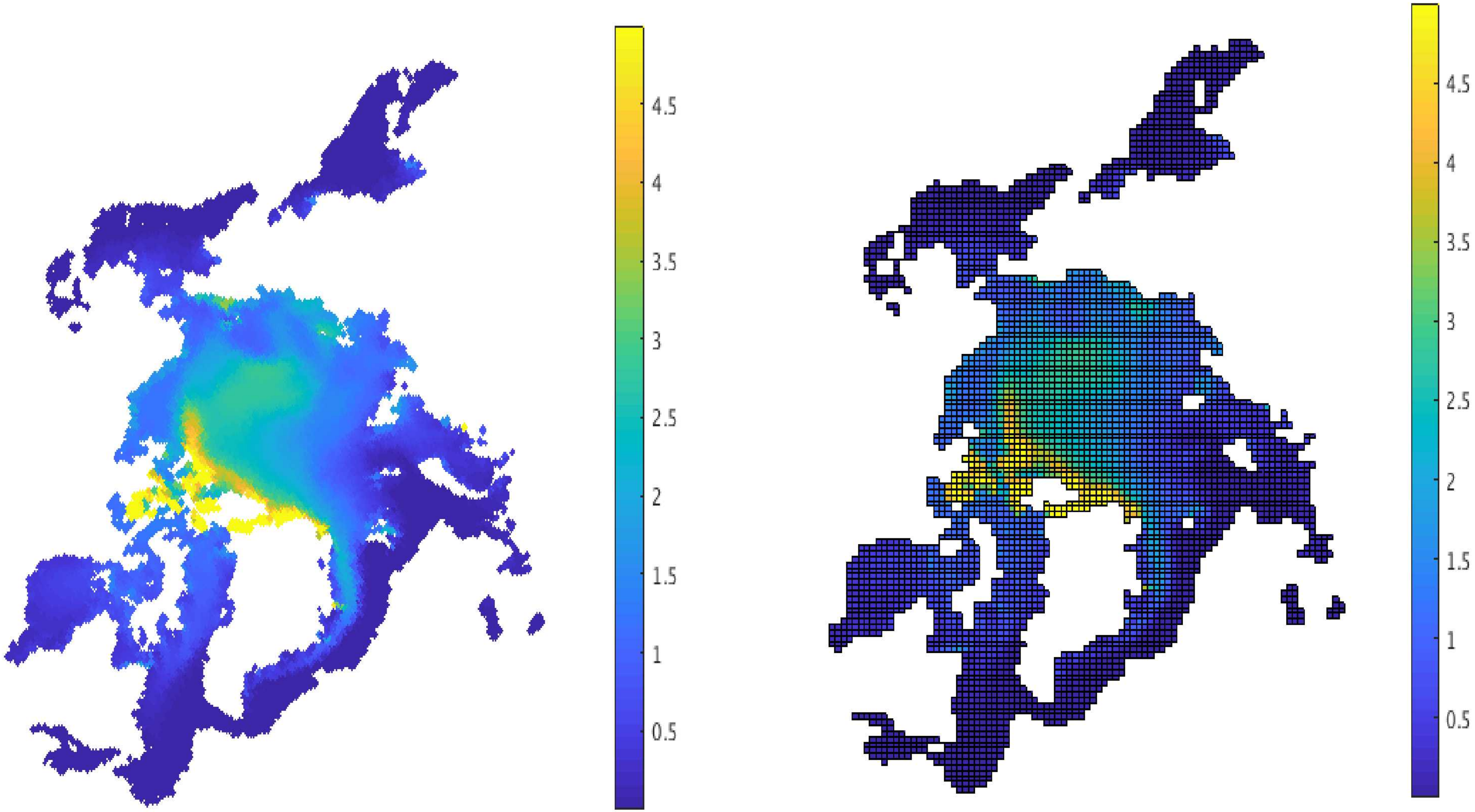
$$b^T = [1 \quad (x_i - x_e) \quad (y_i - y_e)]$$

$$M = \sum_e bb^T N_i(x_e)$$

In cases where the moment matrix is ill-defined, we reduce to first-order Shepard interpolation

$$f_i = \frac{\sum_e N_i(x_e) f_e}{\sum_e N_i(x_e)}$$

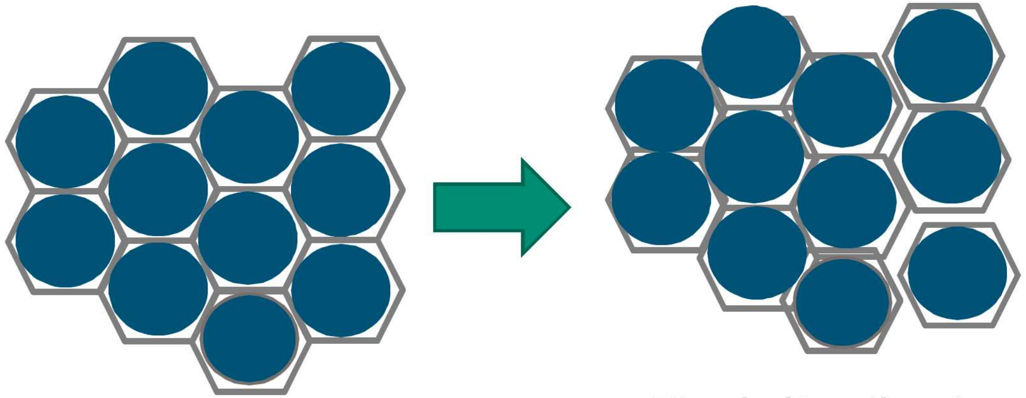
OCEAN/ATMOSPHERE COUPLING



Interpolation of sea ice thickness from particles to grid.

PARTICLE REMAP

- Remap back to an initial particle distribution periodically
- Addresses large particle deformations due to ridging and convergence
- In remapping step activate new particles from thermodynamic ice growth
- Currently in testing phase

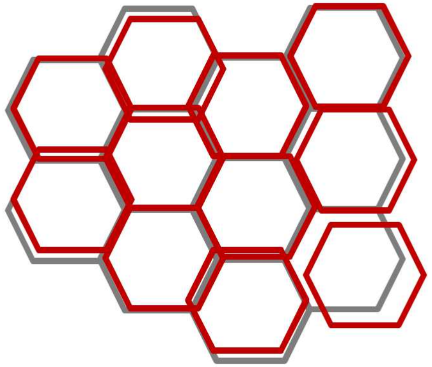


Initial distribution

Final distribution

- Current approach:
  - initialize particle distribution with effective element area defined by Voronoi cells
  - remapping weights defined by Voronoi intersections

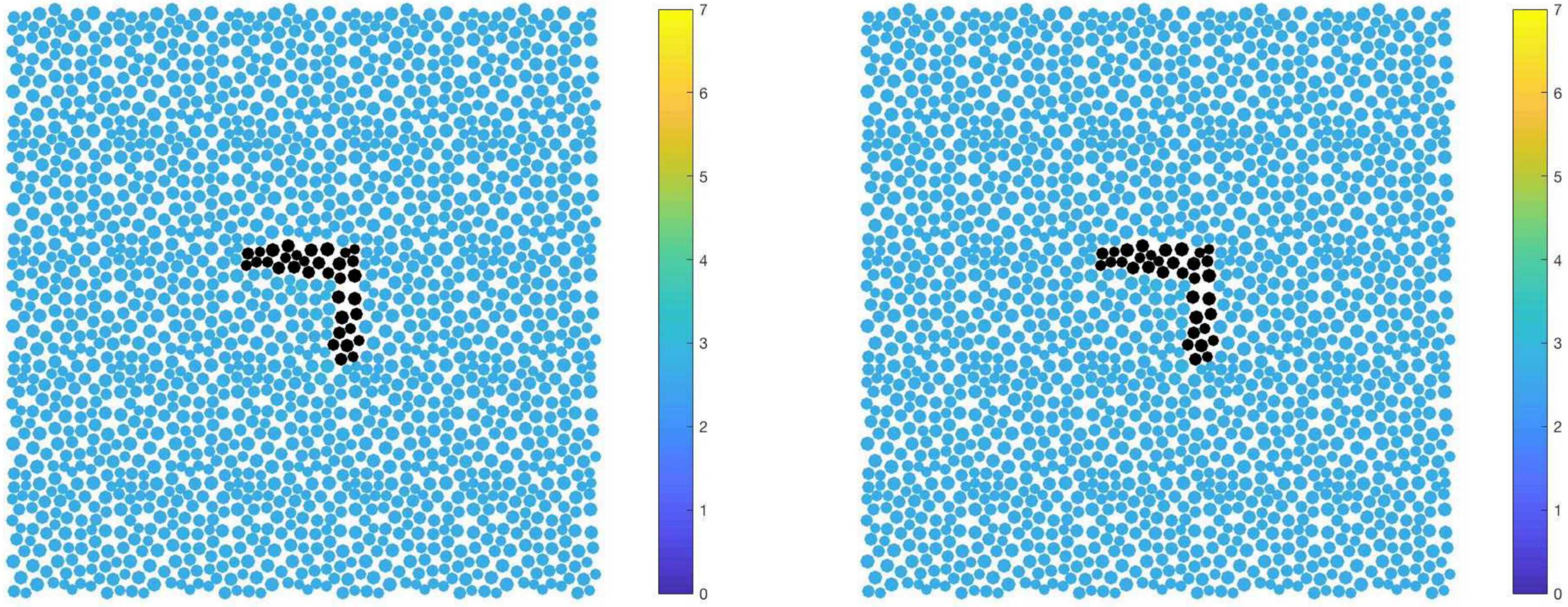
- Flux-based and mass-based methods for conservation and bounds preservation implemented



Intersections

PARTICLE REMAP

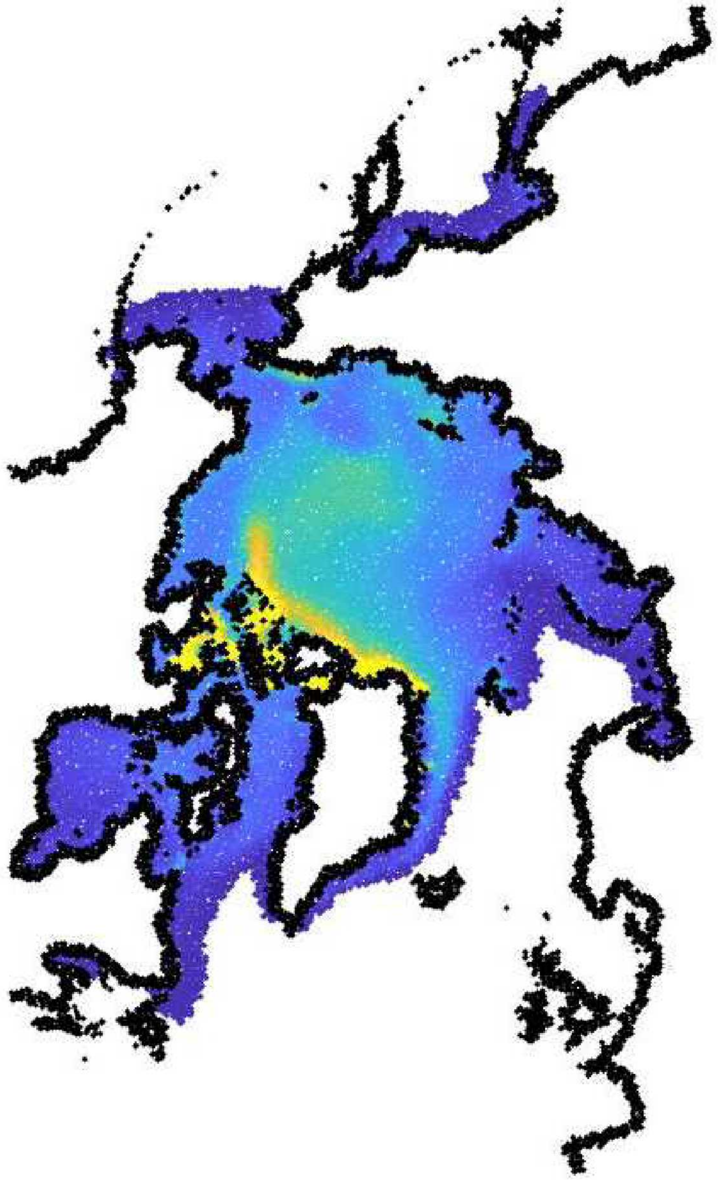
Ridging Test Case



ARCTIC BASIN SIMULATION

- Working towards a realistic Arctic basin simulation
- Including thermodynamics, ridging, fracture

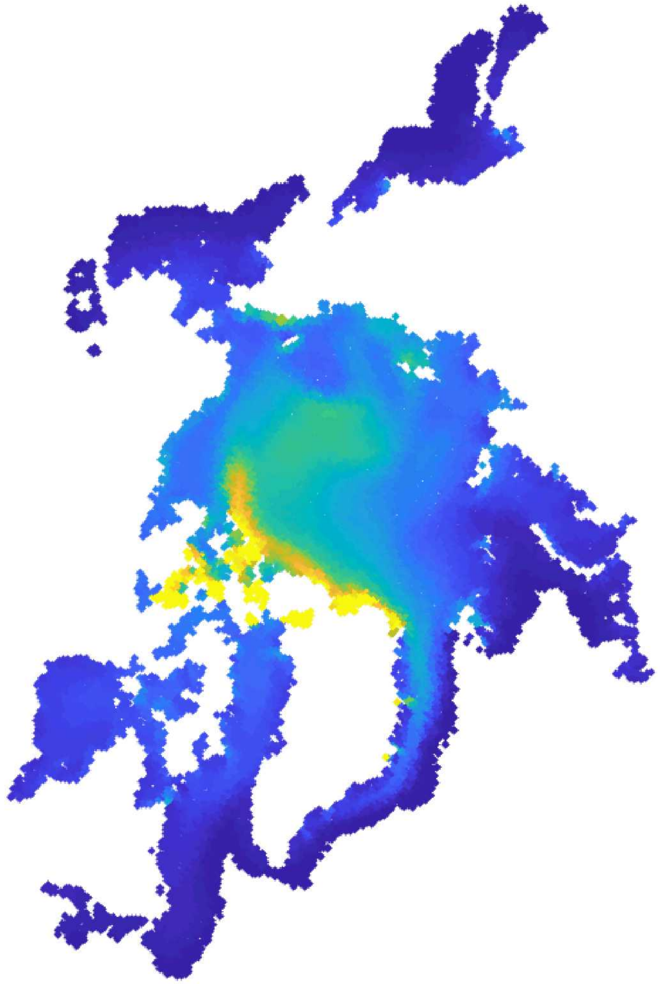
- Preliminary test simulation
  - 16K particles
  - CORE Ocean and atmosphere forcing
  - Slab ocean
  - Remapping to add new ice



CONCLUSIONS

- Developing new DEM sea ice model to better capture sea ice deformation and improve predictions
- Ultimate goal is to incorporate DEMSI as sea ice component in the DOE Energy Exascale Earth System Model (E3SM)

- Ongoing work
  - Arctic basin-scale simulation with validation
  - Continue to improve sea ice contact model
  - Kokkos implementation and performance testing



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