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# DEMSI

## Discrete Element Model for Sea Ice

Sandia National Laboratories

NPS PRAESTANTIA PER SCIENTIAM 1909

**USACM Conference on Meshfree and Particle Methods: Application and Theory**

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SciDAC Scientific Discovery through Advanced Computing

U.S. DEPARTMENT OF ENERGY NNSA

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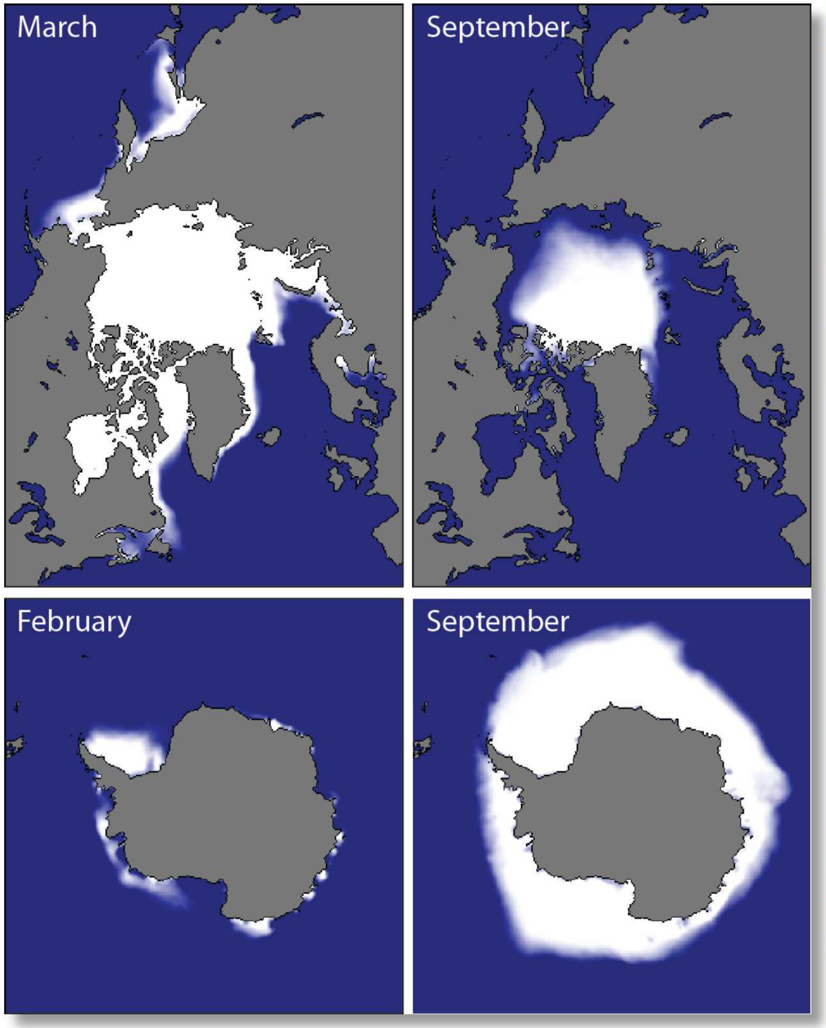
# SEA ICE

- Frozen surface of the ocean at high latitudes
- Covers ~7% of Earth surface and ~12% of ocean surface
- Exhibits strong seasonal cycle
- Important in global climate
  - Reflects solar radiation
  - Insulates ocean from atmosphere
  - Influences ocean circulation
- Accurate modeling of sea ice is important for both global climate and shorter-term forecasting for navigation

Climatology: 1981-2010 (nsidc.org)



# SEA ICE MODELING

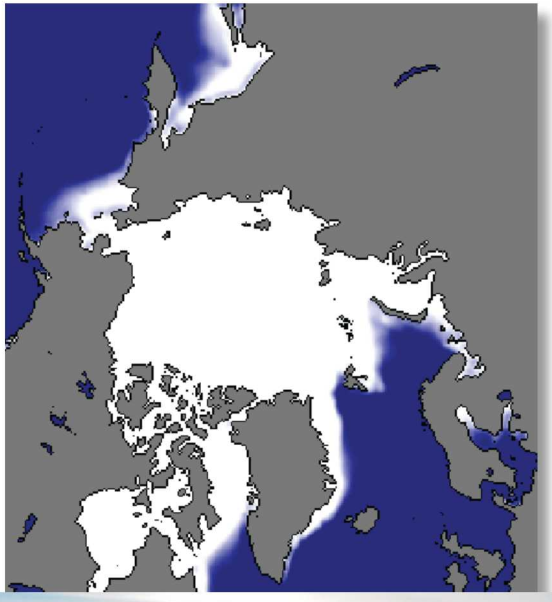
*Important physical processes:*

- Mechanical deformation due to surface winds and ocean currents
- Changes in thickness including lead and ridge formation
- Annual cycle of growth and melt due to radiative forcing

- Dynamics
  - 2-D momentum equation solve for velocity
  - Typically continuum using viscous-plastic rheology
  - More recently, anisotropic rheologies
- Thermodynamics
  - Energy equation solved in column determines temperature and thickness
  - Balance fluxes determines melt/growth of ice
- Ridging
  - Convergent velocity leads to ridging
  - Conserves volume and redistributes ice

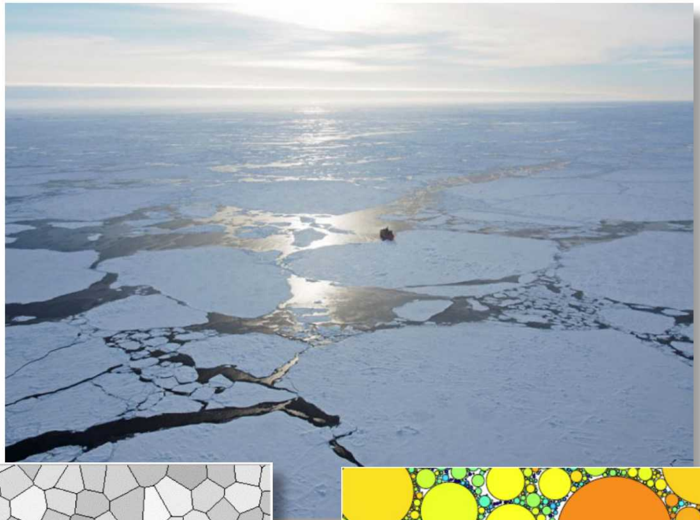
# MODEL LIMITATIONS

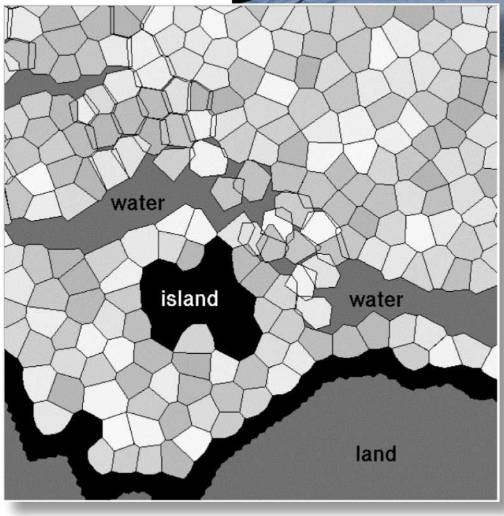
- At high resolutions isotropic continuum models not good approximation of dynamics
- Viscous-plastic model assumes grid cells are large enough that there is an isotropic distribution of leads or cracks in each cell
- Developed when grid cell size was ~100km
- Models now use much higher resolution – e.g. ~6km cells for DOE Energy Exascale Earth System Model (E3SM)/MPAS-Seaice
- Observations suggest viscous-plastic models poor for resolutions < ~10km
- As temperatures are increasing, sea ice may be better represented as a discrete set of floes rather than as a continuous ice cover



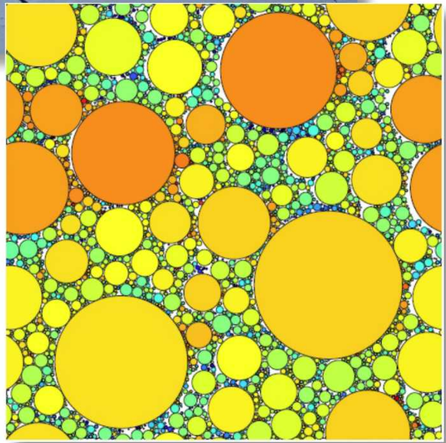
# DISCRETE ELEMENT METHOD

- 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
- Our objective is to develop a computationally efficient global climate scale sea ice model using DEM






Hopkins and Thorndike (2006)



Herman (2012)

# DEMSI

***Dynamics*:** LAMMPS (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 (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, BGC

**DEMSI**: Combines power of LAMMPS and Icepack

- Circular elements to start for efficiency
- Each element represents a region of sea ice, and has its own ice thickness distribution

# PRINCIPLE CHALLENGES

1. Contact model

   How should elements interact to represent sea ice physics?

2. Element distortion

   Convergence of sea ice converts area to thickness – how to manage element distortion?

3. Coupling

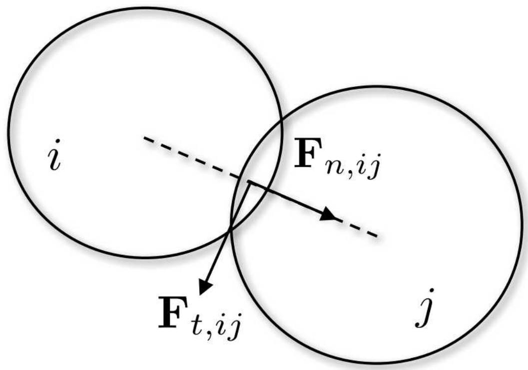
   How to couple particles to Eulerian mesh conservatively?

4. Computational performance

   How to make the model fast enough for global climate applications?

# CONTACT MODEL FOR SEA ICE

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



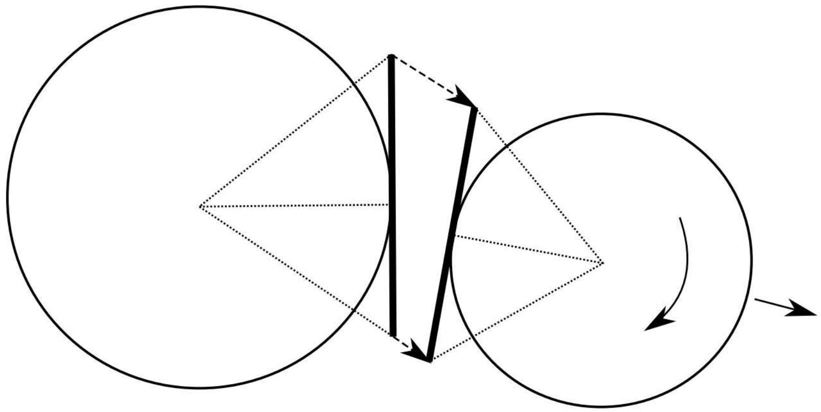

Total force on particle i: $\mathbf{F}_i = \sum_{j,j\neq i}^{N} (\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij}) + \mathbf{F}_{ext}(\mathbf{r}_i)$

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

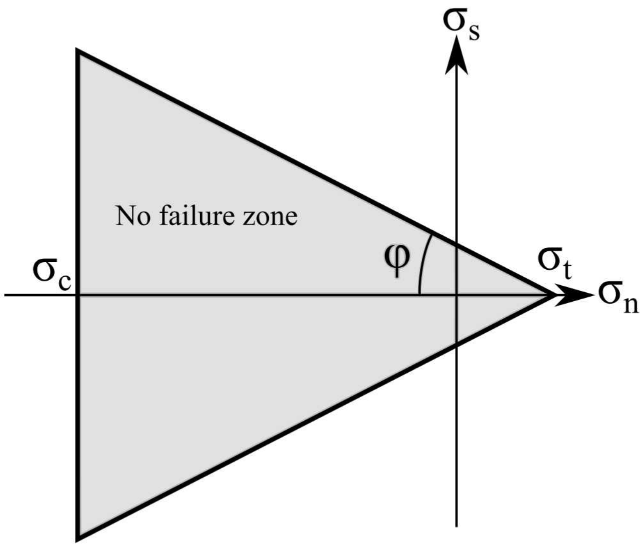
Wind drag — Ocean drag — Coriolis force — Surface tilt

# CONTACT MODEL – 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



Two bonded elements in relative motion

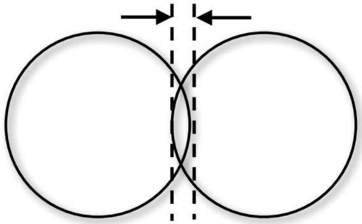


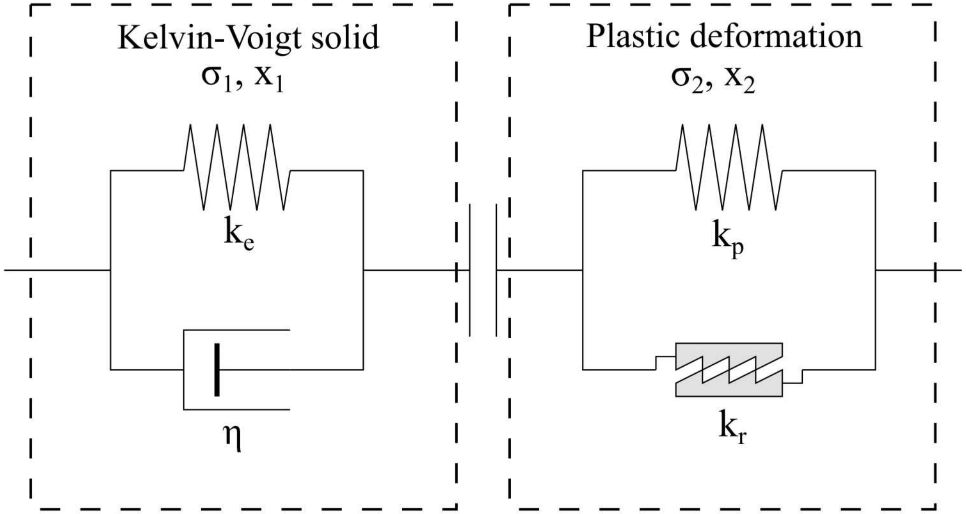

Mohr-Coulomb failure surface

# 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
- Will be implementing new ridging model developed at NPS

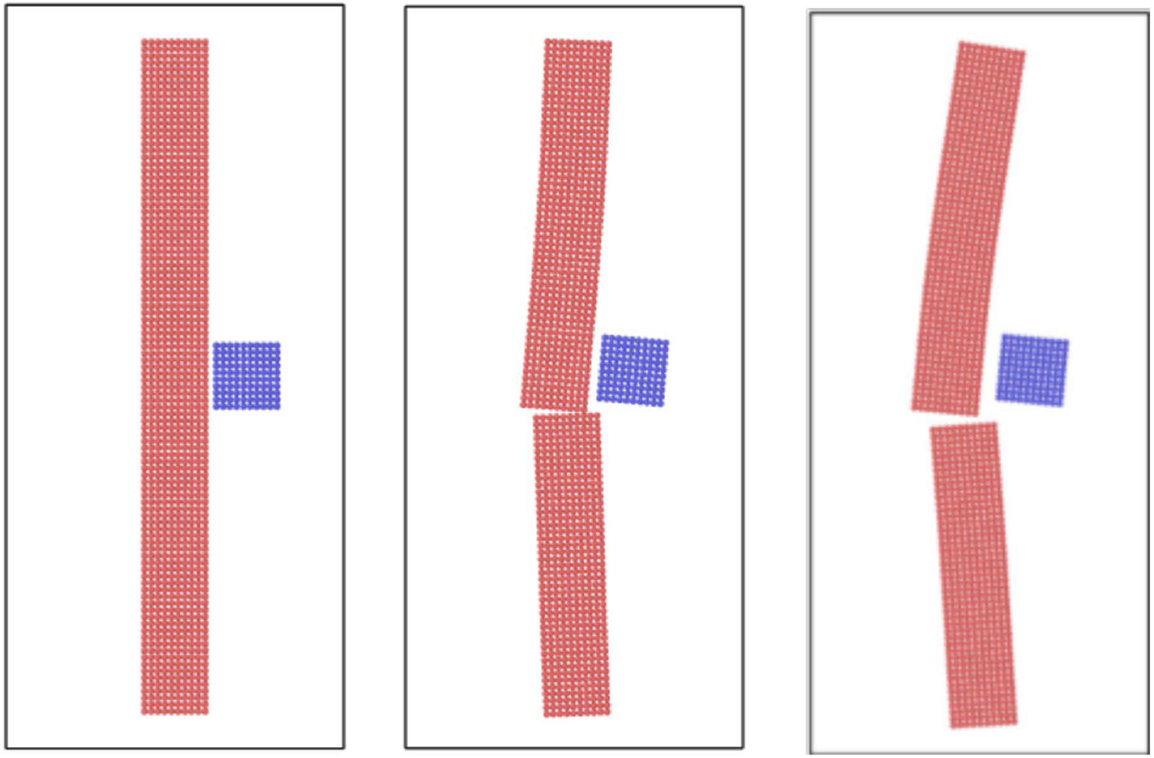
$$\delta = (R_i + R_j) - \|\mathbf{r}_{ij}\|$$





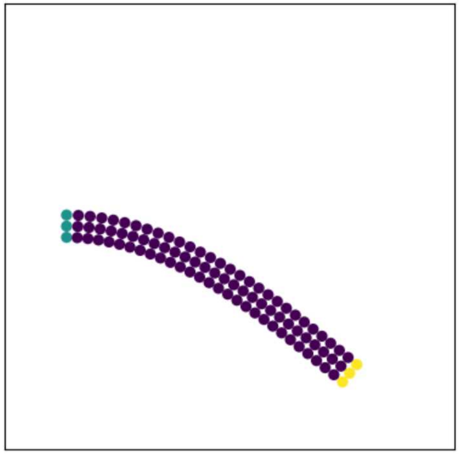
# CONTACT MODEL TESTING

## Impact

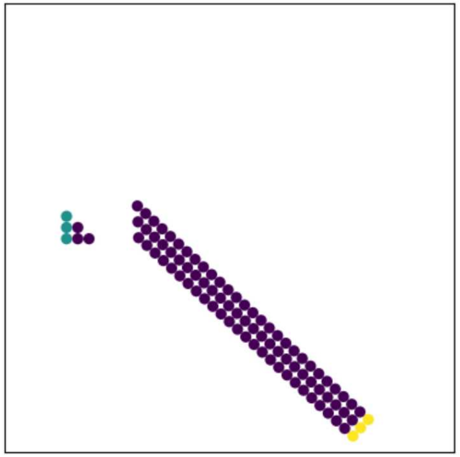


## Cantilever

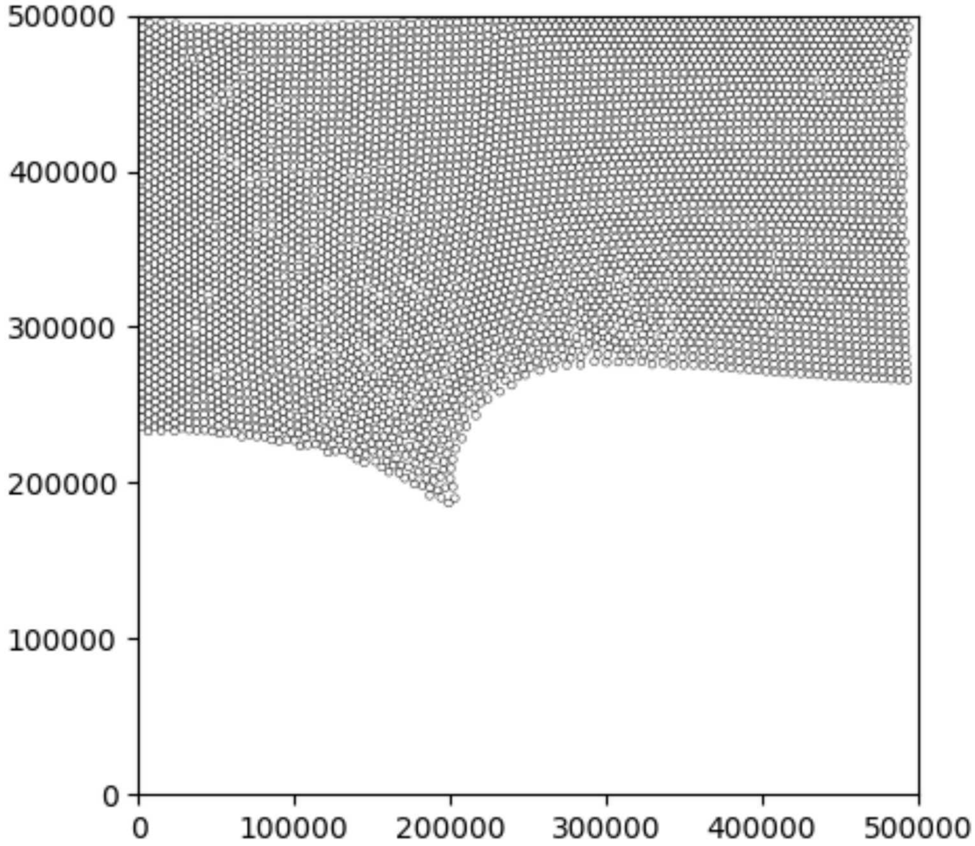
No fracture



With fracture



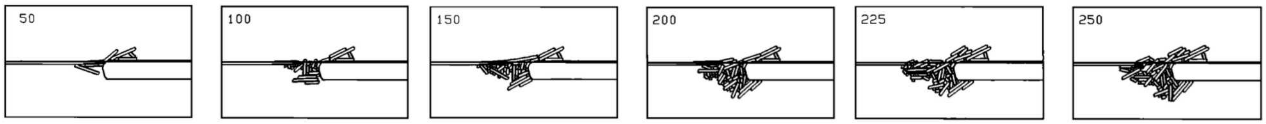
# CONTACT MODEL TESTING




Flato (1993) test case with swirling wind field as forcing

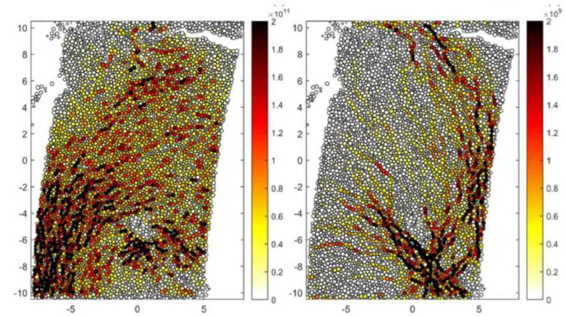
# CONTACT MODEL GOING FORWARD

Individual ridge



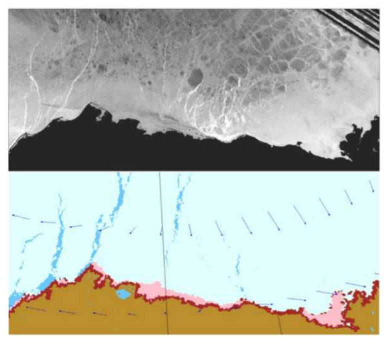

Hopkins 1994

Individual floe experiments



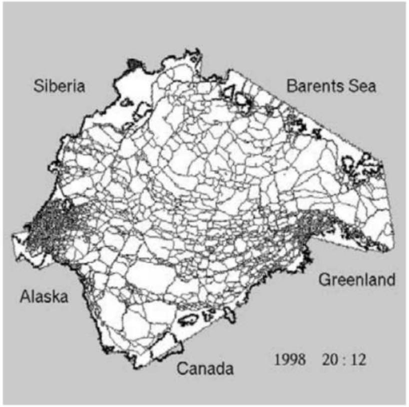
Herman 2016

Regional experiments



Kulchitsky et al. 2017

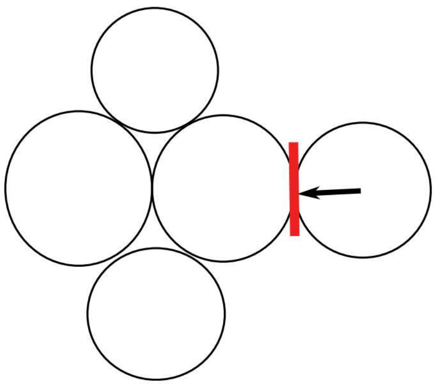
Basin scale experiments

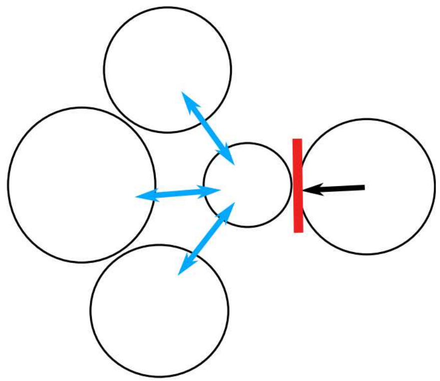



Hopkins et al. 2004

# ELEMENT DISTORTION, CREATION & DESTRUCTION

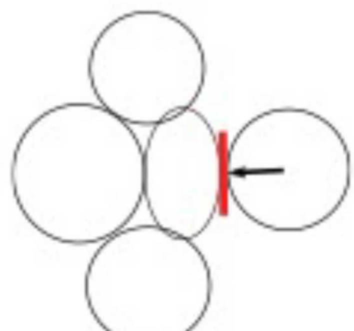
- Convergence of sea ice results in formation of pressure ridges
- Elements need to shrink
  - Decreases time step and increases computational requirements
  - Can result in artificial strain





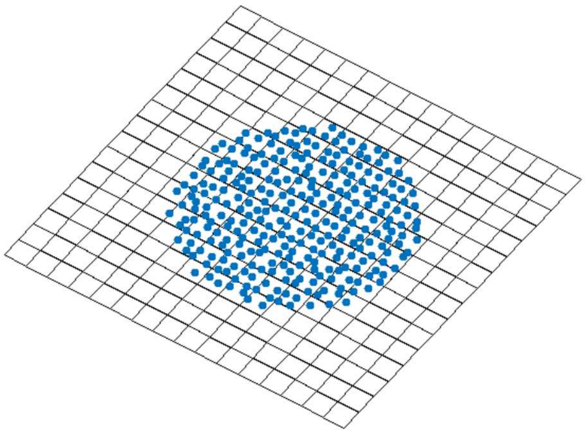
Pressure ridge

- Possible options
  - Use elliptical elements
  - Merge elements that get too small
  - Periodically remap elements



# COUPLING

- DEMSI will need to couple with ocean and atmosphere models for climate simulations
- Requires a method for interpolation between Lagrangian particles and Eulerian grids
- Have implemented a moving least squares (MLS) method for interpolating particle data to a fixed structured grid within DEMSI
- Next steps – implementing optimization-based strategy to ensure conservation



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

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

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

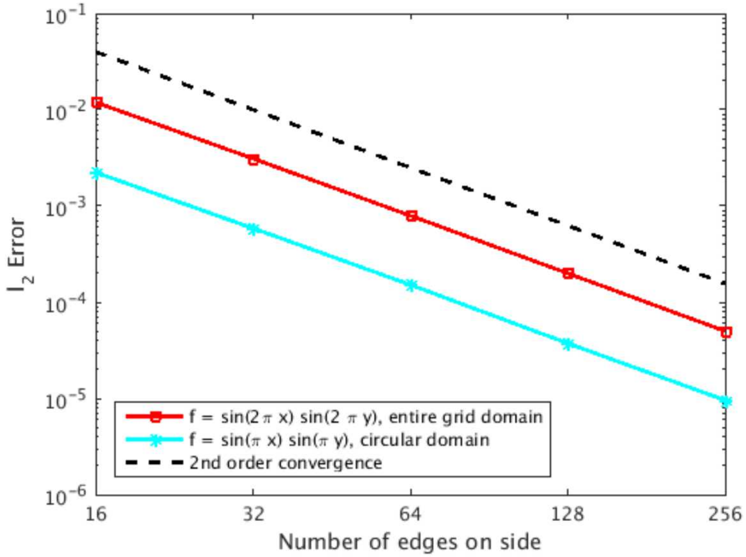
$$M = \sum_e bb^T N_i(x_e)$$

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

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

# PARTICLE-TO-GRID COUPLING

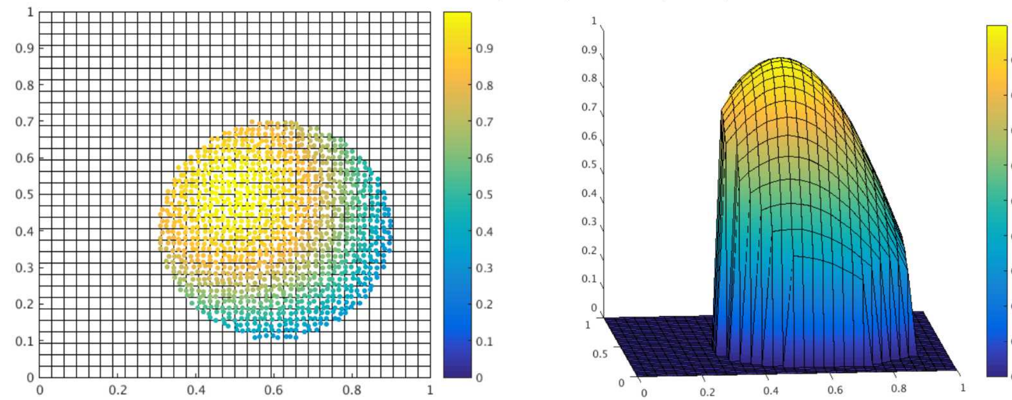
Second-order convergence



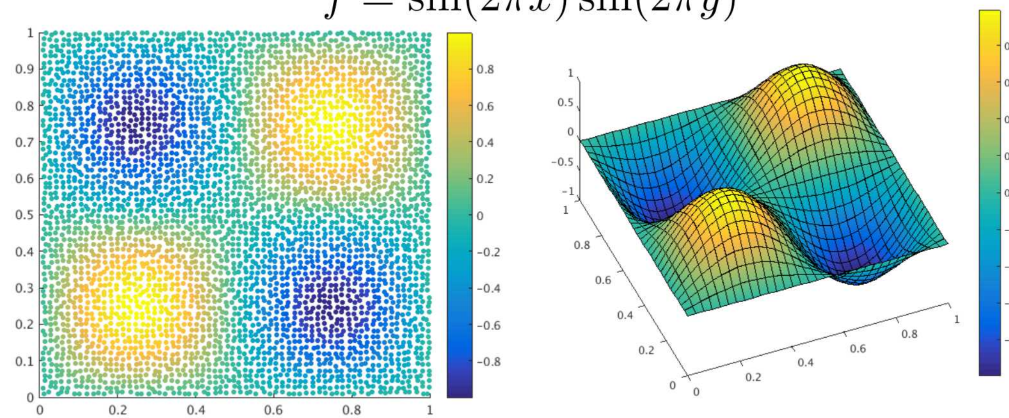

Particle Distribution and Values

Interpolated Grid Values (32x32 cells)

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



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

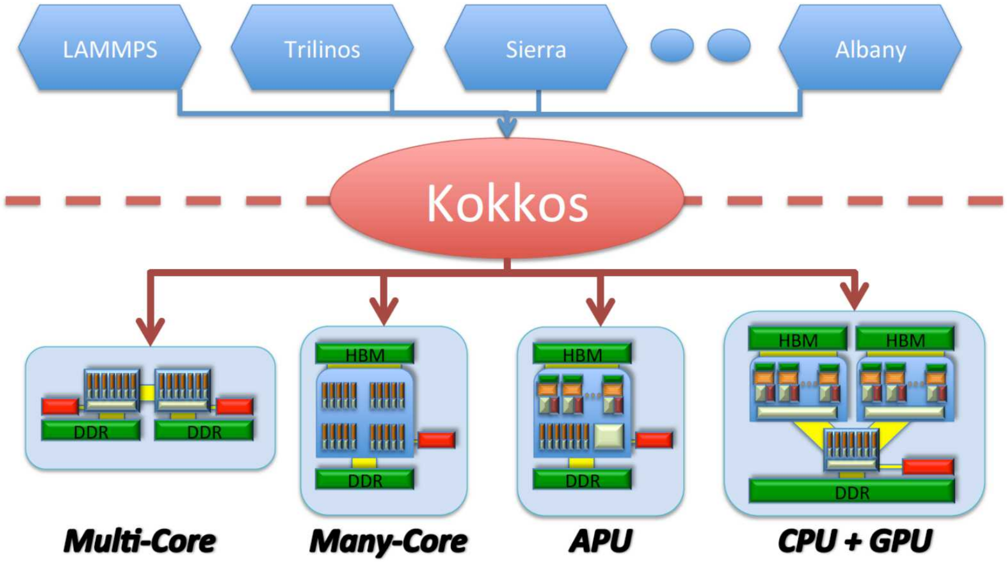


- Approximately 4 particles-per-cell for all grid resolutions
- Particles initialized with random perturbation from structured arrangement
- Errors computed for interior points

# PERFORMANCE

- Global climate simulations are computationally expensive
- Future codes will need to run on DOE next generation computers with heterogeneous architectures
- DEMSI using Kokkos programming model for acceleration

- Shared-memory programming model
- C++ library
- Enables writing algorithms once for many architectures
- Uses multi-dimensional arrays with architecture-dependent layouts

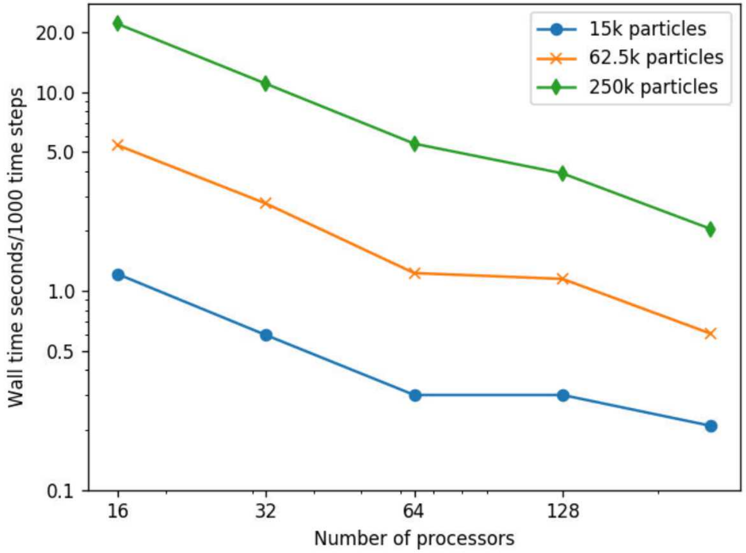



https://github.com/kokkos

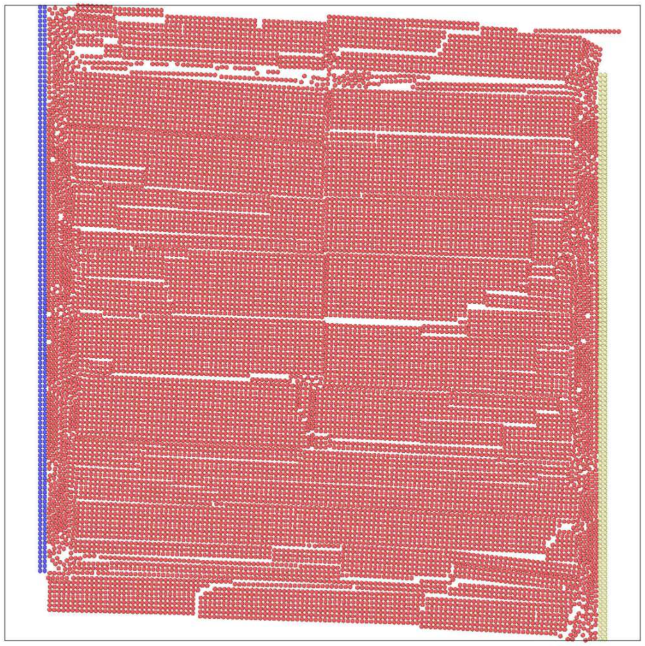
# PERFORMANCE

## Preliminary performance benchmark – MPI only

- Simple shear + compression
- Lattice arrangement of monosized particles
- Need to explore allowable timestep but initial tests suggest competitive
- Future opportunities for performance increase
  - Decrease stiffness for larger time step
  - Kokkos and GPUs




15K particles



# CONCLUSIONS

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

- Ongoing work
  - Continue to improve sea ice contact model
  - Regional and basin-scale testing
  - Test options for element creation and destruction
  - Kokkos implementation and performance testing