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Title: Discrete Element Model for Sea Ice

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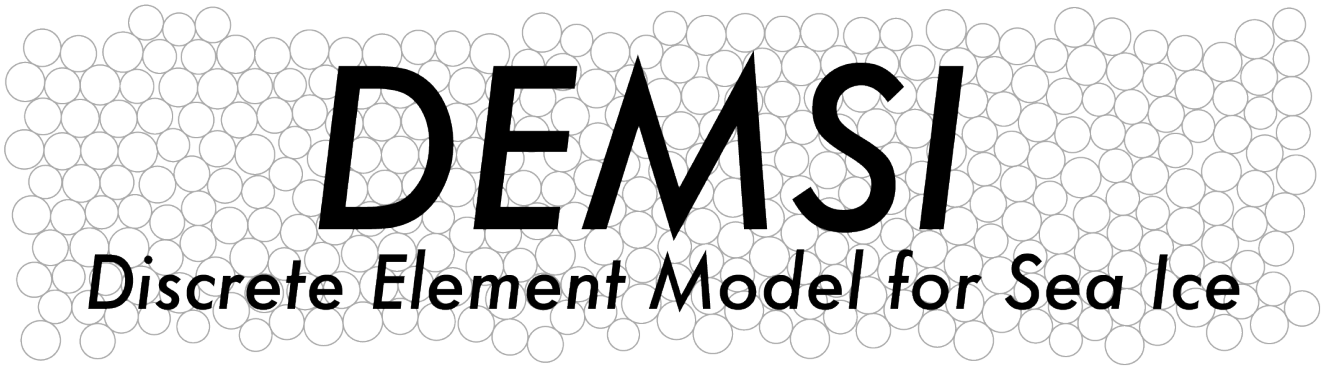
Discrete Element Model for Sea Ice

The DEMSI Team

LANL, SNL, NPS

November 8, 2018

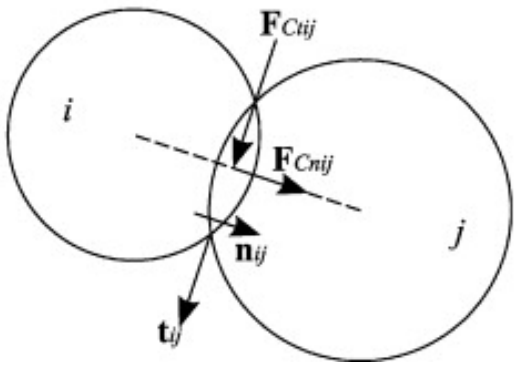


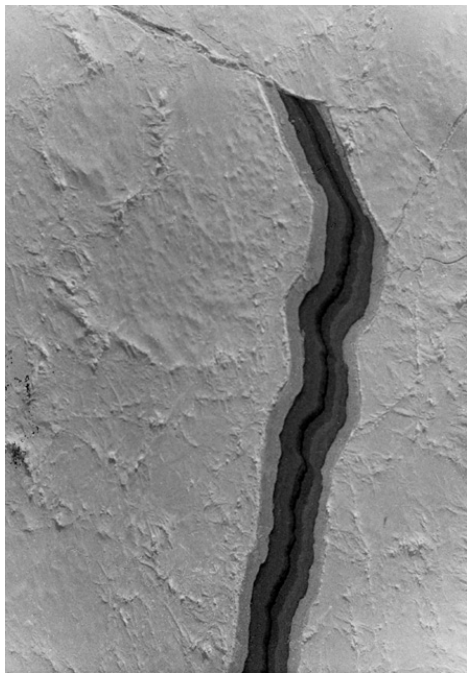
The DEMSI Team

- Los Alamos National Laboratory
  - Adrian Turner (BER PI)
  - Andrew Roberts
  - Min Wang
- Sandia National Laboratories
  - Kara Peterson (ASCR PI)
  - Dan Bolintineaunu
  - Paul Kuberry
  - Dan Ibanez
- Naval Postgraduate School
  - Travis Davis

Discrete Element Method

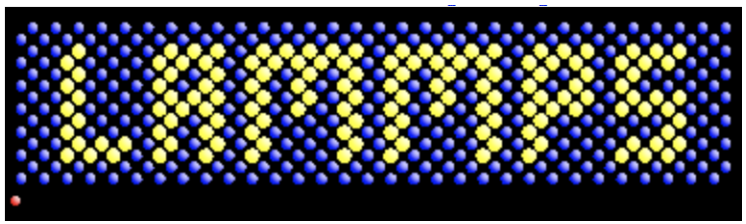
- Regions of sea ice modeled as particles
- Previous models assumed continuous viscous-plastic material – isotropic distribution of leads in grid cell – $\gtrsim$10 km resolution.
- Allows complex physical contact laws, e.g. explicit fracturing
- Project goals:
  - Better utilization of heterogeneous computer architectures
  - Better representation of sea-ice dynamics: spatial/temporal scaling, dispersion, intermittency, heterogeneity, anisotropy





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*: **LAMMPS**
  - SNL 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



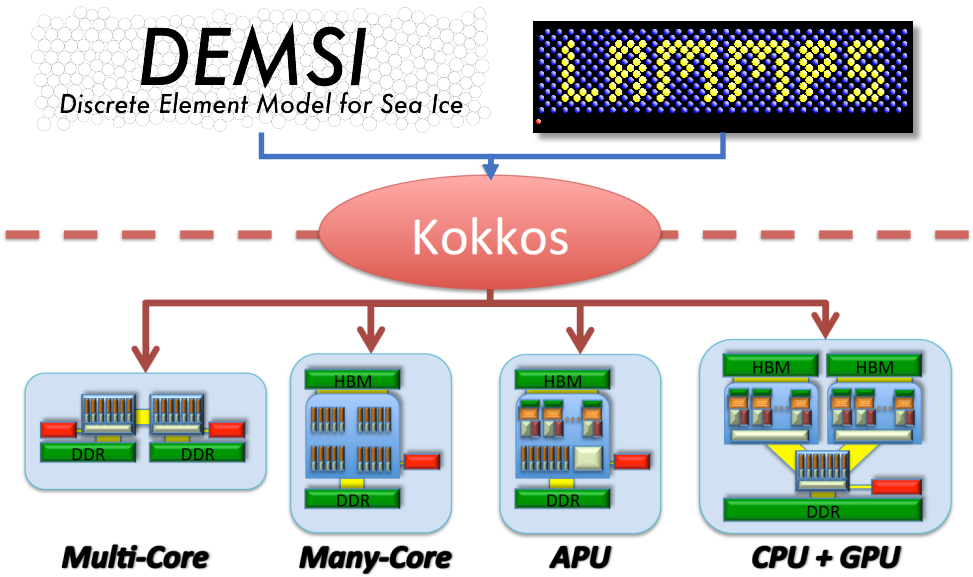
Major Project Challenges

- Performance
- Coupling
- Contact model
- Deformation

Kokkos Acceleration

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

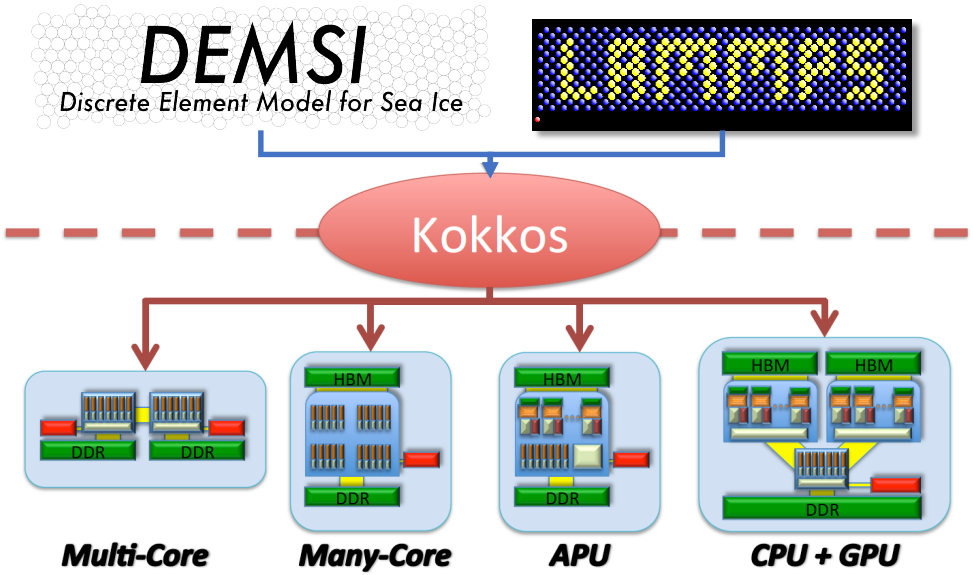
- C++ library
- Shared-memory programming model
- Enables writing algorithms once for many architectures
- Uses multi-dimensional arrays with architecture dependent layouts



https://github.com/kokkos

Current Status

- DEMSI code built using Kokkos data structures
- Currently runs on CPUs and GPUs
- Nearly completed conversion of DEMSI LAMMPS code to Kokkos
- Starting soon on performance optimization



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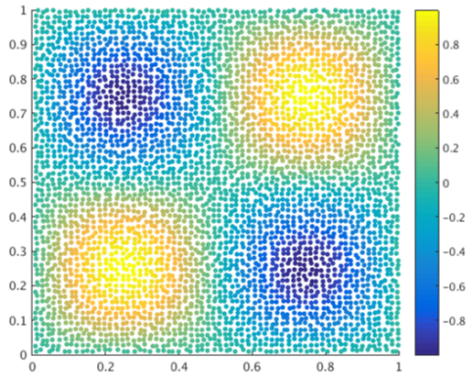
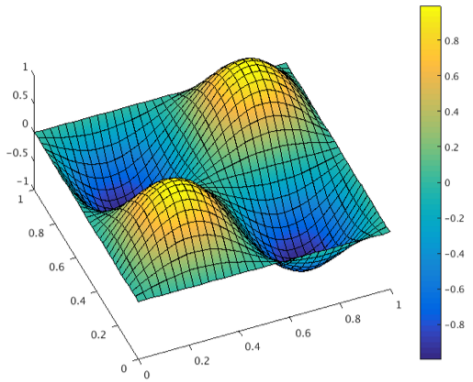
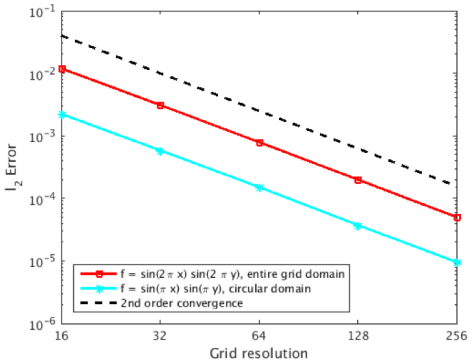
Coupling to Atmosphere/Ocean

- 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

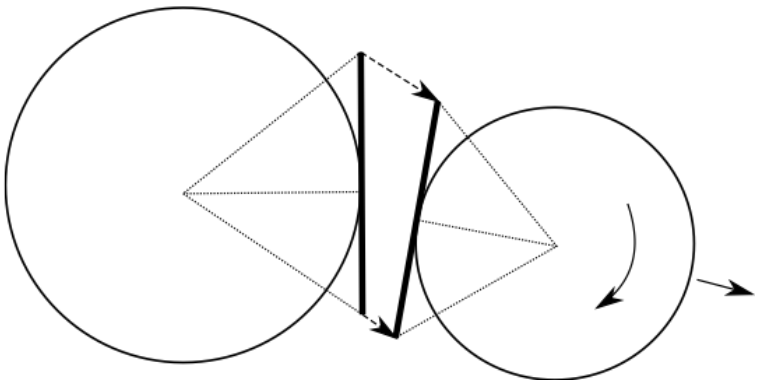


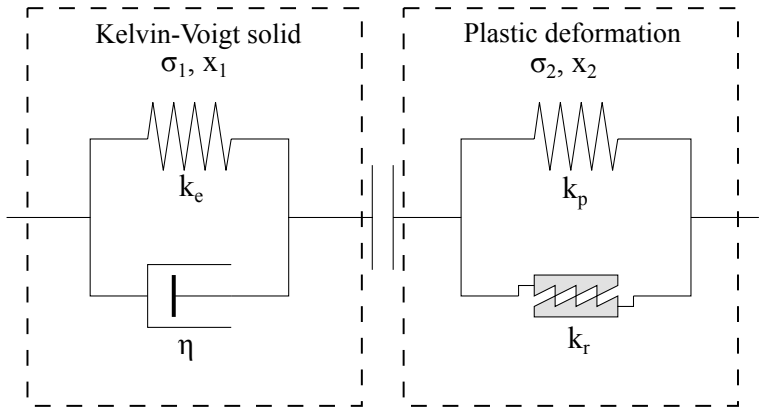




Contact Model

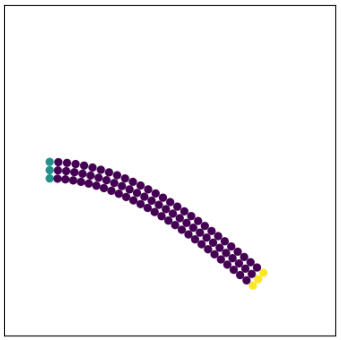
- The element contact model determines the forces between elements in close proximity
- Explicitly represent physical processes
  - Fracturing of bonded elements
  - Ridge formation during ridging
- Initially using contact model developed by Mark Hopkins
- Challenge: how do we determine appropriate contact model for regions of sea ice?



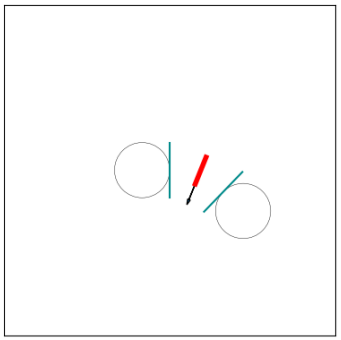


Contact Model Progress

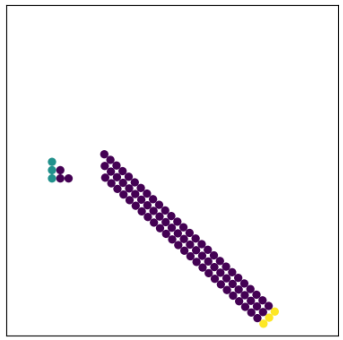
- The history dependence and strength in tension needed special treatment in LAMMPS
- Model verified with the implementation of test cases to demonstrate and test each aspect of the model



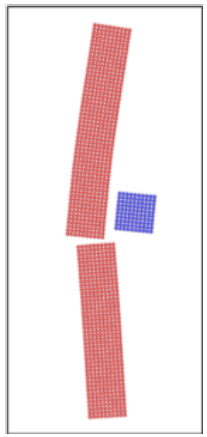
Cantilever no fracture



Two particle fracture



Cantilever with fracture

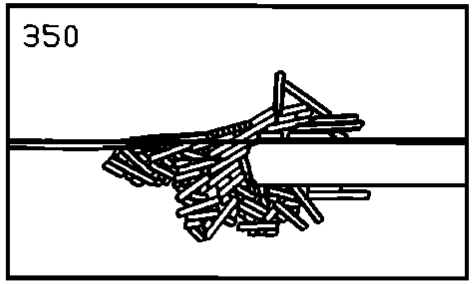


Impact fracture

Further Contact Model Development

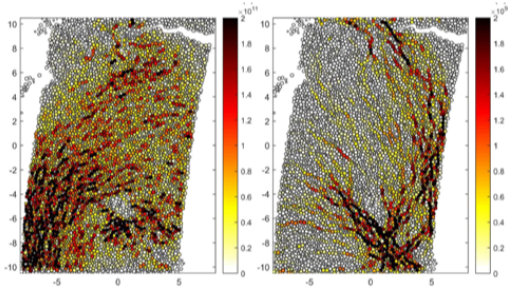
Ridge experiments

Simulations of individual ridges forming



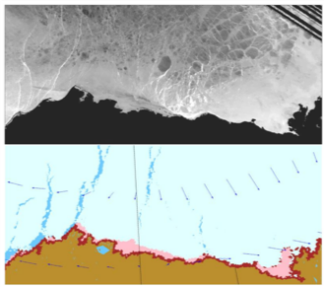
Floe level experiments

Simulations of individual floes



Regional experiments

Simulations of Arctic regions e.g. Barrow, AK

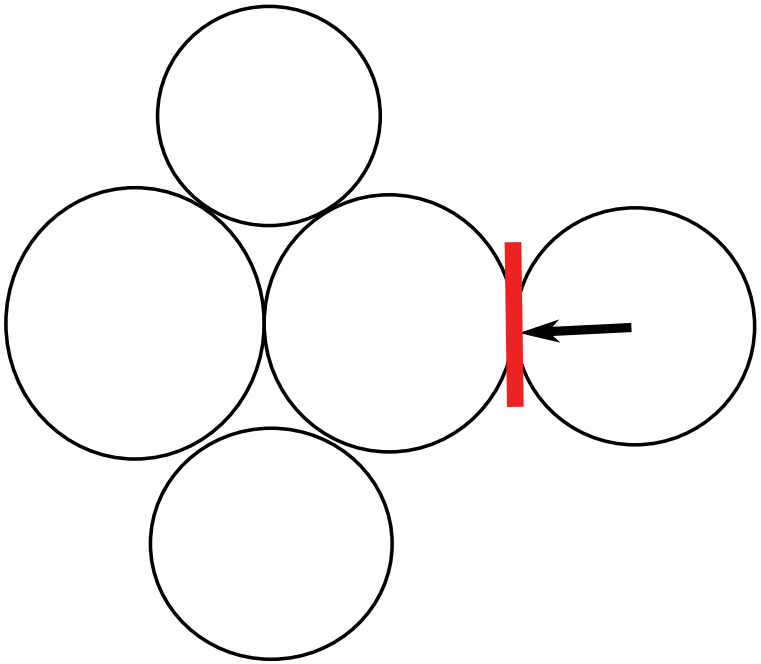


Arctic basin experiments

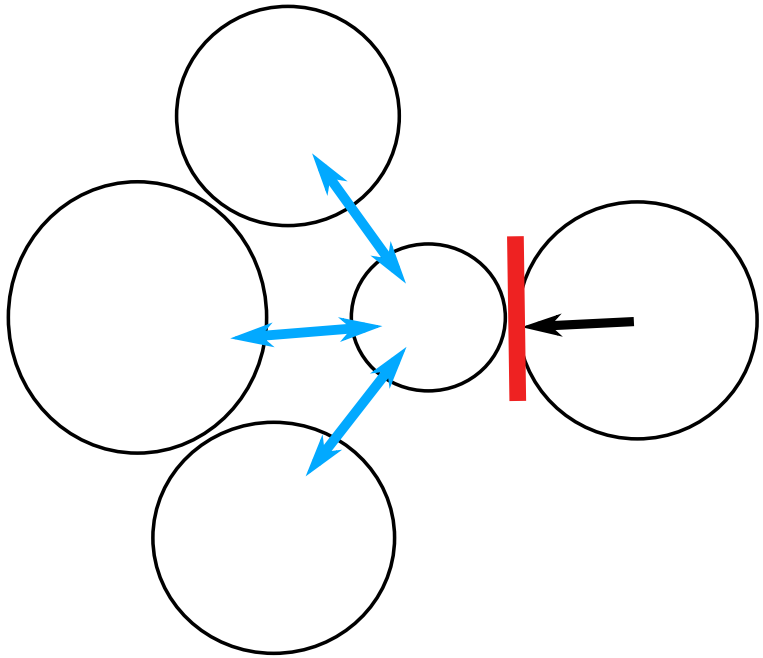
Simulations of Arctic basin

Element deformation

- 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



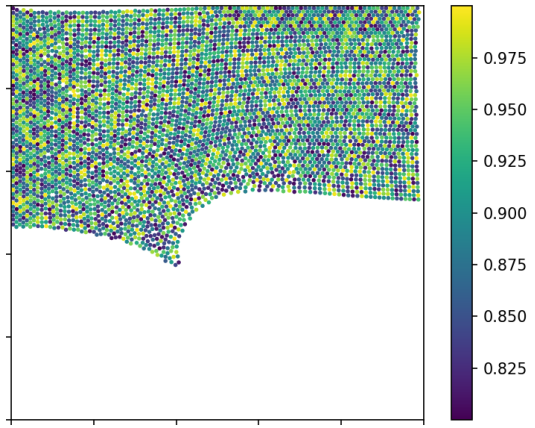
Convergence and ridge formation of two elements in pack



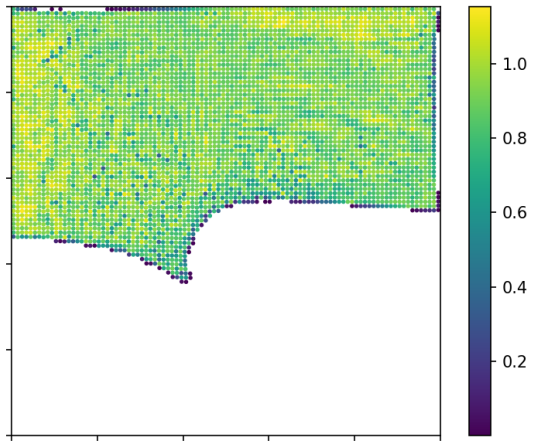
Shrinking of element adds strain to the pack

Element Deformation Solution

- Periodic global remapping of the element distribution back to some "good" initial distribution.
- Initial geometric implementation
  - Circular elements represented as regular polygons
  - Radial Voronoi tessellation of initial distribution (accounts for element radius)
  - Intersection area determined - conserves to machine roundoff
- Will switch to MLS coupling method
- Orientation of bond properties needs to be preserved in remapping



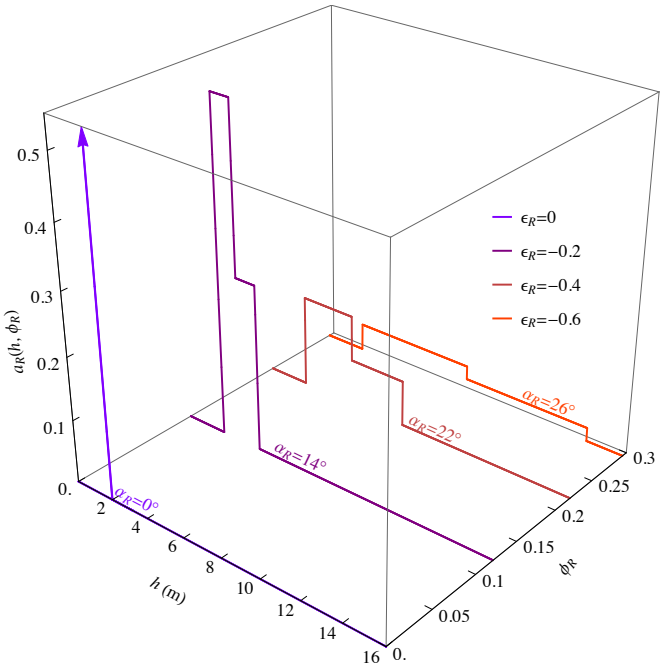
Particle distribution before remapping



Particle distribution after remapping

Variational Morphology

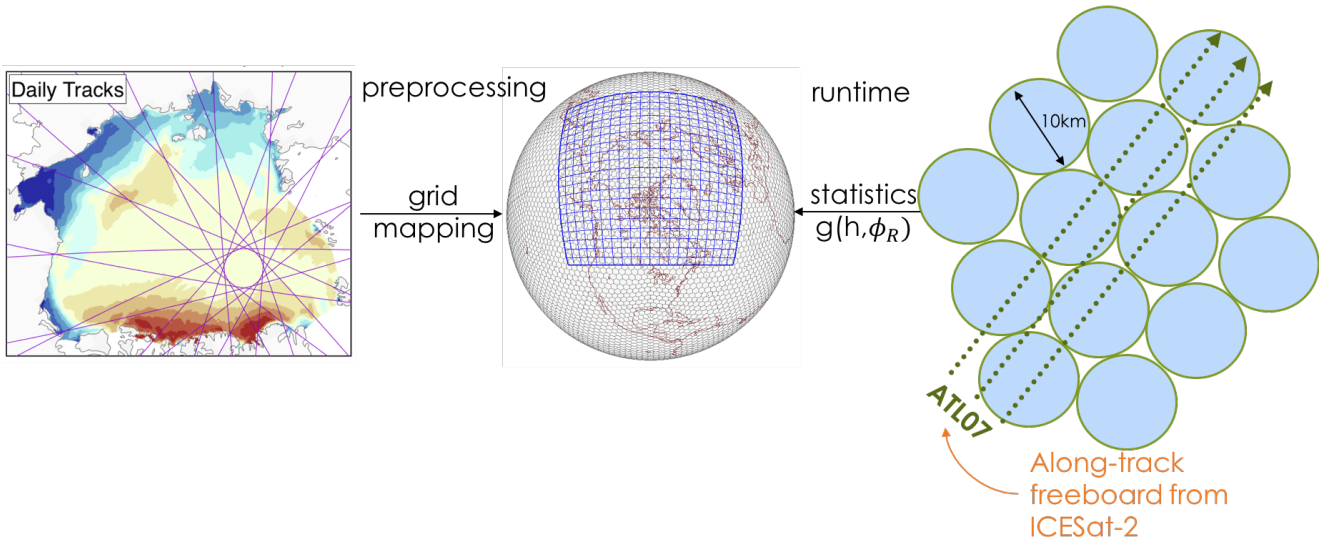
- We will also include recent work to develop a new variational based ice morphology scheme (*Roberts et al. 2018*) to improve the representation of ridging in the model.
- Important for improving coupling
  - Allows better representation of ice roughness - momentum coupling
  - BGC infiltration into porosity
  - Affects snow (albedo) distribution through build up next to ridges
- Porosity affects ice strength - important for navigation



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

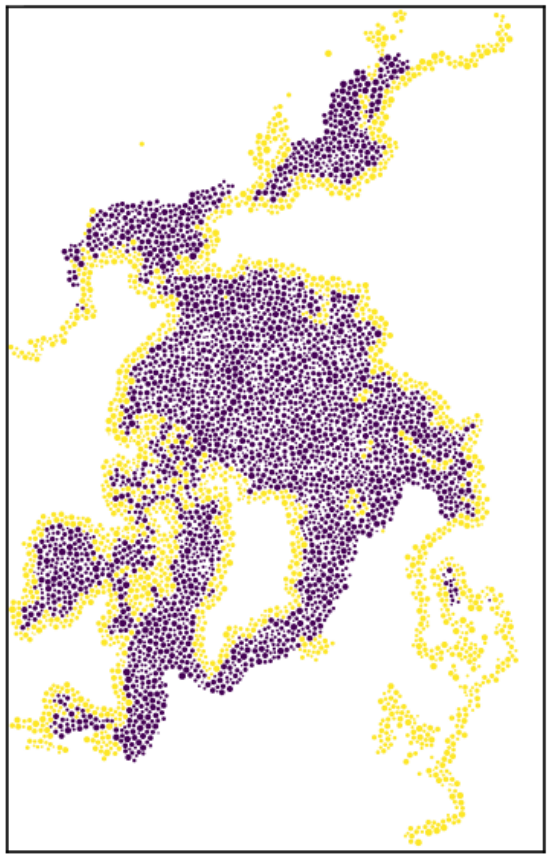
Model validation metrics

- Will be developing metrics to access the physical fidelity of the dynamics:
  - Spatial and temporal scaling of deformation
  - Dispersion of particles initially close together (compare to buoys)
  - Satellite emulator of ICESat-2 and statistically correct comparison with model ice freeboard

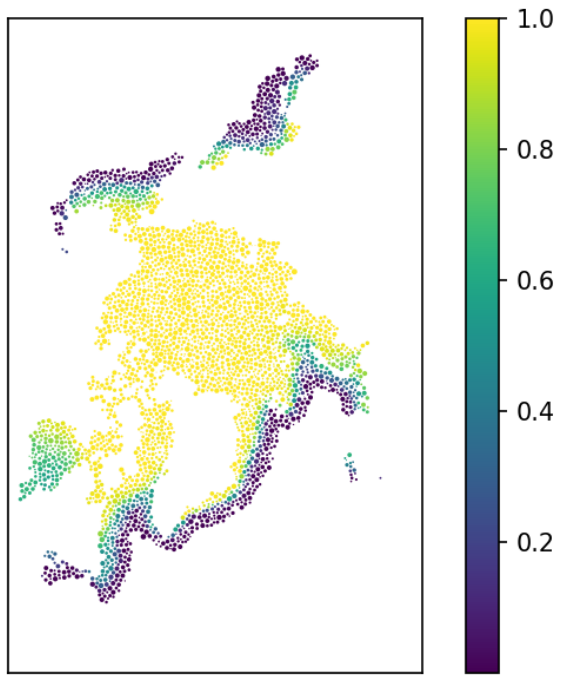


Arctic basin simulations

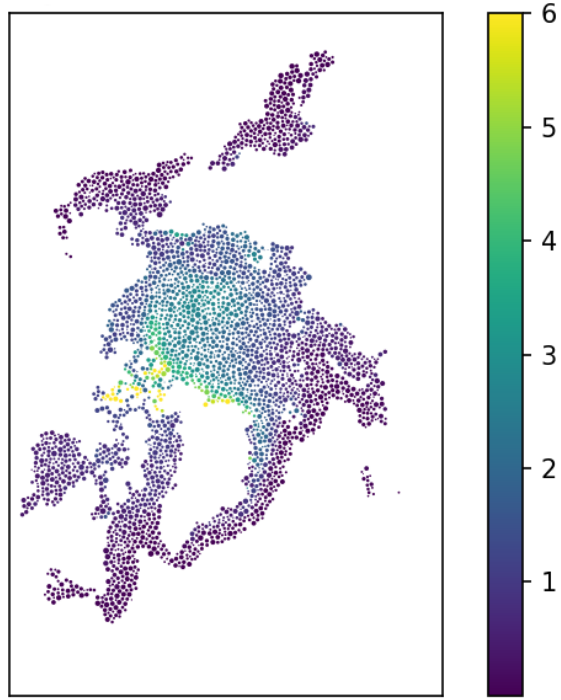
Plan to begin Arctic basin scale simulations soon - already have process to make initial conditions



Element type with coasts



Ice concentration



Ice thickness