Some future cryosphere modeling directions at DOE

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Overview

- Unexhaustive look at some future cryosphere modeling directions at DOE
- Changing computing environments – the rise of heterogeneous computing architectures
- **MPAS-Seaice** – Unstructured sea ice model
- **E3SM** – ESM for DOE mission
- **DEMSI** – Feasibility of discrete element sea-ice model for global climate applications

Future DOE computing environments

- Future (and some current!) DOE machine will be heterogeneous
- **Summit**
  - Oakridge National Lab GPU based machine
  - 27,000 NVIDIA Volta GPUs / 9,000 IBM Power9 CPUs
  - ∼98% compute on GPU!

- **Aurora**
  - Future Argonne National Lab. supercomputer
  - Intel Knights Hill Phi Multicore architecture

- Both machine designed for machine learning
- Future DOE models will need to run effectively on GPUs/KHs

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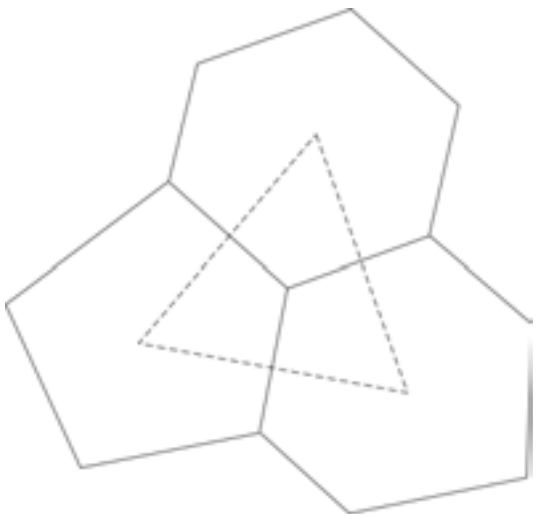
Heterogeneous computing models

- Several programming models being developed to aid heterogenous computing e.g.
  - **Kokkos:** provides abstractions to allow a single implementation of an application to run efficiently on different kinds of hardware
  - **Legion:** Exposes more parallelism through task based parallelism
- Expect to move from Fortran to C++
  - Utilize programming models
  - Availability of good compilers

MPAS-Seaice

- Recently developed unstructured mesh sea-ice model
- Uses Modeling for Prediction Across Scales (MPAS) framework
  - Uses Spherical Centroidal Voronoi Tesselation (SCVT) mesh
- Leverages CICE Consortium Icepack library – same column physics as CICE
- Dynamics of CICE adapted to polygonal elements
- Sea ice component of the DOE Energy Exascale Earth System Model (E3SM)

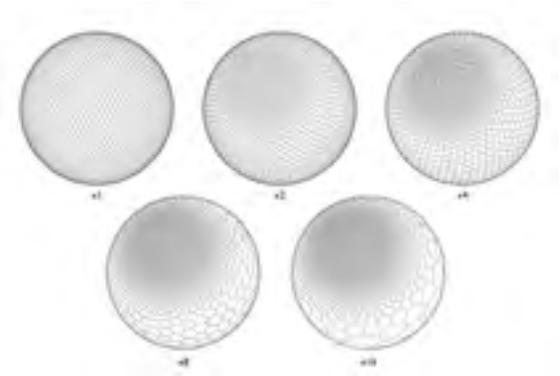
MPAS
Model for Prediction Across Scales



MPAS mesh detail with primary and dual mesh

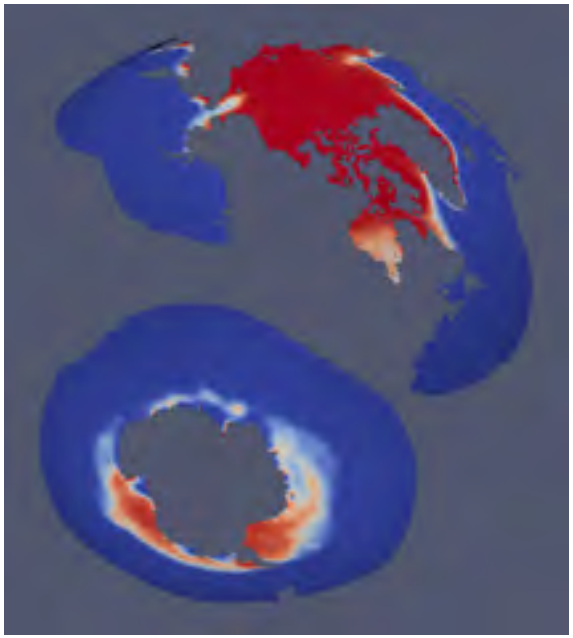
MPAS-Seaice

- MPAS mesh allows variable resolution – focus computational resources in region of interest without lateral boundaries
- Better domain flexibility – remove computationally wasteful equatorial region
- Flexibility in domain decomposition – improved load balancing

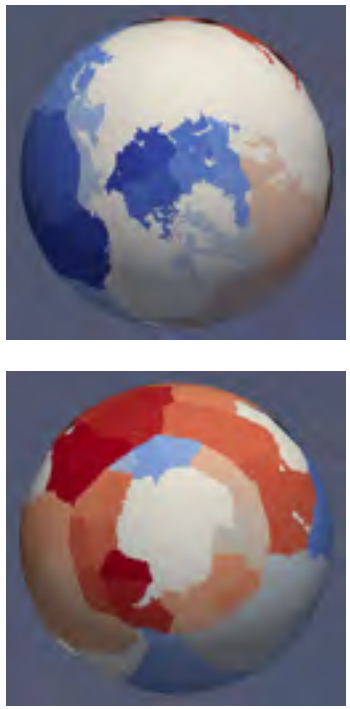


Progressive mesh refinement

North American refined mesh



Two polar cap domain



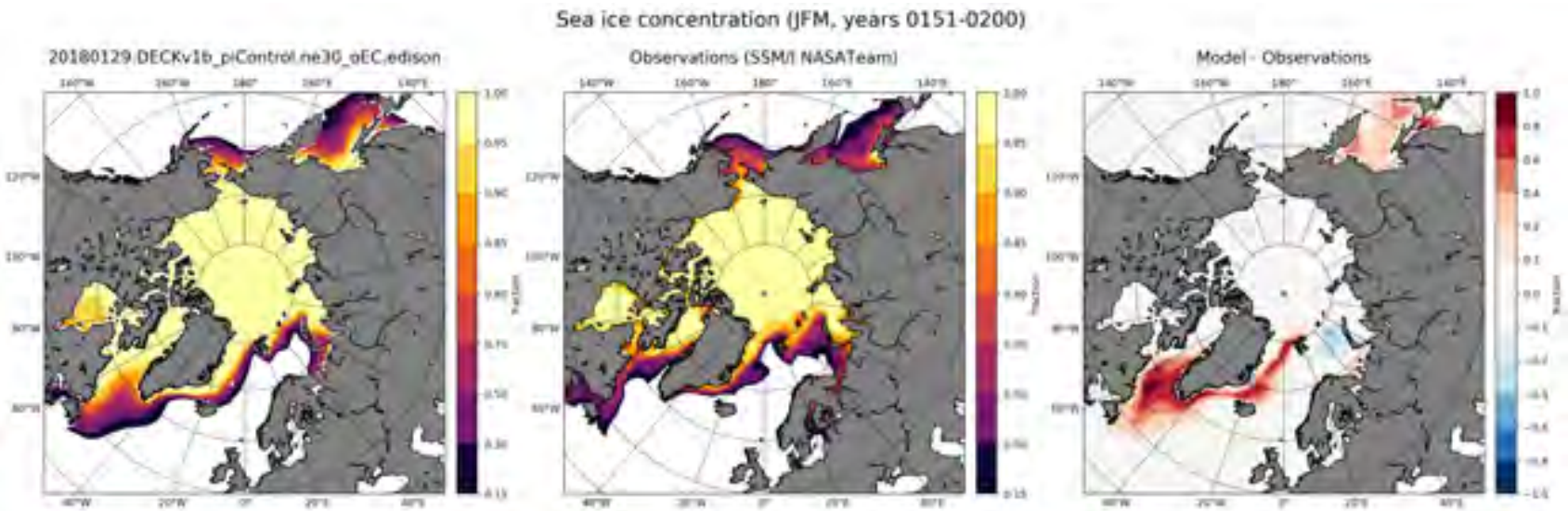
Domain decomposition with sea-ice load balancing

Energy Exascale Earth System Model (E3SM)

- **E3SM** – DOE Earth system model (forked from CESM)
  - Optimized for DOE mission (e.g. SLR (Coastal infrastructure), US drought (water availability for power plants))
  - High- and variable-resolution emphasized (high res. sims: 6km in Arctic for ocean/sea ice)
  - Work done to optimize for new DOE heterogeneous architectures
- Initial focus on three main science questions:
  - **Water cycle:** "How will more realistic portrayals of features important to the water cycle (clouds, aerosols, snowpack, river routing, land use) affect simulations of river flow and associated freshwater supplies at the watershed scale?"
  - **Cryosphere:** "What are the impacts of ocean-ice shelf interactions on melting of the Antarctic Ice Sheet, the global climate, and sea level rise?
  - **BGC:** "What are the effects of nitrogen and phosphorous on climate-biogeochemistry interactions, and how sensitive are these interactions to model structural uncertainty?"

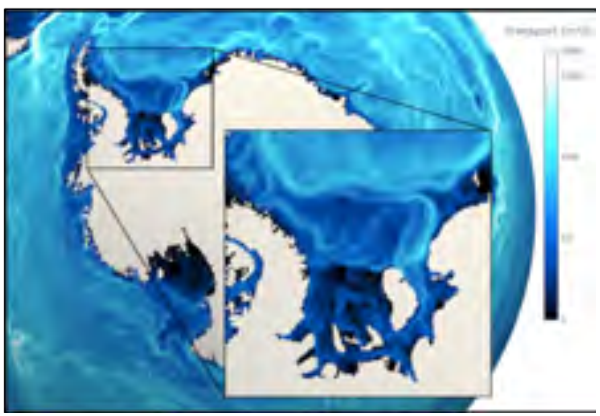
Sea-ice in E3SM

- MPAS-Seaice coupled as sea ice component
- Started assessment of sea ice in simulation output
  - Lower res simulations have excessive sea ice in Labrador sea
  - High res simulations have warm bias in Arctic
- MPAS-Seaice struggles to scale to sufficient number of processors on Cori-KNL for high-res
  - Exploring deactivation of equatorial cells to improve performance (Sea ice and ocean required to have same mesh)

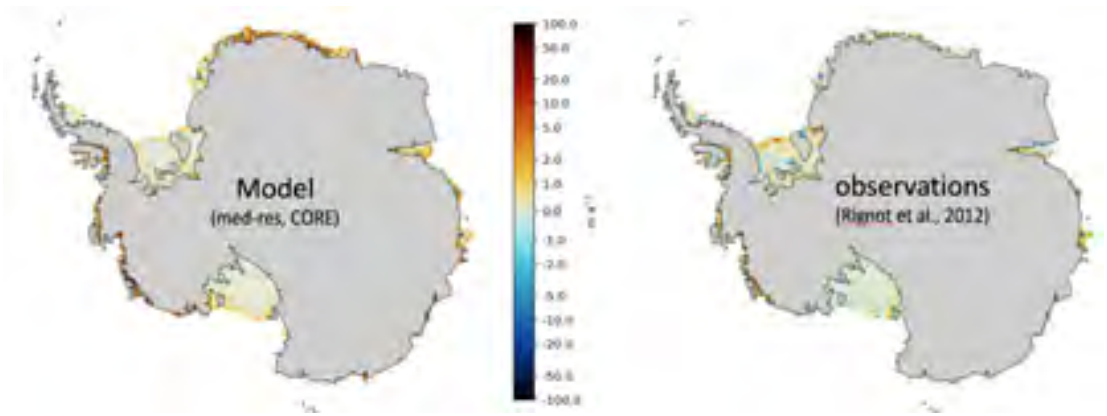


Under shelf cavities (Xylar Asay-Davis, Mark Peterson)

- Under ice-shelf cavities have been added to E3SM
- Allow simulation of ice shelf melt from warm water intrusion
- Work ongoing to assess under shelf melt rates



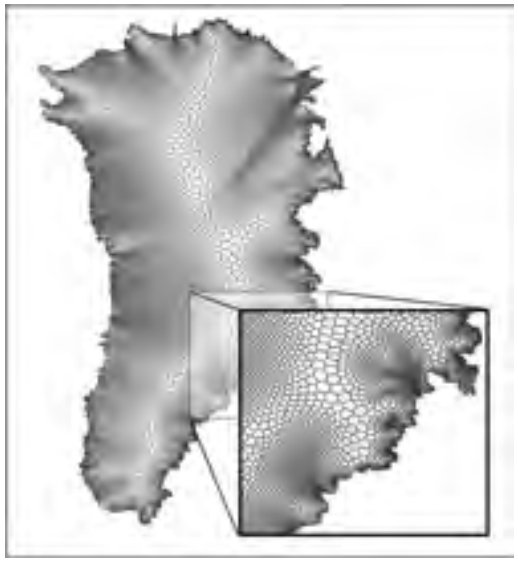
Flow under ice shelves around Antarctica



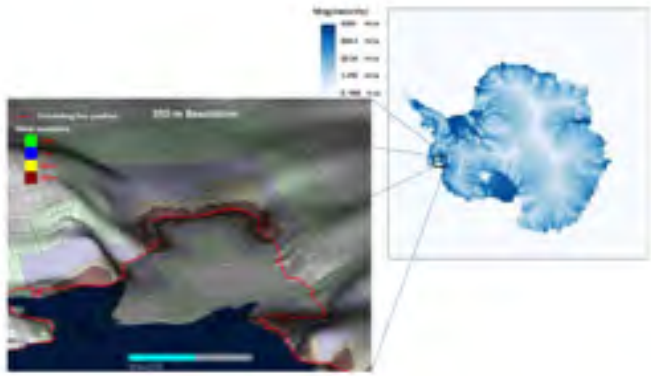
Under shelf melt rates in E3SM compared to observations

Dynamic ice-sheet modeling

- DOE developing two ice sheet models for climate applications
- **MPAS-Albany Land Ice (LANL/SNL)**:
  - MPAS mesh using the Albany FE/Trilinos solver
  - Uses variable resolution meshes for performance
  - Uses Kokkos programming model for use on heterogeneous architectures
  - Includes adjoint capability for initialization
- **Bisicles (LBL)**:
  - Adaptive mesh refinement with Chombo framework



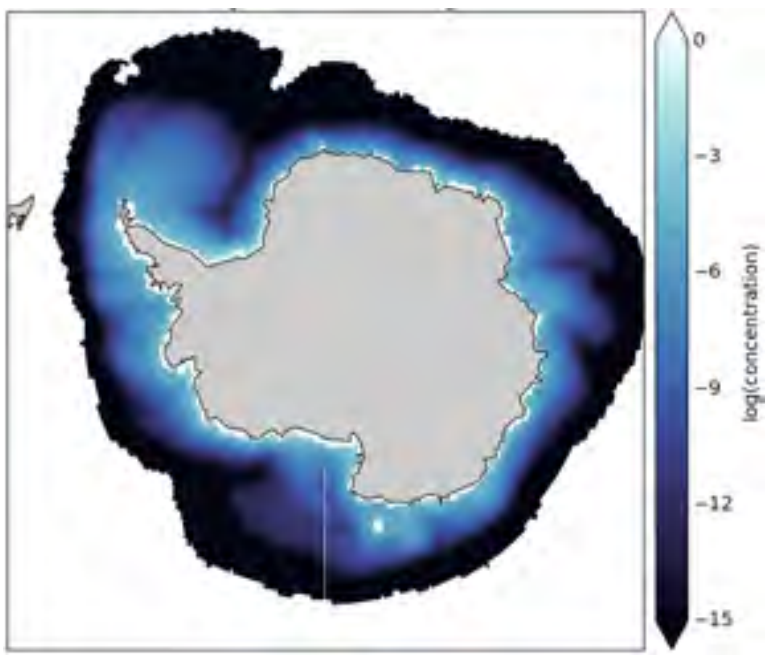
MALI Greenland variable resolution mesh



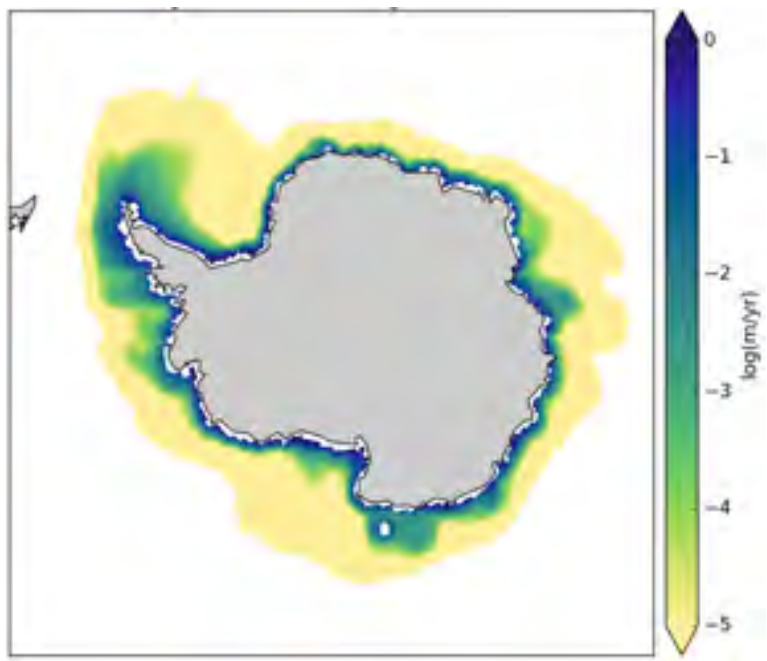
Detail of adaptive mesh around grounding line in Bisicles

Icebergs (Darin Comeau)

- Icebergs represent about half of the mass flux from Antarctica to the Southern Ocean
- Eulerian based iceberg model has been added MPAS-Seaice – direct interaction with sea ice
- Is being coupled into E3SM – will perform fully coupled simulations
- Hope to improve Southern Ocean stratification and circulation

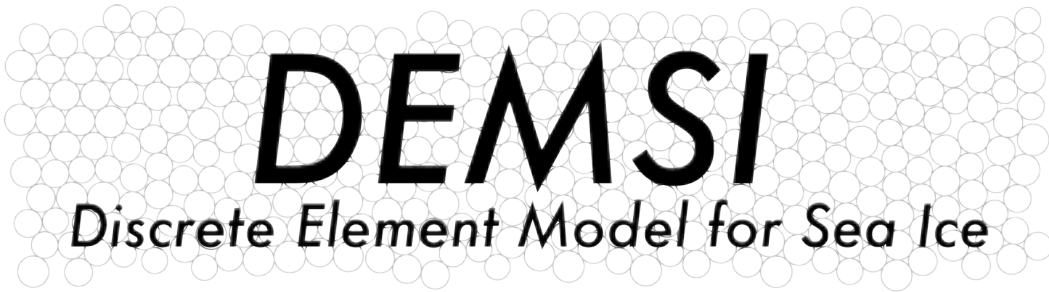


Iceberg area fraction



Iceberg fresh water melt flux

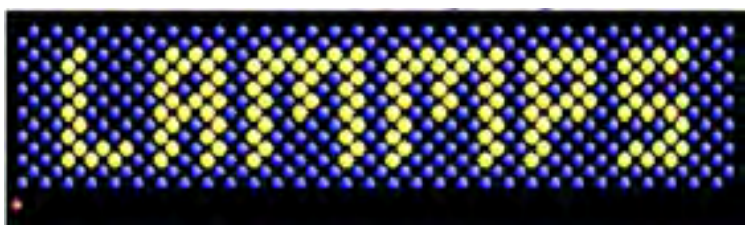
DEMSI: Discrete Element Model for Sea Ice (LANL/SNL)



- Joint DOE Advanced Scientific Computing Research (ASCR) / Biological and Environmental Research (BER) project
- Explore challenges to create a Discrete Element Based sea ice model for global climate applications
- Ultimately want to use it as the sea-ice component of E3SM
- Objectives:
  - Better utilize future heterogeneous computing architectures
  - Improved representation of sea-ice dynamical processes - intermittency, anisotropy, heterogeneity
- Particle based method where circular elements represent regions of sea-ice with ice thickness distribution

DEMSI

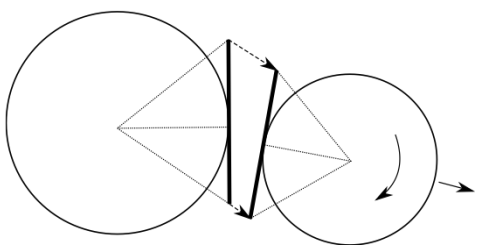
- DEMSI leverages two pre-existing model libraries
- *Dynamics*: **LAMMPS**
  - SNL particle based molecular dynamics code
  - Built in support for DEM methods including history dependent contact models
  - Computationally efficient with massive parallelization
- *Thermodynamics*: **CICE consortium Icepack library**
  - State-of-the-art sea-ice thermodynamics package
  - Vertical thermodynamics, salinity, shortwave radiation, snow, melt ponds, ice thickness distribution, BGC



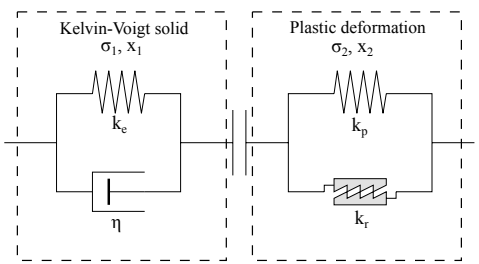
CICE Consortium

Major challenges: contact model

- The element contact model determines the forces between elements in close proximity – sea-ice dynamics
- Explicitly represent physical processes
  - Fracturing of bonded elements
  - Ridge formation during ridging
- Initially using modified version of contact model developed by Mark Hopkins
- Also researching new contact models with hierarchy of models: Individual ridge, Floe scale, Process

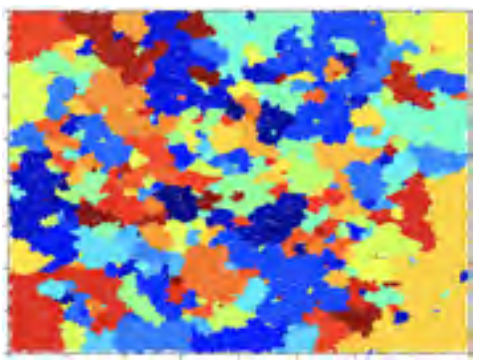


Linear bond between two elements



Plastic deformation for unbonded elements

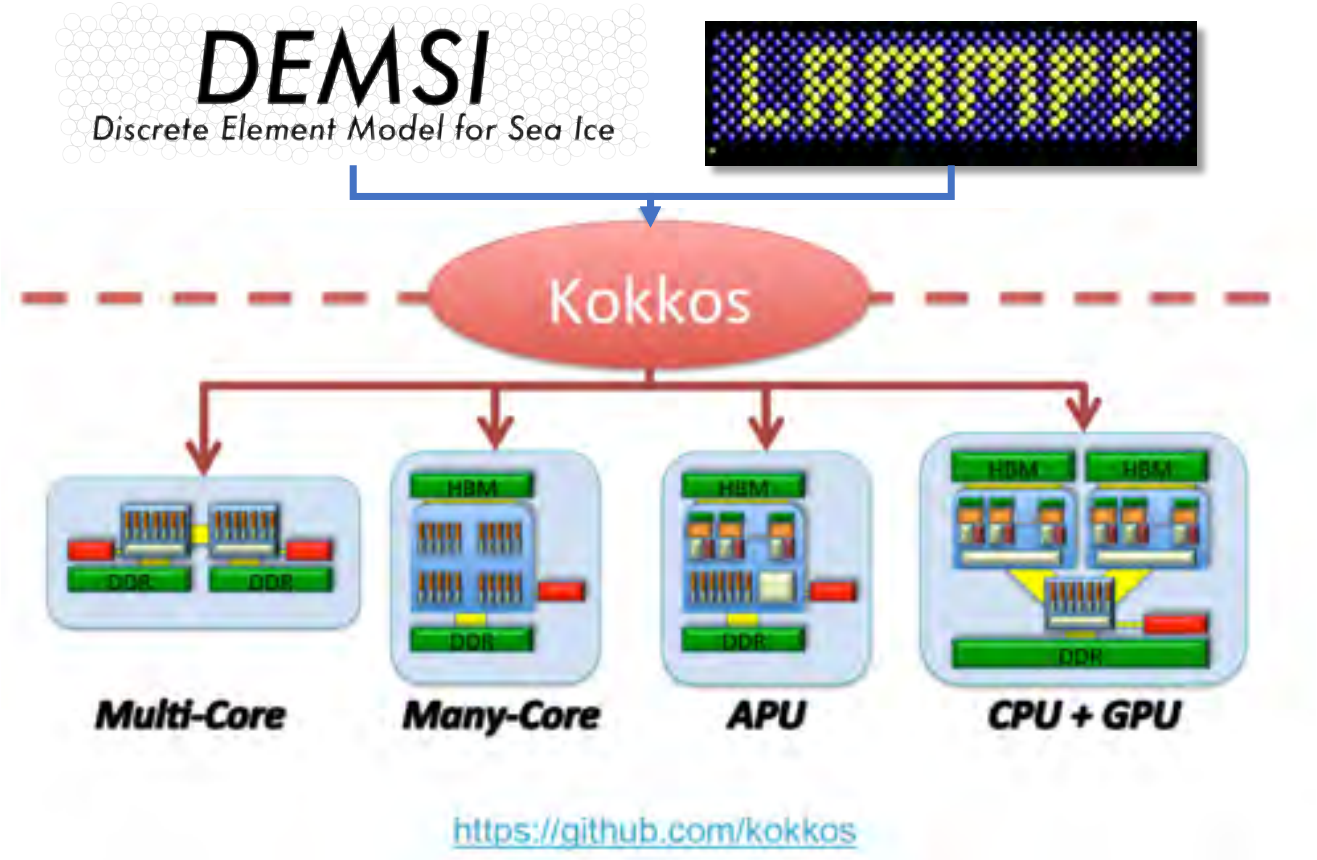
Cantilever test case



Break up of pack in idealized constant stress experiment

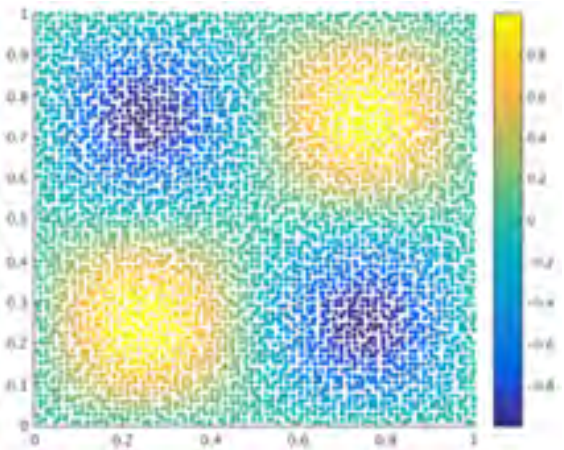
Major challenges: Performance

- Added Kokkos support to LAMMPS for DEM part
- Performance testing has begun
- Optimize DEM algorithms for DEMSI soon

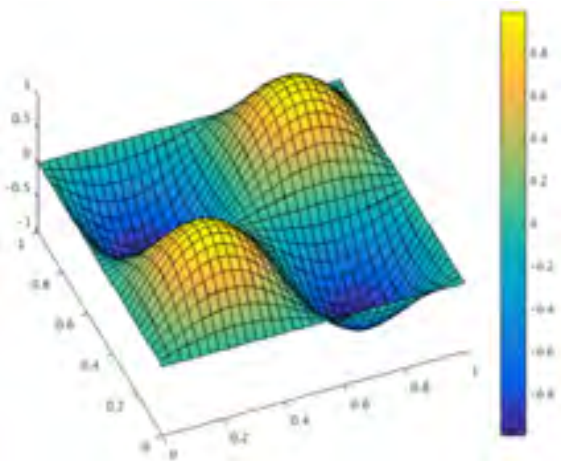


Major challenges: Coupling

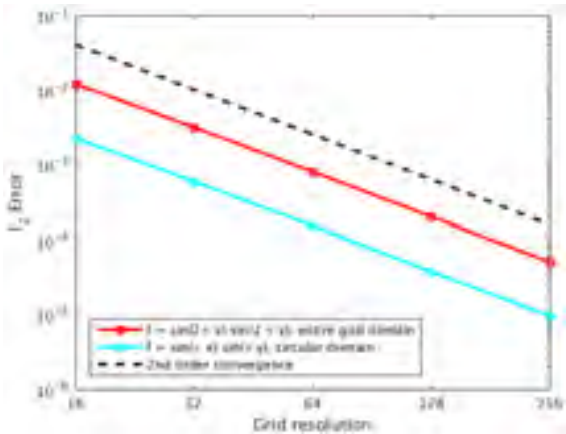
- Need to couple from particles to Eulerian mesh
- Implemented a moving least squares method
- Developing optimized version for conservation



Trial particle distribution



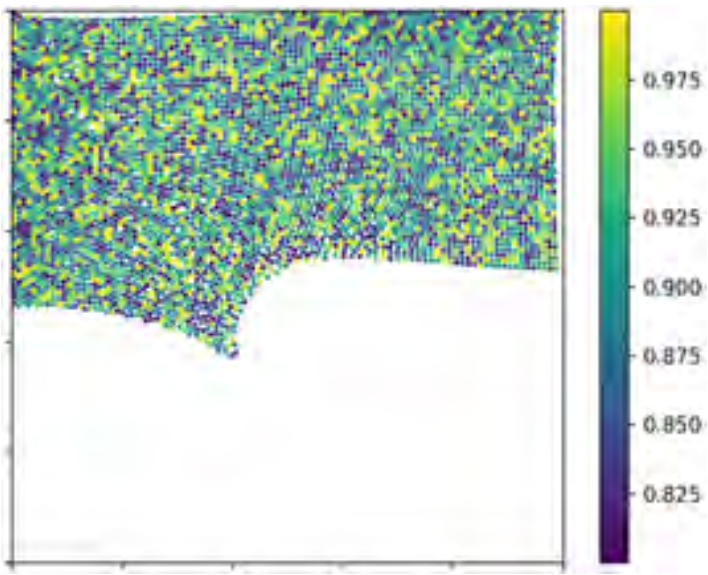
Interpolated function



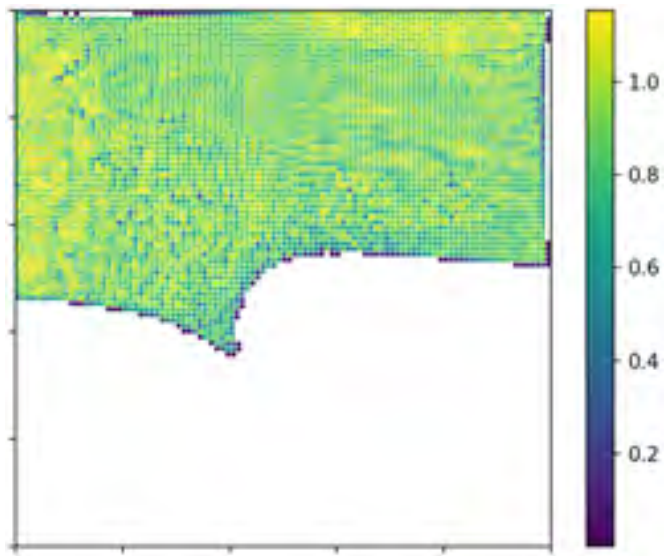
Convergence of coupling system

Major challenges: Deformation

- Convergence of sea ice produces pressure ridges – ice area converted to thickness while volume conserved
- Elements need to get smaller – decreases allowable time step, add artificial strain to the pack
- Investigating periodic global remapping back to an initial "good" distribution
- Orientation of bond properties needs to be preserved in remapping



Particle distribution before remapping



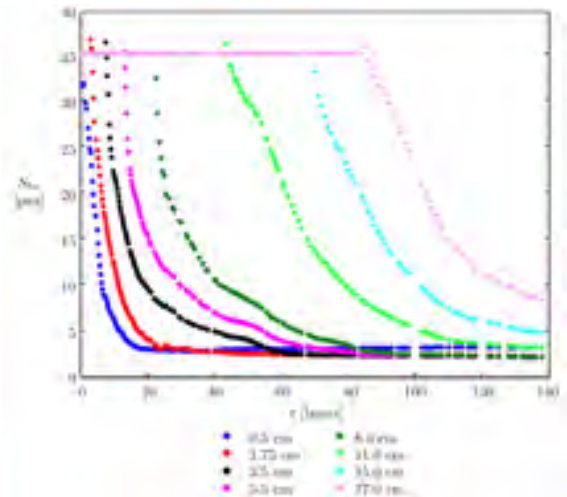
Particle distribution after remapping

Improved observations

- Improved meltpond measurements (basin scale and in situ)

- Improved in-situ observations of gravity drainage

Wire harp instrument (D. Notz)



Desalination of sea-ice during gravity drainage (D. Notz)