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DEMSI
Discrete Element Model for Sea Ice

Methods for Coupling a Lagrangian Discrete Element Sea Ice Model to an Eulerian Ocean Model



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MS731 Advances in Rigorous and Agile Coupling of Conventional and Data-Driven Models for Heterogeneous Multi-Scale, Multi-Physics Simulations

SciDAC
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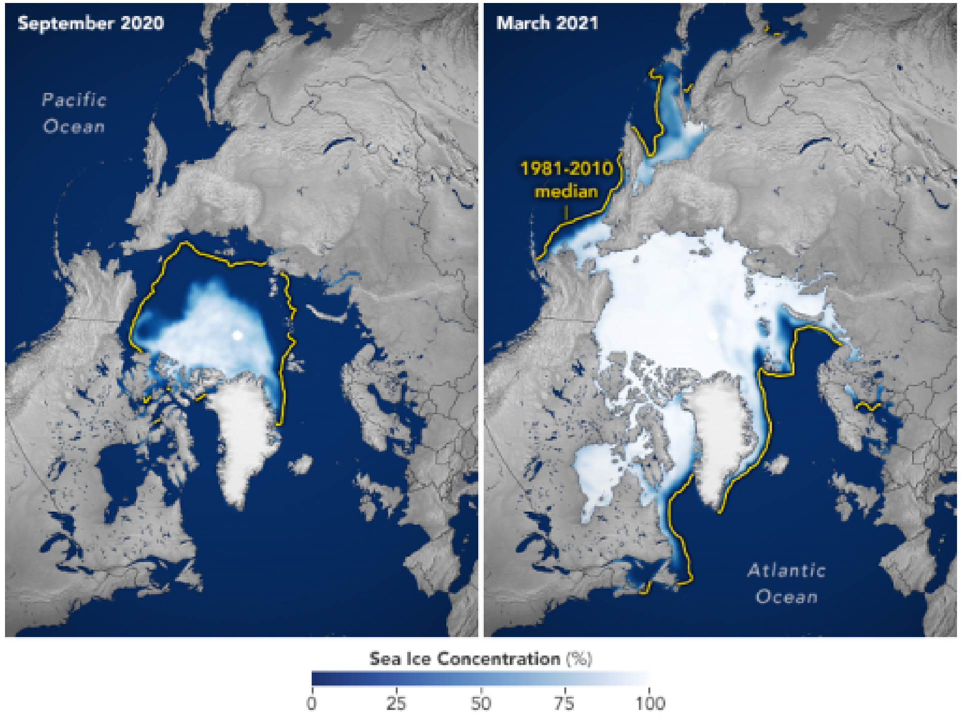
SEA ICE IN THE EARTH SYSTEM

Importance in global climate

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

Sea ice models must capture

- 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

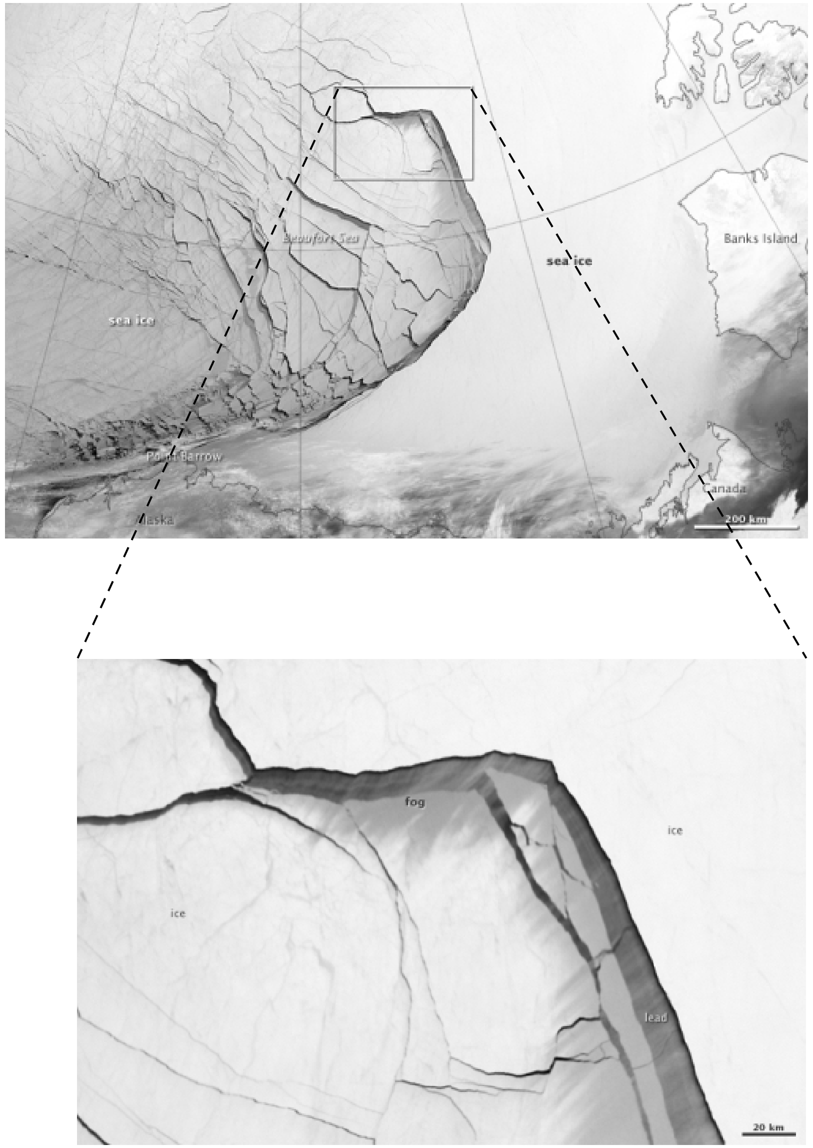


NASA Earth Observatory images by [Joshua Stevens](), using data from the [National Snow and Ice Data Center]().

SEA ICE MODELING

- Most sea ice models in coupled Earth system models use a continuum formulation (Turner et al. 2022, Rampal et al. 2016)
- At high resolutions (~5-6 km) isotropic continuum models do not approximate the dynamics well
- Discrete element method
  - Lagrangian particles
  - Captures anisotropic, heterogenous nature of sea ice deformation
  - Explicit fracture and break-up of pack
- Previous DEM sea ice modeling efforts focused primarily on regional scale, short-term simulations (Hopkins 2004)

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



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

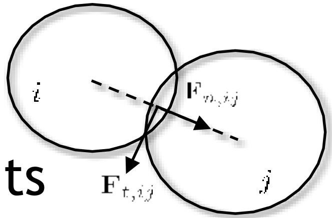
DISCRETE ELEMENT MODEL FOR SEA ICE (DEMSI)

Dynamics: Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Thompson et al. 2022)

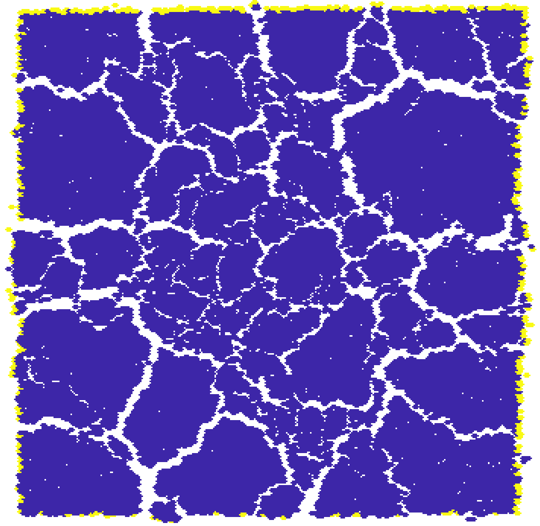
- Particle based molecular dynamics code
- Includes support for DEM and history dependent contact models

Thermodynamics: CICE Consortium Icepack Library (Hunke et al. 2018)

- State-of-the-art sea-ice thermodynamics package
- Includes vertical thermodynamics, salinity, shortwave radiation, snow, melt ponds, ice thickness distribution, biogeochemistry



- Dynamics are computed using circular Lagrangian elements
- Interactions via contact forces for bonded and unbonded elements
- Enables capture of complex anisotropic deformation and fracture



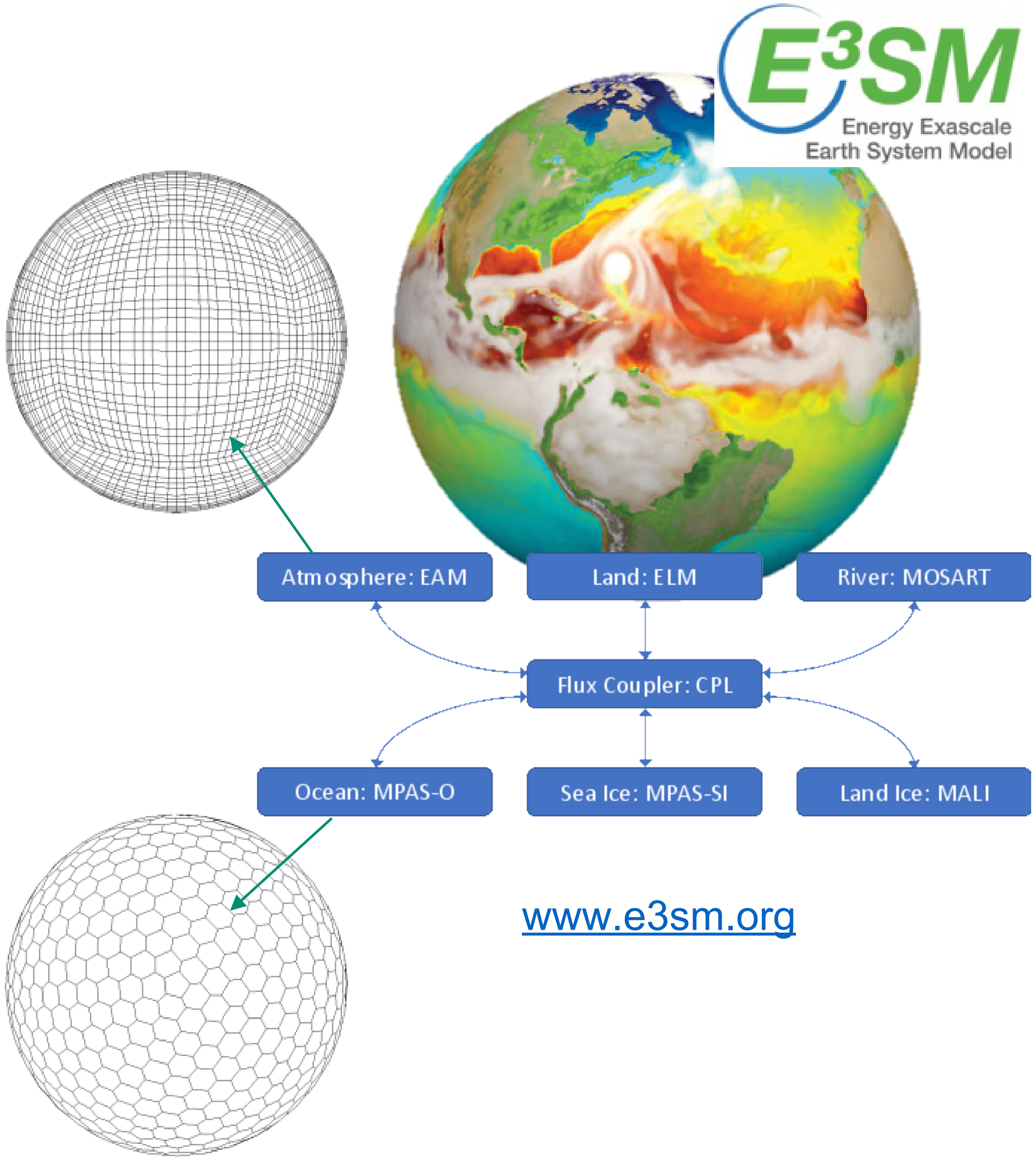
INTERPOLATION & REMAP IN DEMSI

Coupling with ocean and atmosphere models

- DEMSI under development for the Energy Exascale Earth System Model (E3SM)
- Requires interpolation between Lagrangian particles and Eulerian grids
- Work to incorporate unstructured Voronoi grid in DEMSI is ongoing

Particle-to-particle remap

- Periodic remap to initial particle distribution to manage large deformations and particle clustering
- Provides method for adding new particles due to thermodynamic growth

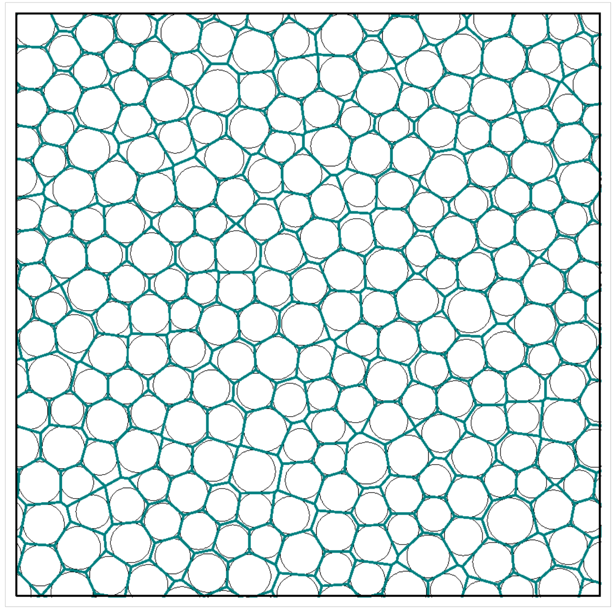


www.e3sm.org

REPRESENTATION OF SEA ICE IN DEMSI

Each circular discrete element particle represents a region of ice with varying thickness including open water

- Ice thickness distribution, k thickness categories
  - Ice concentration (c) in each category
  - Thickness (h) in each category
- Vertical levels for ice thermodynamics
  - Ice enthalpy (q) in each vertical layer (l) and category (k)
- Use an effective particle area (e)
  - Defined by Voronoi tessellation of particles
  - Provides a method to define conserved quantities covering the domain



REQUIREMENTS FOR REMAP/INTERPOLATION ALGORITHMS

- Conservation
  - Need to conserve area, volume, energy, and fluxes
- Bounds preservation or monotonicity
  - No new extrema generated by the remapping algorithm
- Accuracy
  - Want at least 2nd -order accuracy
- Compatibility
  - Consistency between primitive tracer fields and conserved variables

Conserved Quantities

Total ice area per thickness category

$$\mathcal{A}_k = \sum_i e_i c_{ik}$$

Total ice volume per thickness category

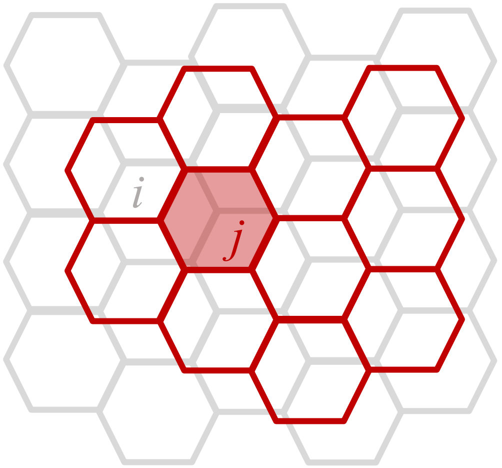
$$\mathcal{V}_k = \sum_i e_i c_{ik} h_{ik}$$

Total ice energy per thickness category and layer

$$\mathcal{Q}_{kl} = \sum_i e_i c_{ik} h_{ik} q_{ikl}$$

GEOMETRIC REMAP STEPS

1. Determine overlap polygons and remap effective element area
2. Compute linear reconstructions of average tracer fields
3. Integrate conserved variable reconstructions over intersection polygons
4. Enforce bounds preservation using flux correction



$$e_j = \sum_i e_{ij} = \sum_i \frac{A_{P_{ij}}}{A_{P_i}} e_i.$$

Turner, *et al*. GMD 2022

GEOMETRIC REMAP STEPS

1. Determine overlap polygons and remap effective element area
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Mean-preserving reconstructions (Lipscomb and Hunke 2001)

$$c^p(\mathbf{r}) = c + \alpha_c \nabla c \cdot (\mathbf{r} - \bar{\mathbf{r}})$$

$$\bar{\mathbf{r}} = \frac{1}{A} \int_A \mathbf{r}\, dA,$$

$$h^p(\mathbf{r}) = h + \alpha_h \nabla h \cdot (\mathbf{r} - \widetilde{\mathbf{r}})$$

$$\widetilde{\mathbf{r}} = \frac{1}{cA} \int_A c^p(\mathbf{r}) \mathbf{r}\, dA$$

$$q^p(\mathbf{r}) = q + \alpha_q \nabla q \cdot (\mathbf{r} - \hat{\mathbf{r}})$$

$$\hat{\mathbf{r}} = \frac{1}{chA} \int_A c^p(\mathbf{r}) h^p(\mathbf{r}) \mathbf{r}\, dA$$

Gradients are approximated as multivariate linear regression of values in neighboring source particles. Van Leer limiting of the gradients is used.

Turner, *et al*. GMD 2022

GEOMETRIC REMAP STEPS

1. Determine overlap polygons and remap effective element area
2. Compute linear reconstructions of average tracer fields
3. Integrate conserved variable reconstructions over intersection polygons
4. Enforce bounds preservation using flux correction

$$\mathcal{A}_{jk} = \sum_i e_{ij} \frac{1}{A_{P_{ij}}} \int_{A_{P_{ij}}} c^p_{ik}(\mathbf{r})\, dA, \longrightarrow c_{jk} = \frac{\mathcal{A}_{jk}}{e_j}$$

$$\mathcal{V}_{jk} = \sum_i e_{ij} \frac{1}{A_{P_{ij}}} \int_{A_{P_{ij}}} c^p_{ik}(\mathbf{r}) h^p_{ik}(\mathbf{r})\, dA \longrightarrow h_{jk} = \frac{\mathcal{V}_{jk}}{e_j c_{jk}}$$

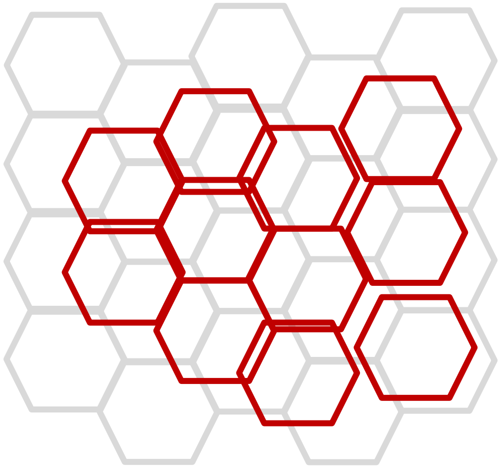
$$\mathcal{Q}_{jkl} = \sum_i e_{ij} \frac{1}{A_{P_{ij}}} \int_{A_{P_{ij}}} c^p_{ik}(\mathbf{r}) h^p_{ik}(\mathbf{r}) q^p_{ikl}(\mathbf{r})\, dA \longrightarrow q_{jkl} = \frac{\mathcal{Q}_{jkl}}{e_j c_{jk} h_{jk}}$$

Turner, *et al*. GMD 2022

GEOMETRIC REMAP STEPS

1. Determine overlap polygons and remap effective element area
2. Compute linear reconstructions of average tracer fields
3. Integrate conserved variable reconstructions over intersection polygons
4. Enforce bounds preservation using flux correction to adjust remapped effective element area

Flux correction is required in cases of non-uniform motion where there can be gaps and overlaps between effective element polygons



$$\begin{aligned} &\text{minimize} \quad \tfrac{1}{2}\mathbf{f}^T\mathbf{P}\mathbf{f} \\ &\text{subject to} \quad \mathbf{l} \le \mathbf{B}\mathbf{f} \le \mathbf{u} \end{aligned}$$

$$l_j = -e_j$$

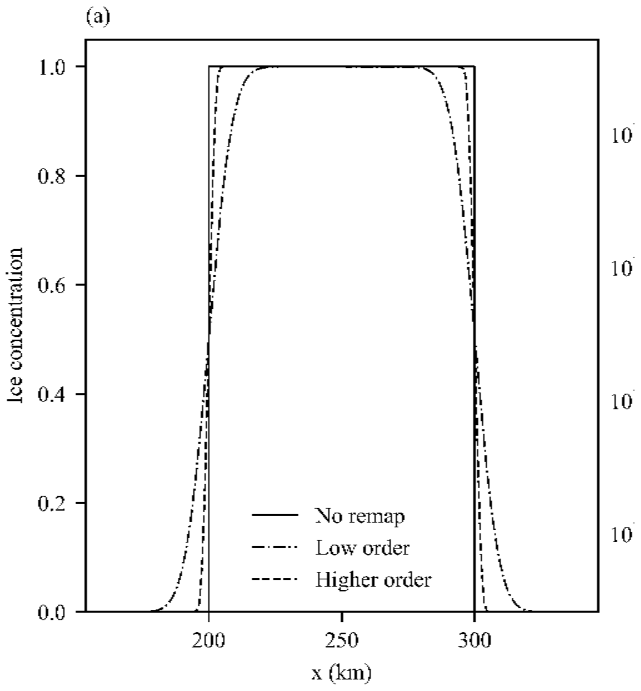
$$u_j = A_{P_j} - e_j$$

Turner, *et al*. GMD 2022

COMPUTATIONAL EXAMPLES – 1D

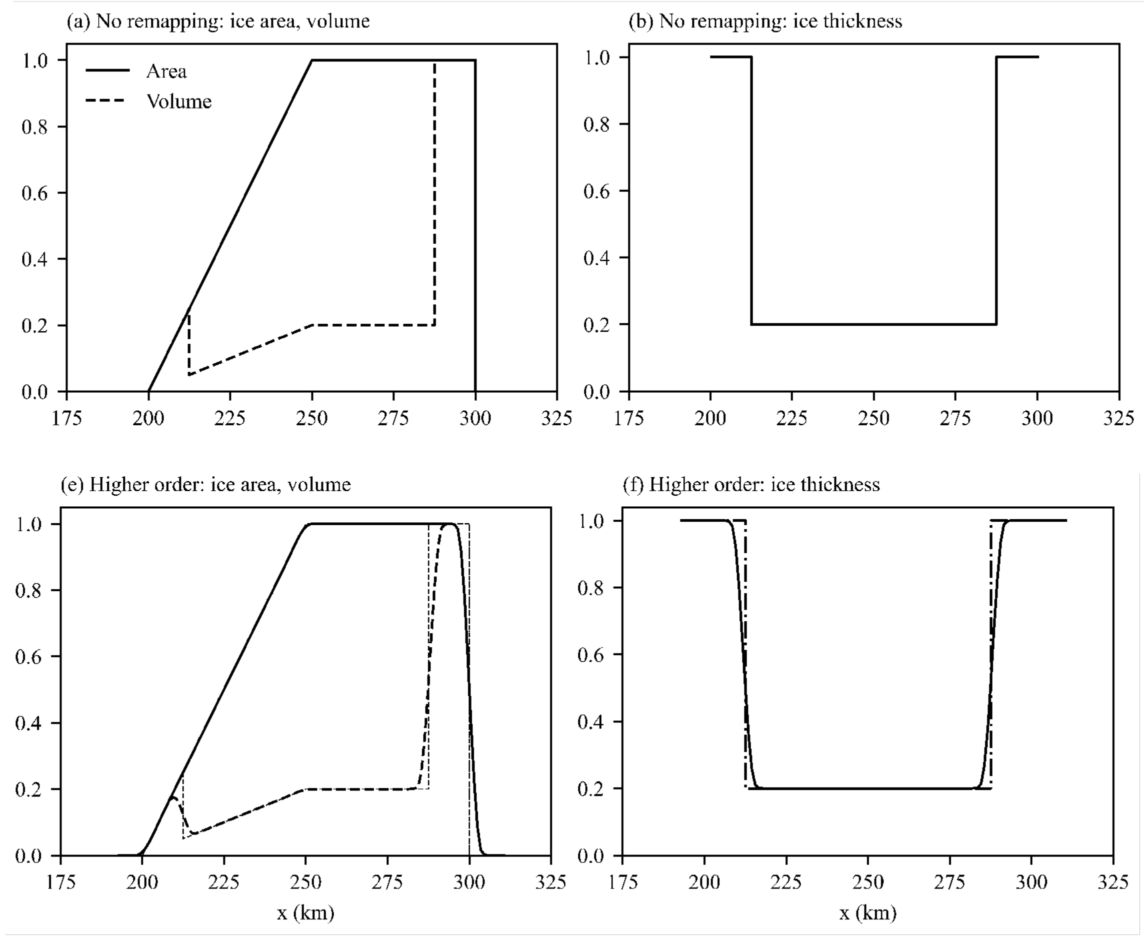
Simple 1-D uniform motion

Translation of square pulse 100 km



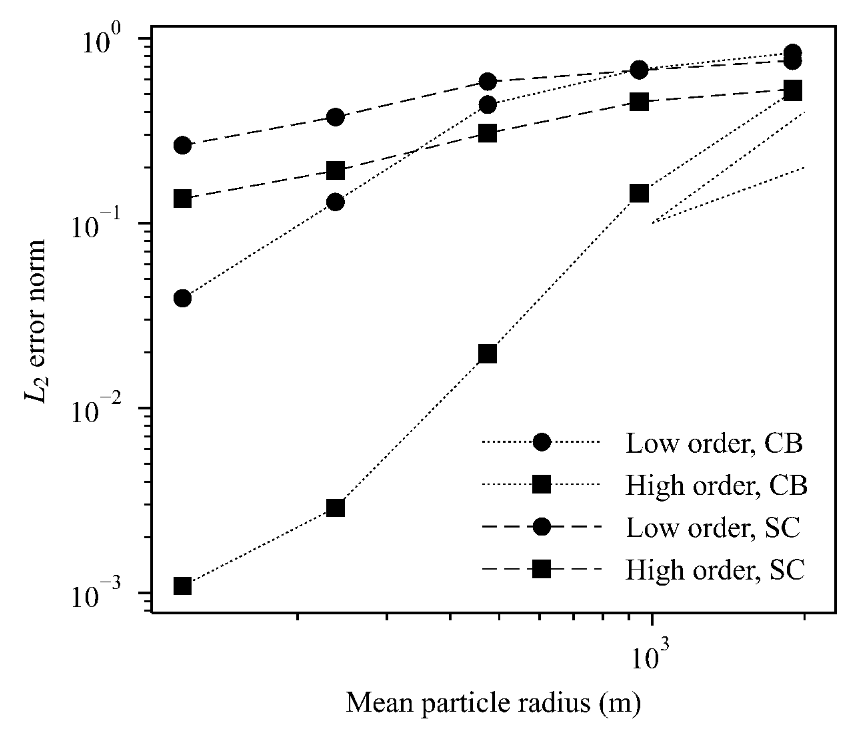
Compatibility test case

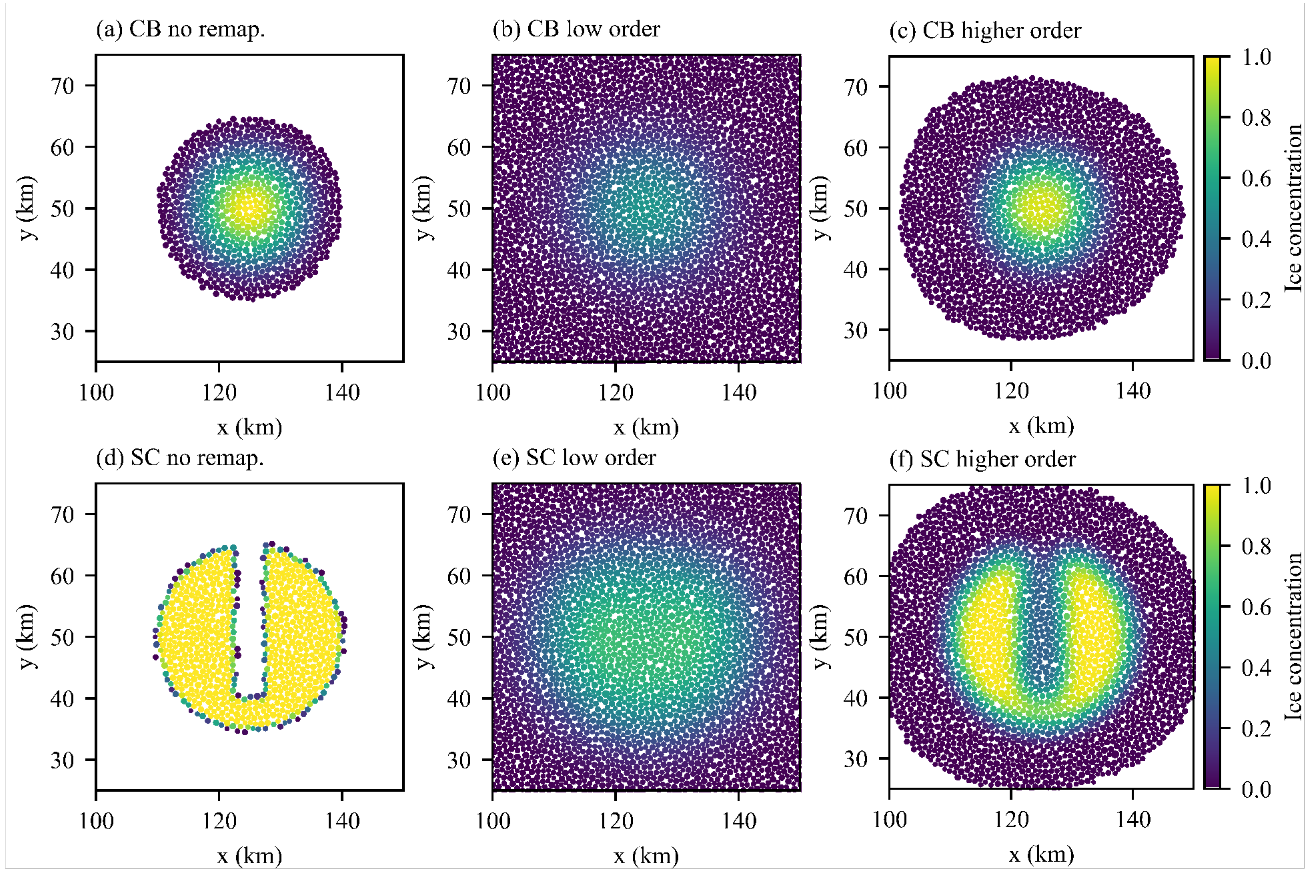
Translation of distributions 100 km



COMPUTATIONAL EXAMPLES – 2D TRANSLATION

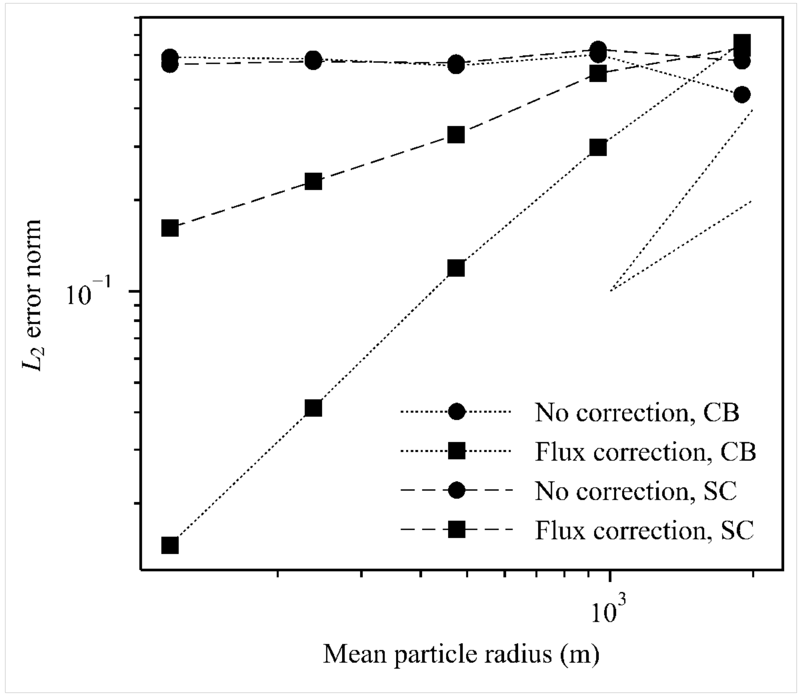
- Cosine bell and slotted cylinder
- Irregular initial particle distribution
- 100 km of translation

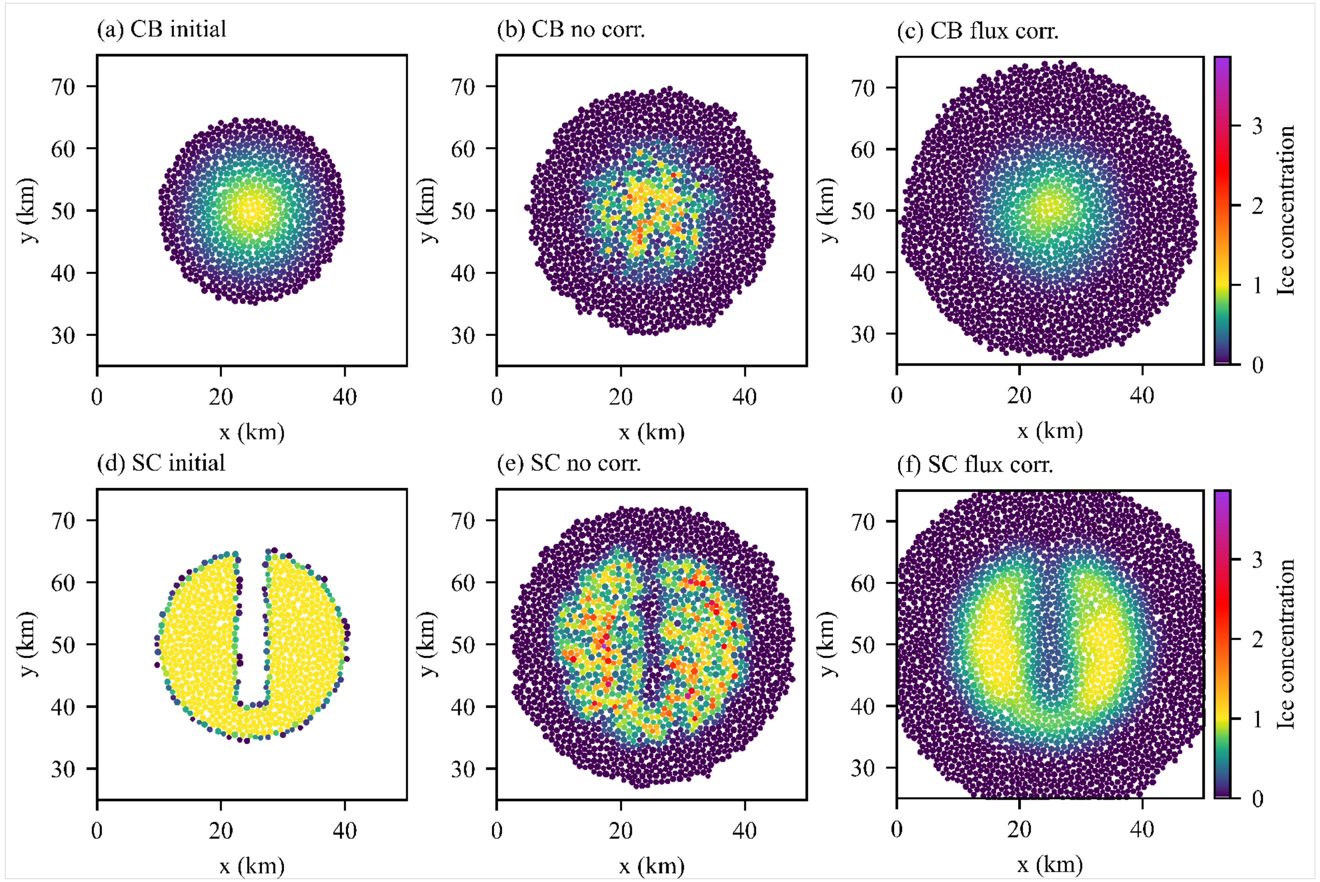




COMPUTATIONAL EXAMPLES – 2D TRANSLATION

- Cosine bell and slotted cylinder
- Irregular initial particle distribution
- Randomized element orientations to test flux correction
- 100 km of translation





MOVING LEAST SQUARES (MLS) INTERPOLATION

- Also investigating MLS algorithms for remapping and interpolation in DEMSI
- Using Compadre toolkit (Kuberry et al. 2019)
- Compadre has already been used for grid-based interpolation within E3SM
- Have implemented point-based reconstruction in DEMSI

Given a set of sampling functionals λ_j and a vector space V, we seek the element of V that best matches a set of scattered degrees of freedom, and use that to approximate a target functional τ over V

$$p^* = \underset{p \in V}{\arg\min} \ \frac{1}{2} \sum_{j=1}^{N} (\lambda_j(u) - \lambda_j(p))^2 \omega(\tau; \lambda_j).$$

$$\tau(u) \approx \tau(p^*)$$

MLS REMAP MASS-BASED CORRECTION

- MLS interpolation is not inherently mass conserving or bounds preserving
- For each tracer we apply an optimization algorithm to enforce physical properties (Bochev et al. 2013, 2014)
- Local min/max are computed from values of old elements used in MLS reconstruction
- Prior to optimization the concentration is multiplied by effective element area

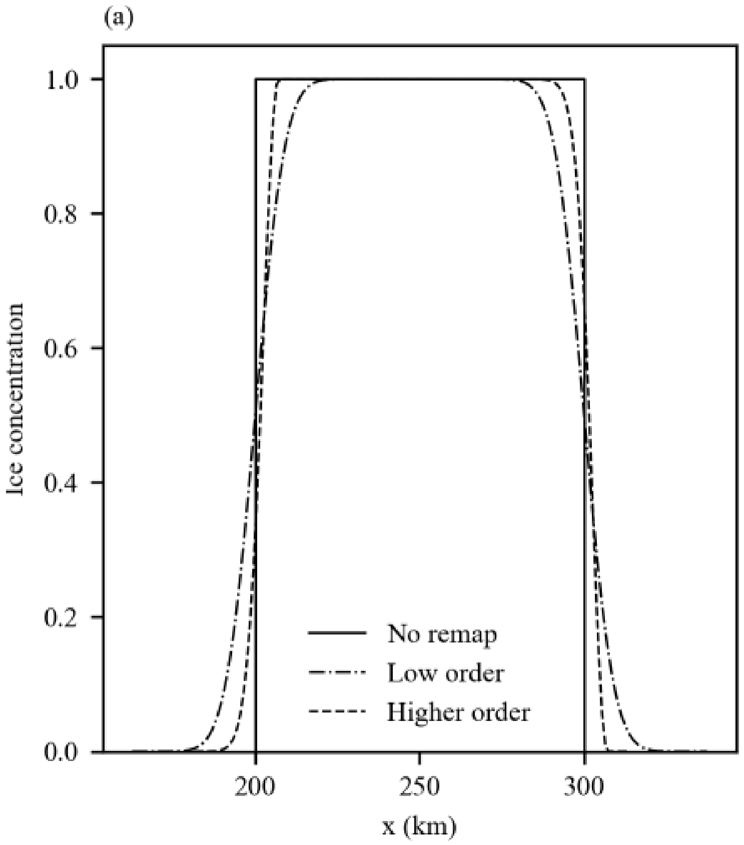
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widehat{c} - c^{\mathsf{T}}\|_{\ell_2}^2 \qquad \text{subject to} \\ \sum \widehat{c}_q A_q = A_{ice} \quad \text{and} \quad c_q^{\min} \leq \widehat{c}_q \leq c_q^{\max} \quad q = 1, \ldots, N. \end{cases}$$

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widehat{h} - h^{\mathsf{T}}\|_{\ell_2}^2 \qquad \text{subject to} \\ \sum \widehat{c}_q \widehat{h}_q A_q = V_{ice} \quad \text{and} \quad h_q^{\min} \leq \widehat{h}_q \leq h_q^{\max} \quad q = 1, \ldots, N. \end{cases}$$

MLS COMPUTATIONAL EXAMPLES – 1D

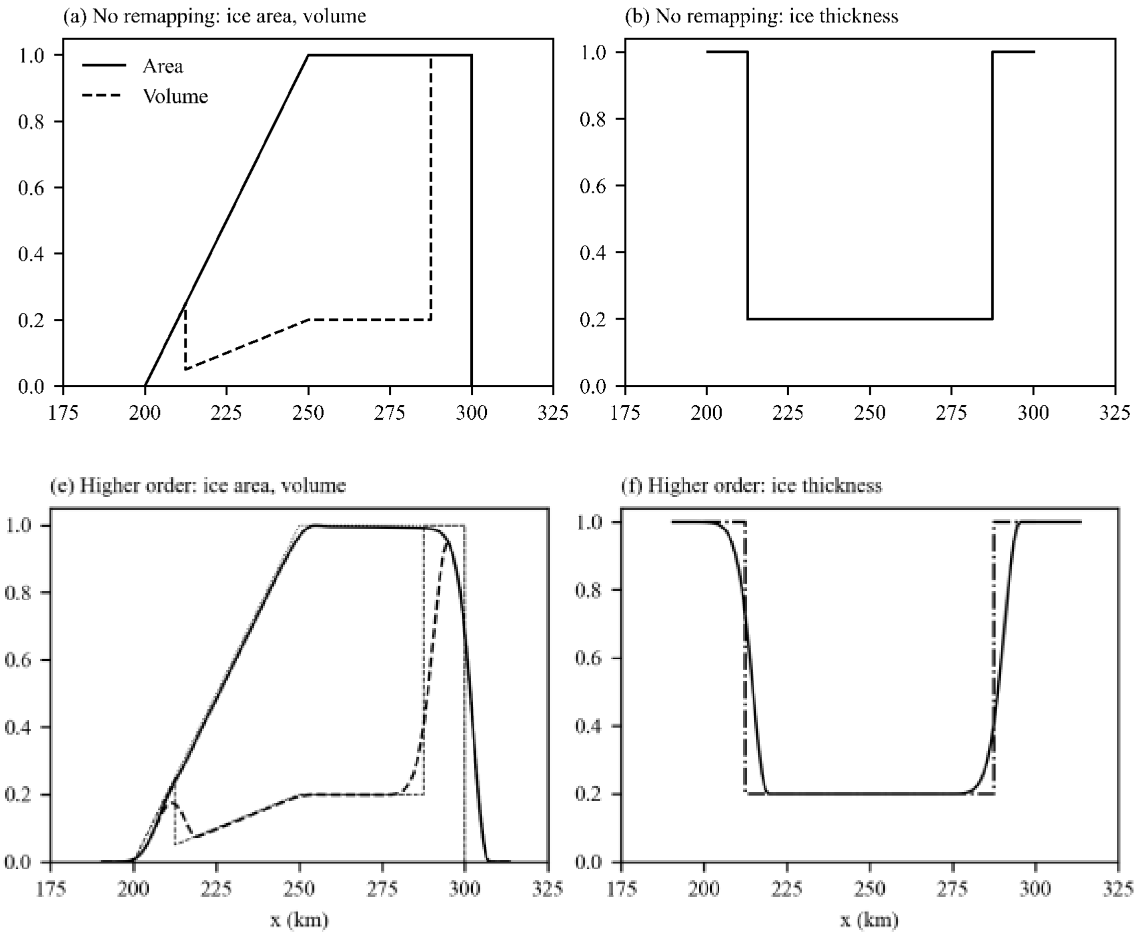
Simple 1-D uniform motion

Translation of square pulse 100 km



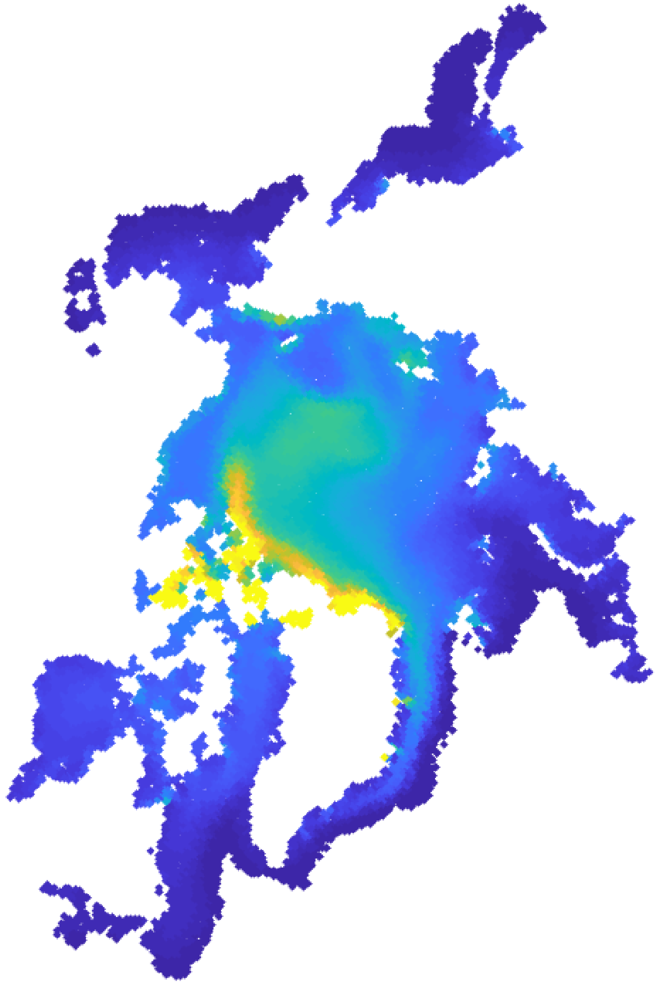
Compatibility test case

Translation of distributions 100 km



CONCLUSIONS

- Discrete elements can better capture fracture and anisotropic deformation in sea ice dynamics
- New approaches for particle remapping as well as coupling to Eulerian ocean and atmosphere are required for Lagrangian particle methods
- Presented geometric particle remap method
  - Ensures conservation and bounds preservation
  - Method can also be used for particle to grid interpolation
- Investigating MLS approaches for computationally efficient interpolation and remap



Arctic Sea Ice Thickness in DEMSI

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