DEMSI
Discrete Element Model for Sea Ice

Sandia National Laboratories

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Conservative Remap and Interpolation for the Discrete Element Model for Sea Ice



Kara Peterson, Dan Bolintineanu
Sandia National Laboratories

Adrian Turner
Los Alamos National Laboratory

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MS233 Approaches, Applications, and Analysis of Heterogeneous Numerical Methods

SciDAC
Scientific Discovery through Advanced Computing

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DEMSI

New sea ice model under development for use in coupled Earth system models

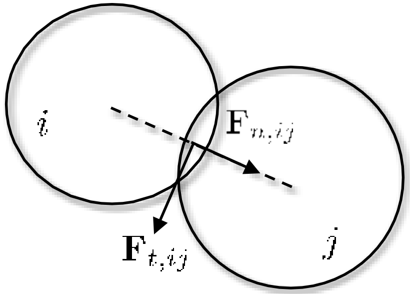
Dynamics: Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

- https://lammps.sandia.gov
- Particle based molecular dynamics code
- Includes support for DEM and history dependent contact models

Thermodynamics: CICE Consortium Icepack Library

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

- Dynamics are computed using circular Lagrangian elements that interact via contact forces for bonded and unbonded elements
- DEM enables capture of complex anisotropic deformation that continuum sea ice models have difficulty reproducing



INTERPOLATION & REMAP IN DEMSI

Coupling with ocean and atmosphere models

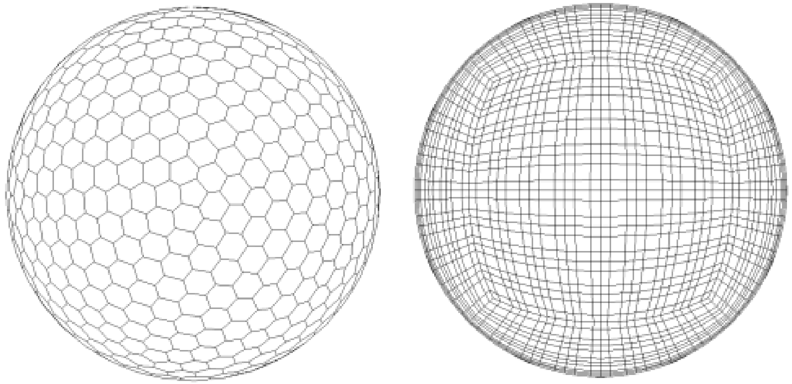
- Requires interpolation between Lagrangian particles and Eulerian grids

Particle-to-particle remap

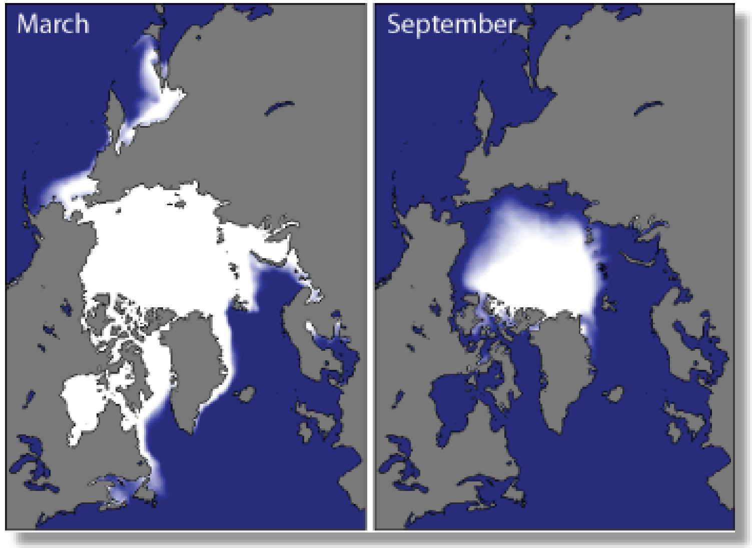
- Periodic remap to initial particle distribution to manage large deformations and particle clustering
- Provides method for adding new particles due to thermodynamic growth

For this presentation will focus on the particle-to-particle remap

Example global grids



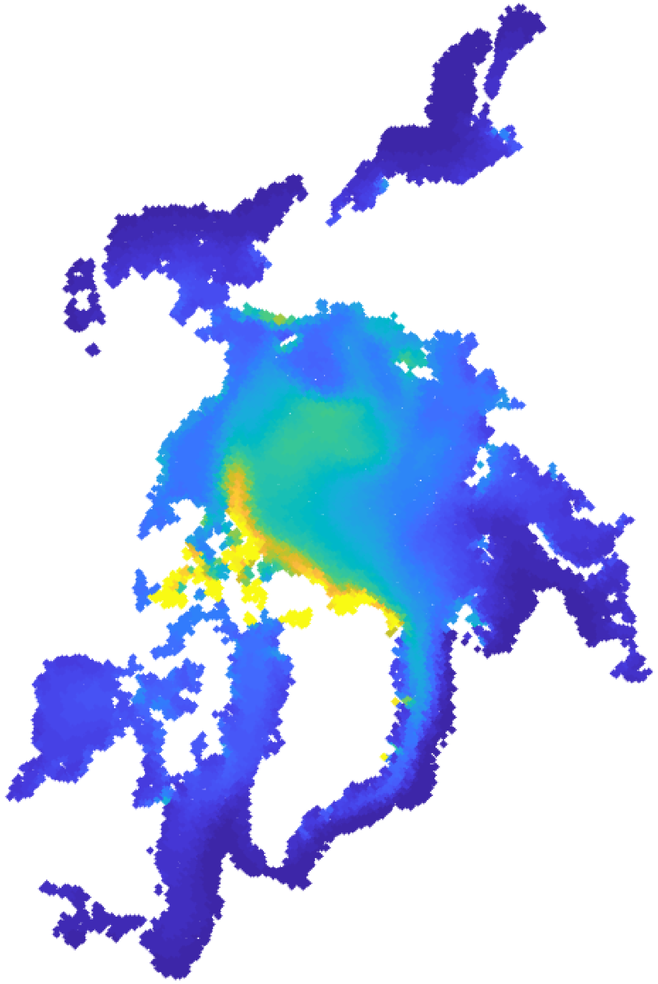
Satellite sea ice concentration illustrating large seasonal variation in sea ice domain



Climatology: 1981-2010 (nsidc.org)

OUTLINE

- Remap challenges in DEMSI
- Remap implementations
  - Geometric remap
  - Moving Least Squares
- Computational results



Arctic Sea Ice Thickness in DEMSI

CHALLENGES

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

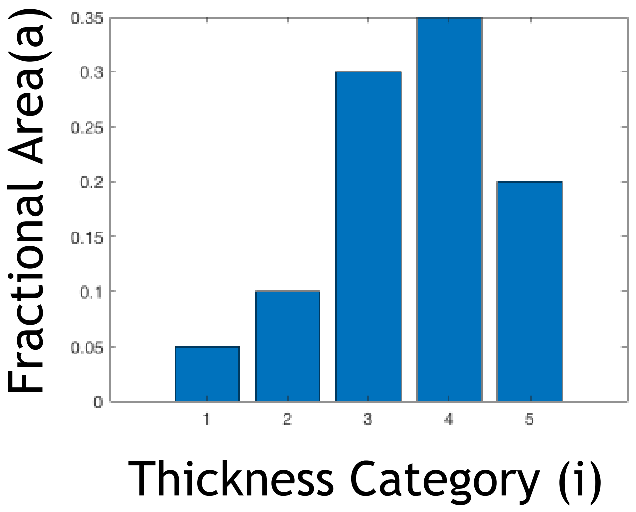
Fractional area in thickness category i: a_i

Fractional volume in thickness category i: v_i

Concentration (fraction of ice in particle) : $$c_p = \sum_i a_{i,p}$$

Fractional Volume : $$v_p = \sum_i v_{i,p}$$

Thickness: $$h_p = v_p / c_p$$



Additional quantities like ice enthalpy and snow thickness are also modeled, leading to a system of hierarchical tracers for remap

CHALLENGES

Physical constraints including conservation and bounds preservation

- Remap algorithms must
  - Conserve total ice area and volume
  - Maintain bounds for remapped quantities
  - Maintain consistency between tracer quantities $h_p = v_p/c_p$

Conserved Quantities

Total ice area: $A_{ice} = \sum_p c_p A_p = \sum_p \sum_i a_{ip} A_p$

Total ice volume: $V_{ice} = \sum_p c_p h_p A_p = \sum_p \sum_i v_{ip} A_p$

Physical Bounds

$0 \leq c_p \leq 1$ $\quad 0 \leq h_p$ $\quad 0 \leq v_p$

CHALLENGES

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  - Maintain consistency between tracer quantities $h_p = v_p / c_p$
- For conservation we use an effective element area A_p
  - Define Voronoi cells associated with initial partial distribution
  - Effective element areas are transported with Lagrangian particles

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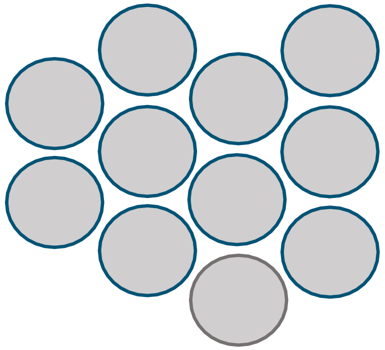

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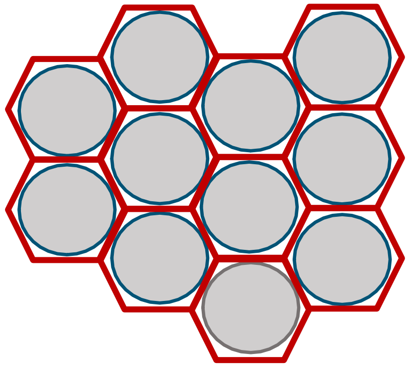
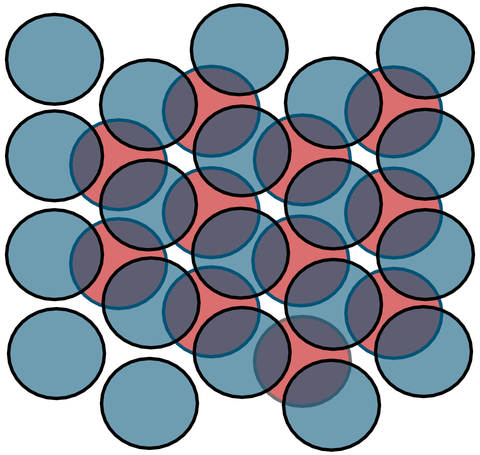


GEOMETRIC REMAP

Procedure

- Compute intersections between old and new effective element areas
- Compute mean preserving linear reconstructions of tracer for each old particle using neighbor values
- Integrate reconstruction over area intersections and sum to get area average on the new particle



Linear reconstructions

$$c_p(\mathbf{x}) = \bar{c}_p + \alpha_c \nabla c_p \cdot (\mathbf{x} - \mathbf{x_c})$$

$$v_p(\mathbf{x}) = \bar{v}_p + \alpha_v \nabla v_p \cdot (\mathbf{x} - \mathbf{x_c})$$

Limiting coefficients (van Leer limiting)

$$0 \leq \alpha_c \leq 1 \qquad 0 \leq \alpha_v \leq 1$$

Element centroid $\mathbf{x_c}$

Lipscomb and Hunke (2004) Modeling Sea Ice Transport Using Incremental Remapping. *Mon. Wea. Rev.*, **132**, 1341–1354.

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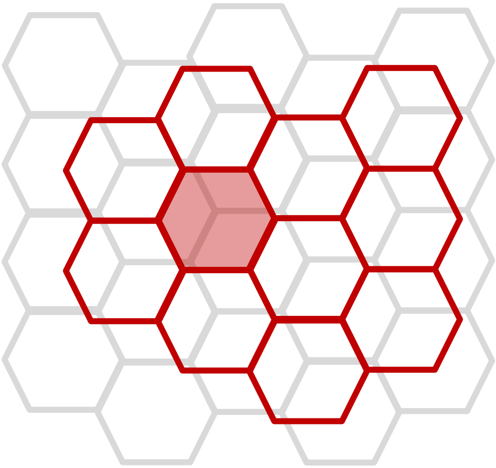


Intersections Ω_{pq}

Old particles p

New particles q

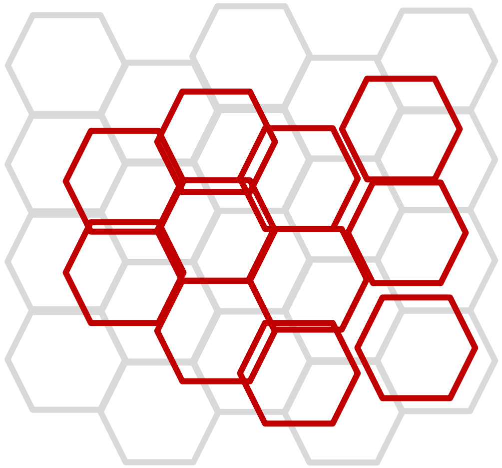
Lipscomb and Hunke (2004) Modeling Sea Ice Transport Using Incremental Remapping. *Mon. Wea. Rev.*, **132**, 1341–1354.

GEOMETRIC REMAP FLUX CORRECTION

- This algorithm is conservative and bounds preserving when remapping between well-defined grids
- In practice there are gaps and overlaps between effective cell areas
- Use flux-based optimization algorithm to correct the remapped areas
- Fluxes are then used in an iterative procedure to modify the tracer values to ensure conservation
- Permon (https://github.com/permon/permon) used to solve resulting quadratic program

Flux correction

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widehat{f} - f^{\mathsf{T}}\|_{\ell_2}^2 \qquad \text{subject to} \\ A^{\min} \leq \widehat{A} + \mathsf{D}\widehat{f} \leq A^{\max} \end{cases}$$



Intersections Ω_{pq}

Old particles p

New particles q

$$A_q \neq \sum_p \Omega_{pq}$$

MOVING LEAST SQUARE REMAP

Procedure

- Find old particle neighbors of new particle
- Compute moment matrix and solve
- Compute remapped variable
- Implemented with interpolatory weight function, but tests indicate weight function does not make much difference to solution

- In practice the choice of neighborhood for the reconstruction makes a large difference for elements on edge of the particle distribution

Moment matrix

$$M = \sum_{p \in N_q} b b^T w_p$$

$$b^T = [1 \quad (x - x_p) \quad (y - y_p)]$$

Interpolant

$$c(x,y) = \sum_{p \in N_q} b^T M^{-1} b c_p w_p$$

$$h(x,y) = \sum_{p \in N_q} b^T M^{-1} b h_p w_p$$

Weight function $w_p = \dfrac{\exp(-d^2)}{d^2 + \epsilon}$

Formulation based on Sulsky and Gong (2016). Improving the Material-Point Method. 10.1007/978-3-319-39022-2_10.

MOVING LEAST SQUARE 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
- Local min/max are computed from values of old elements used in MLS reconstruction
- Prior to optimization the concentration is multiplied by approximate fractional area in the case of boundary cells $c_q = c_q(\sum_p \Omega_{pq})/A_q$

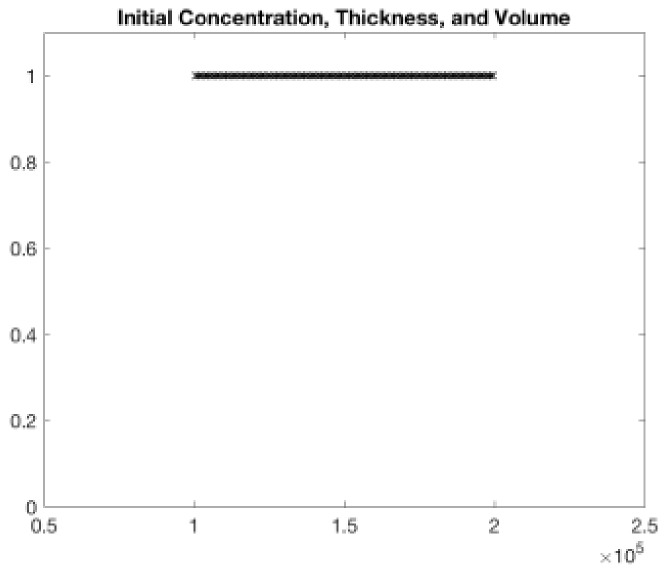
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widehat{c} - c^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum \widehat{c}_q A_q = A_{ice} \quad \text{and} \quad c_q^{\min} \le \widehat{c}_q \le c_q^{\max} \quad q = 1, ..., N. \end{cases}$$

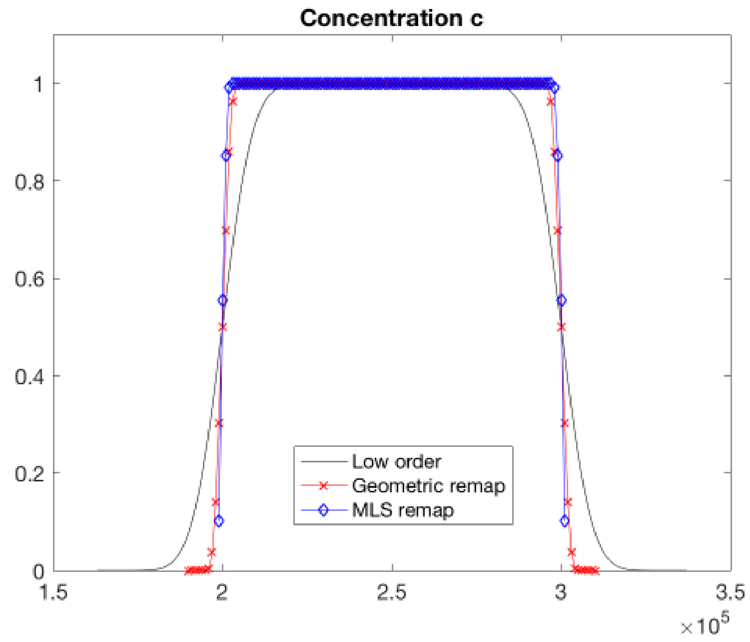
$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widehat{h} - h^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum \widehat{c}_q \widehat{h}_q A_q = V_{ice} \quad \text{and} \quad h_q^{\min} \le \widehat{h}_q \le h_q^{\max} \quad q = 1, ..., N. \end{cases}$$

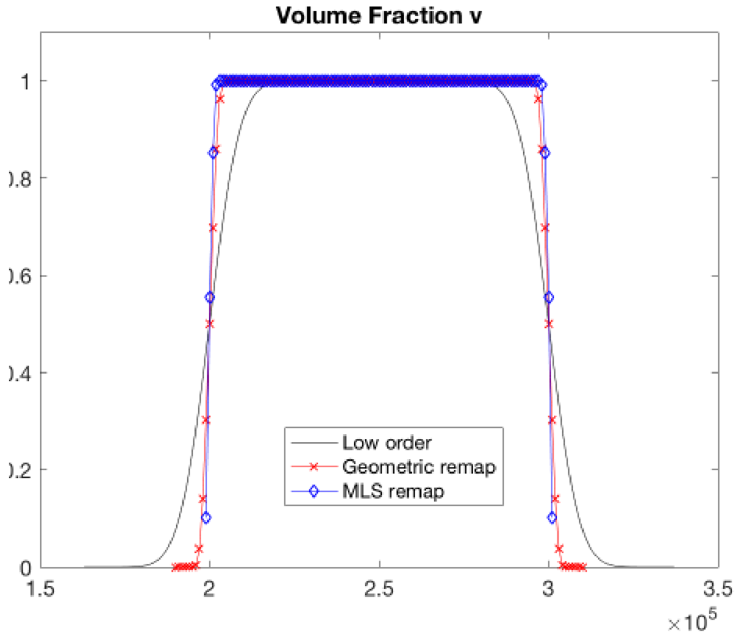
Bochev, Ridzal, Shashkov (2013) Fast optimization-based conservative remap of scalar fields through aggregate mass transfer, *JCP*
Bochev, Ridzal, Peterson (2014) Optimization-based remap and transport: a divide and conquer strategy for feature-preserving discretizations, *JCP*

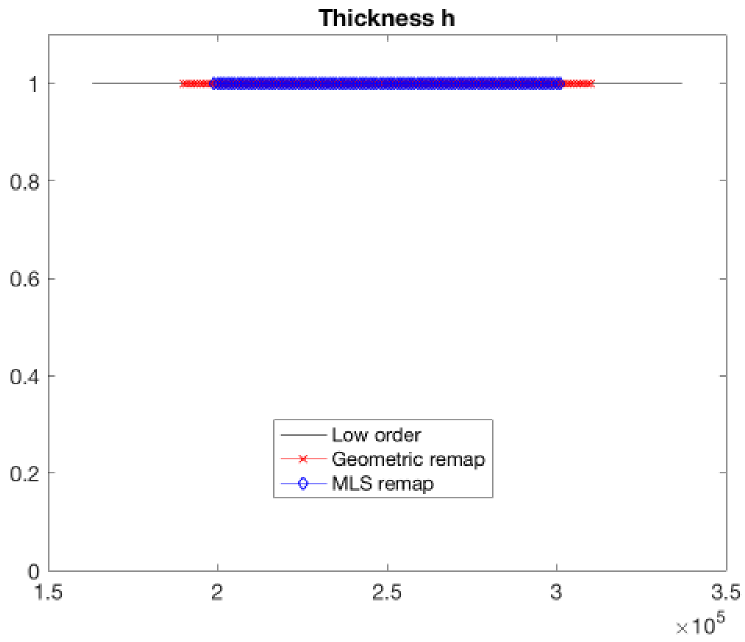
EXAMPLE PROBLEM: 1-D TRANSLATION

- Translation of constant concentration, thickness, and volume
- X total time steps
- Remap performed at each time step
- Both Geometric and MLS remap options resolve the boundary well and maintain bounds and consistency between thickness, volume, and concentration



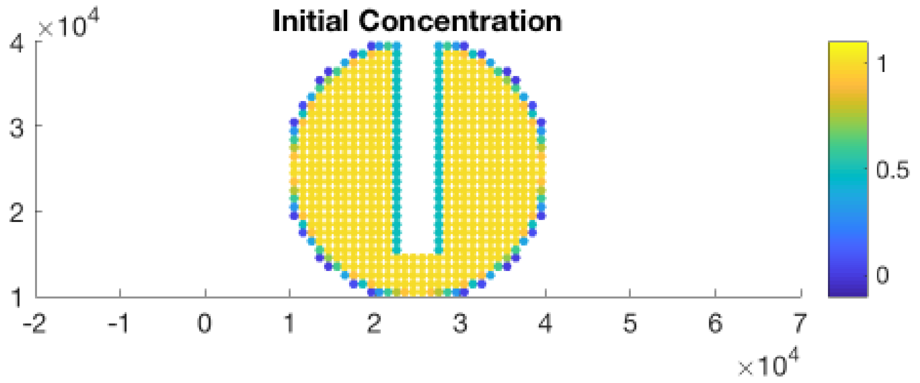


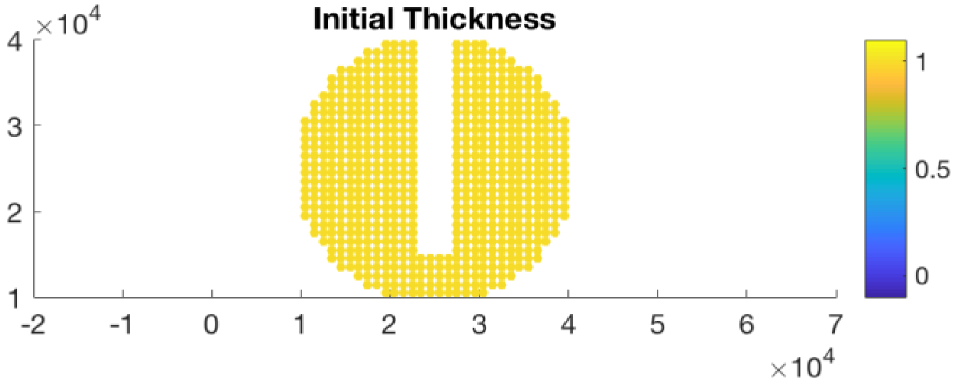




EXAMPLE PROBLEM: 2-D TRANSLATION

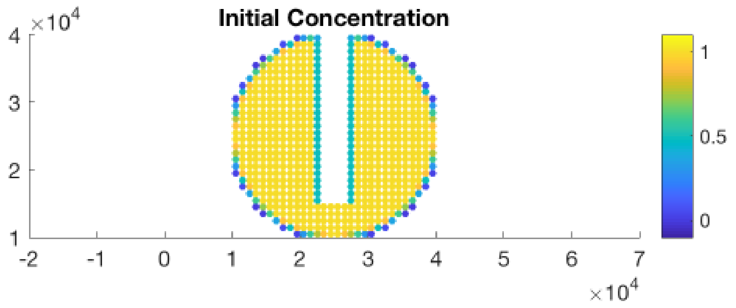
- Regular Particle Distribution
- Translation of discontinuous concentration, thickness, volume



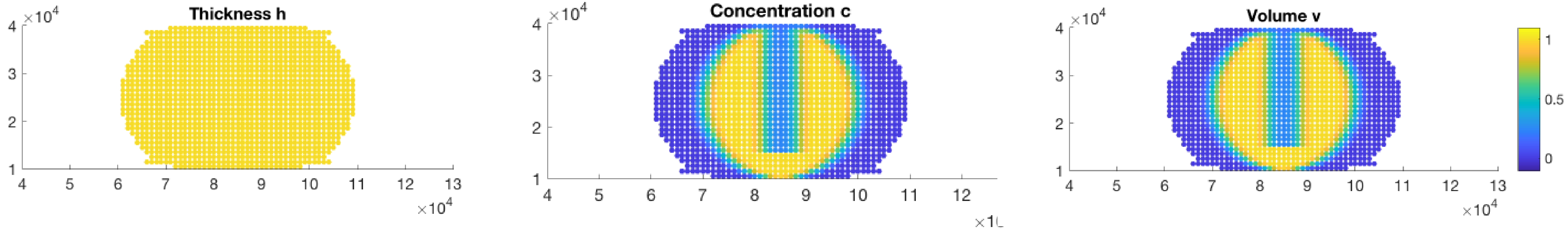


EXAMPLE PROBLEM: 2-D TRANSLATION

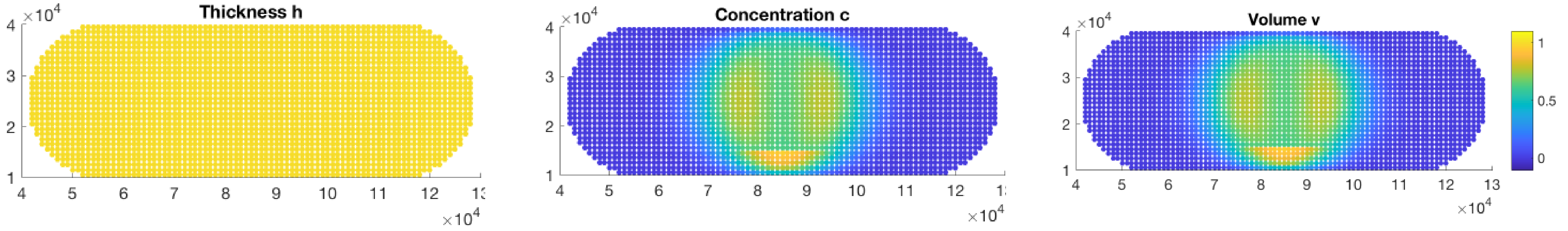
- Regular Particle Distribution
- Translation of discontinuous concentration, thickness, volume
- Plots at 120 remap steps



Geometric Remap



Low Order Remap



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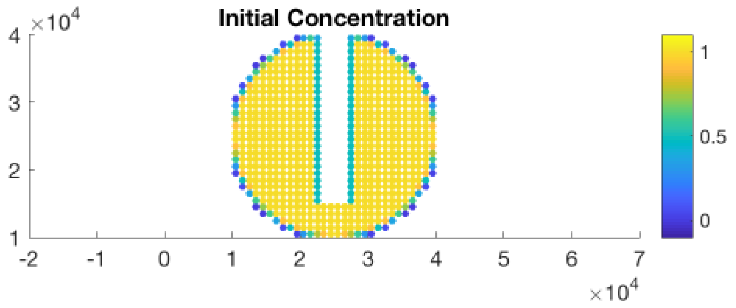

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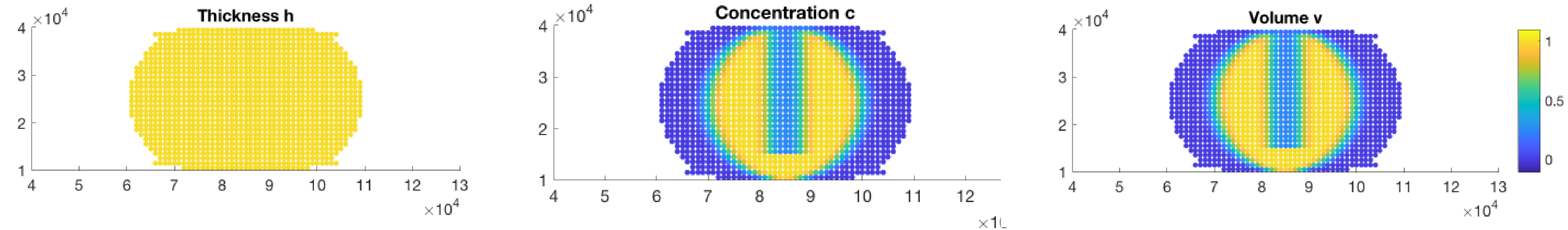
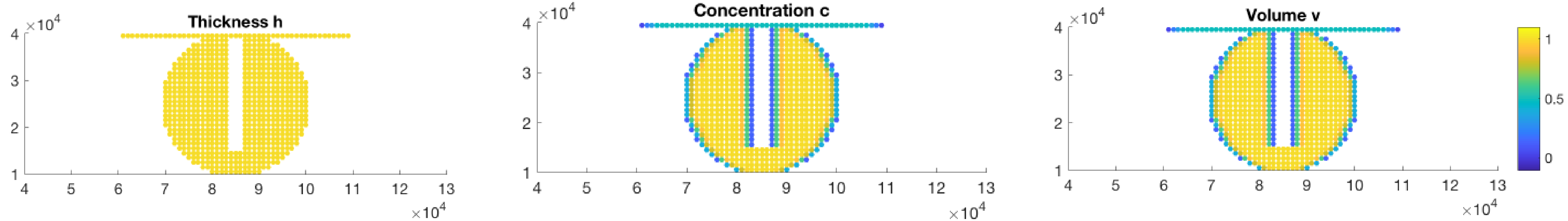


MLS Remap



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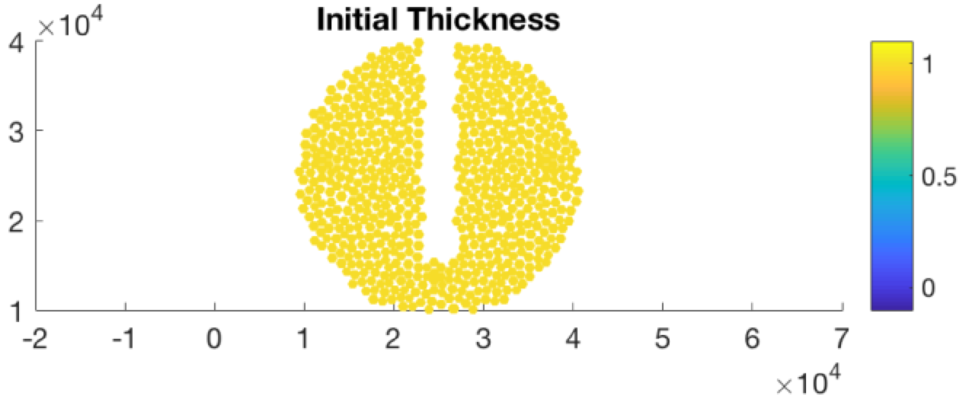

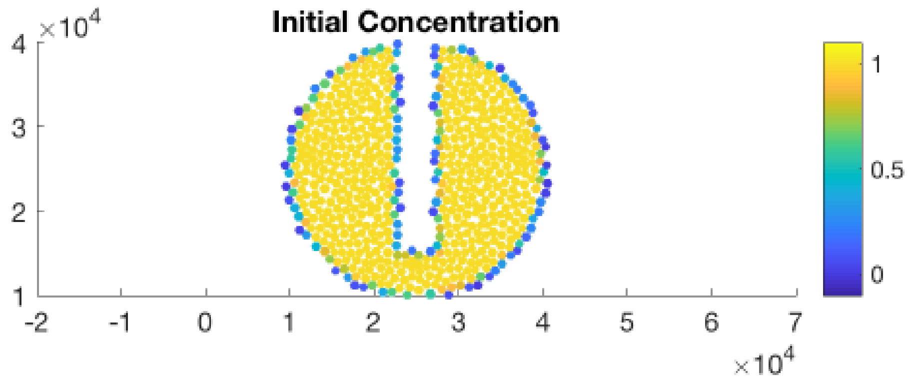

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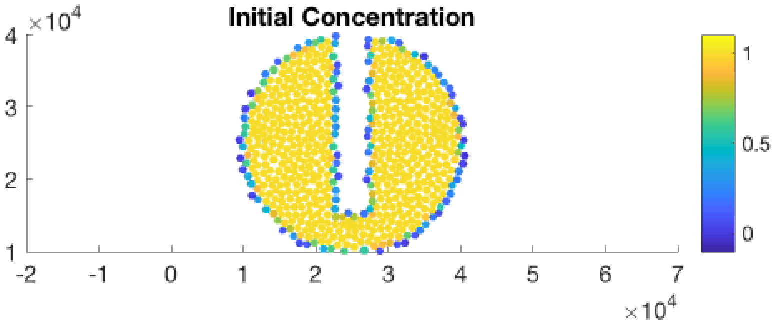
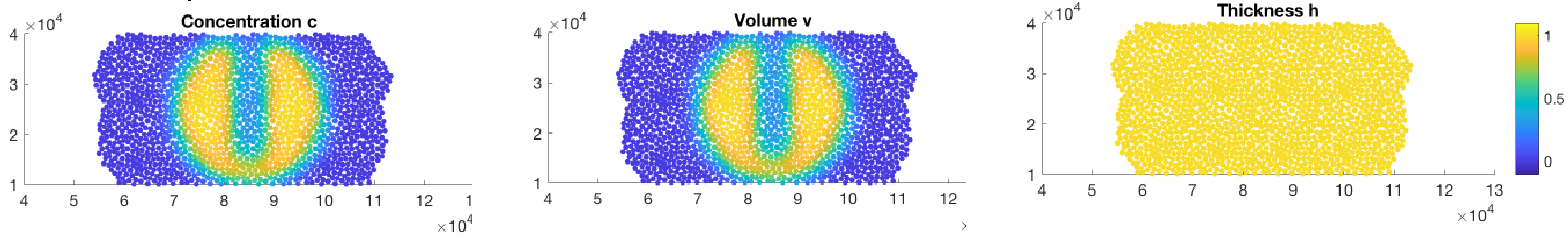
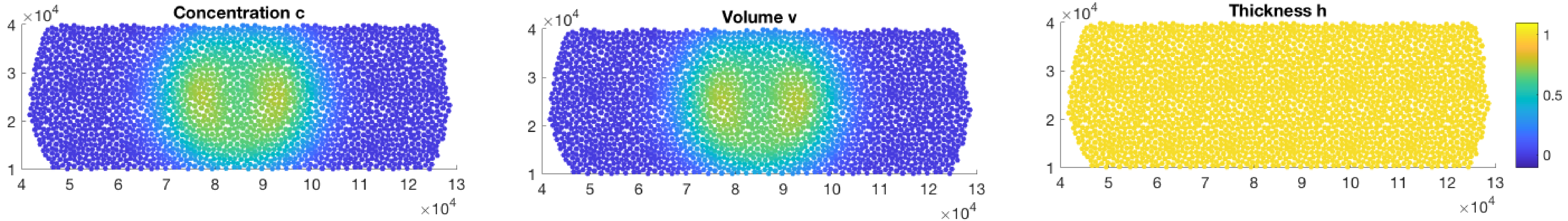


Geometric Remap



Low Order Remap



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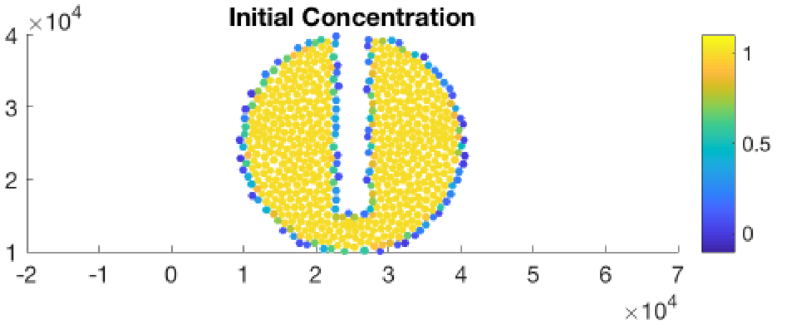

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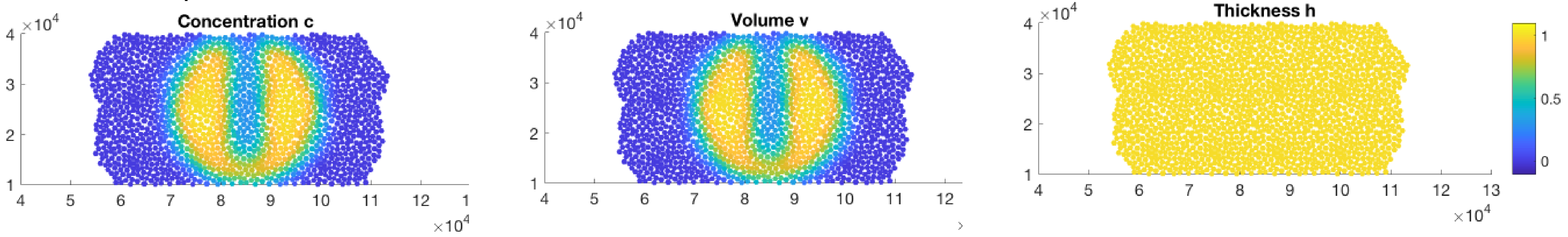

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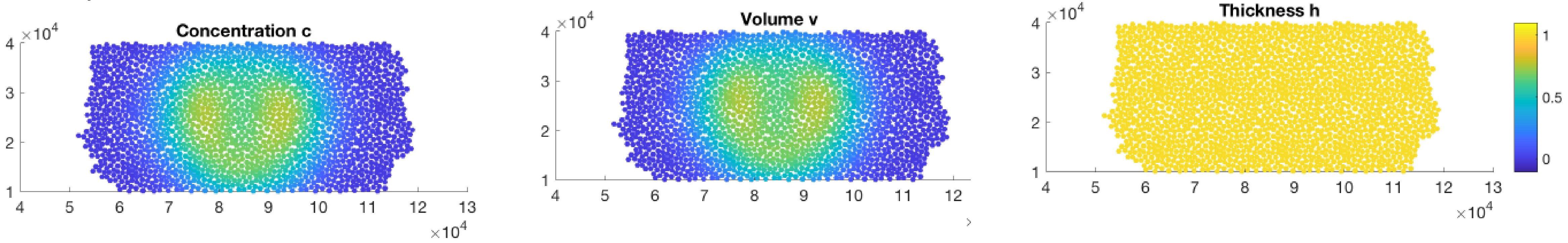
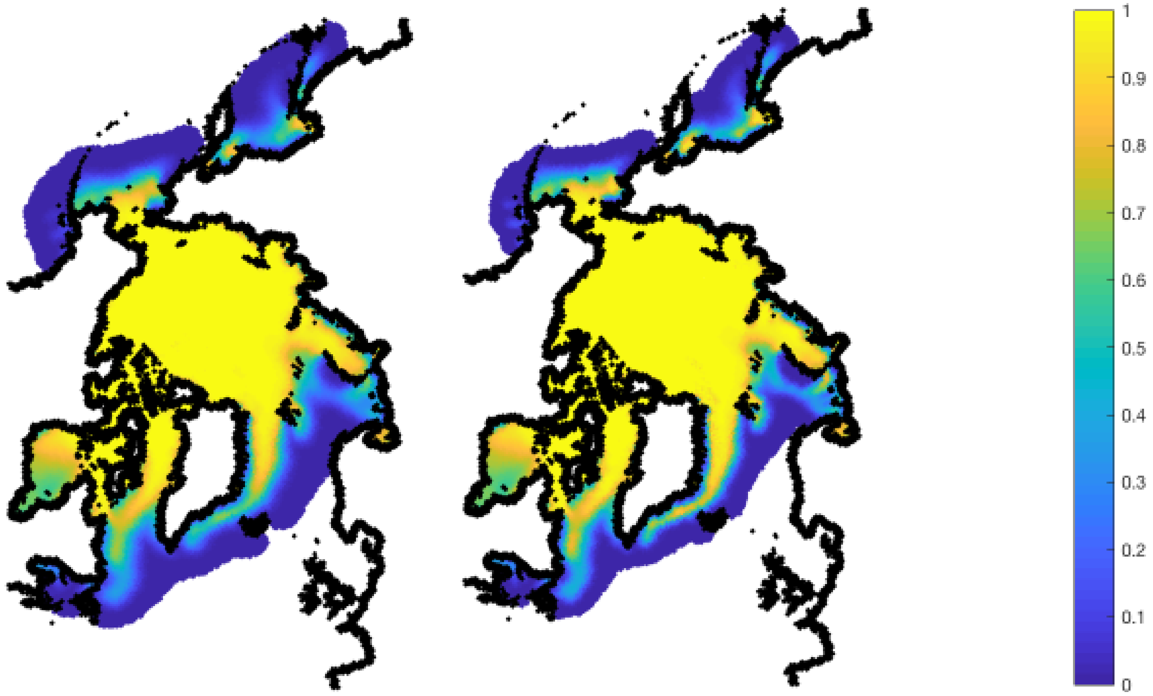


EXAMPLE PROBLEM: ARCTIC BASIN

- Realistic particle distribution and forcing
- 30 days of simulation
- Remap performed once per simulated day
- Dynamic timestep of 3600 seconds

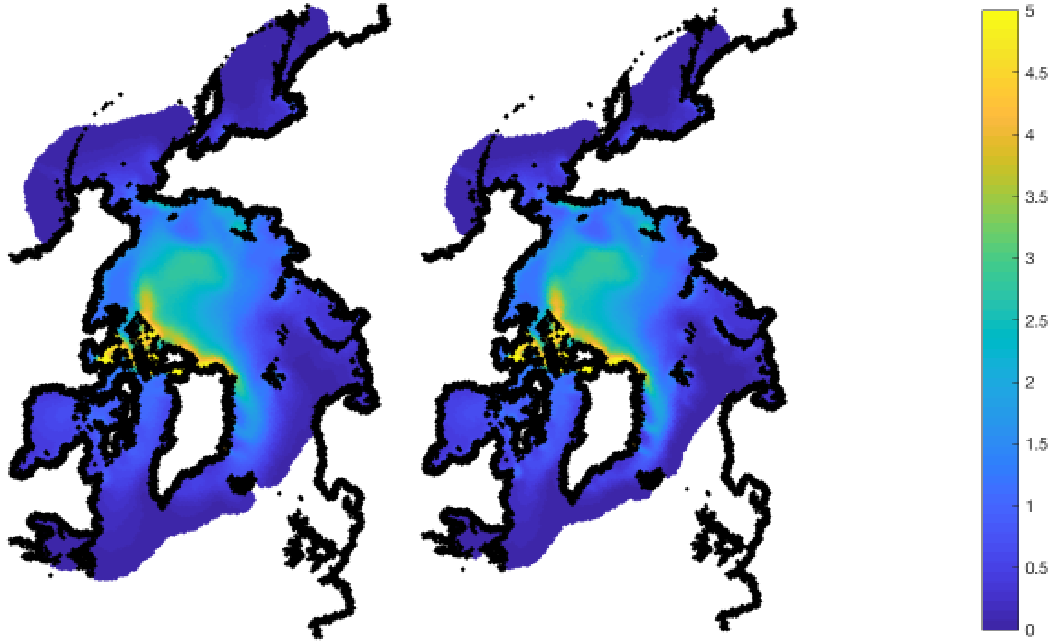
Concentration

Low Order | Geometric Remap



Thickness

Low Order | Geometric Remap



CONCLUSIONS

- Described two remap methods for particle-to-particle remap in DEMSI
  - Geometric with flux correction
  - MLS with mass correction
- Geometric remap works well for all test cases
- MLS is potentially more computational efficient, but exhibits significant numerical diffusion for irregular particle distributions

- Ongoing and future work
  - Additional testing and debugging of MLS remap
  - Investigate alternative algorithms for enforcing physical constraints