



Overview of MPAS-SI-MPM

Improved Coupled Climate Simulations in E3SM
Through Enhanced Sea-Ice Mechanics

A BER-SciDAC5 Partnership

Participants

- University of New Mexico
 - Deborah Sulsky (PI)
 - Howard Schreyer
 - Han Tran
- University of Nebraska - Lincoln
 - Yawen Guan (co-PI)
- Rensselaer Polytechnic Institute (FASTMath)
 - Onkar Sahni (co-PI)
 - Mark Shephard
 - Cameron Smith
- Los Alamos National Laboratory
 - Adrian Turner (co-PI)
 - Andrew Roberts
- Sandia National Laboratories
 - Kara Peterson (co-PI)
 - Devin O'Connor
 - Svetoslav Nikolov

Project Objective

Enhance the representation of sea ice mechanics, deformation, and leads in MPAS-Seaice to improve accuracy and reduce uncertainties in coupled climate simulations by improving predicted fluxes between atmosphere, ocean, and sea ice. (Leads occupy ~2% of area but account for ~66% of heat flux. Responsible for localized dense water formation through brine ejection.)

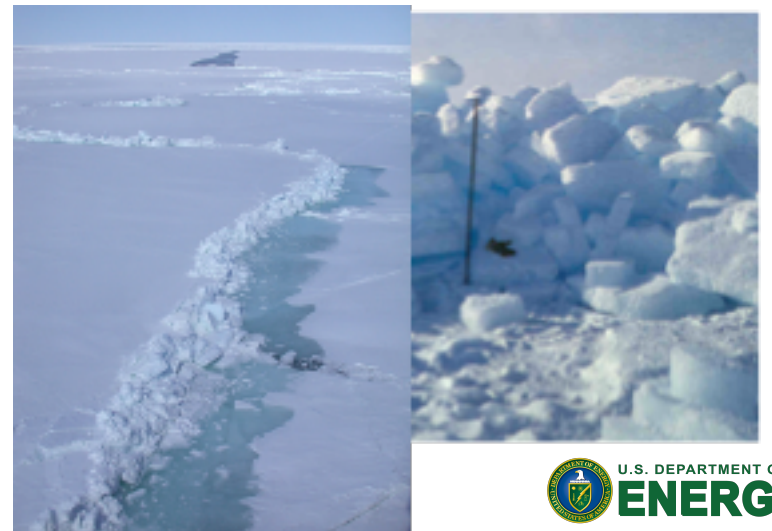
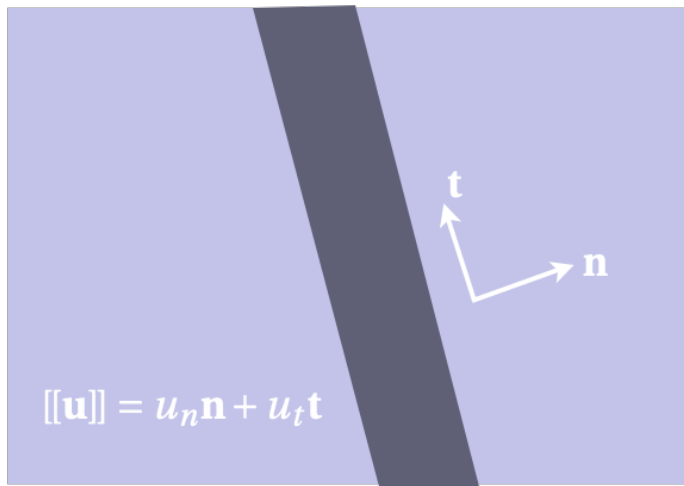
- Leads are included through the elastic-decohesive constitutive model for sea ice which treats intact ice as an elastic solid that can fracture to form areas of open water. Closing and refreezing of leads is included.
- Techniques for parameter calibration and model validation (especially for leads) to be developed.
- Sea ice dynamics to be run on GPUs using the PUMIPic Library

Approach

- **Model Development and Implementation:** Use the material-point method with the elastic-decohesive constitutive model on MPAS meshes for CPUs and GPUs.
- **Validation and Verification:** Design a test suite and sequence of milestone simulations. Identify new metrics for model performance and quantitatively compare different models and their impact on coupled climate simulations. Provide metrics to assess performance of the new model for prediction of lead opening and lead distribution.
- **Model Calibration:** Apply new and standard metrics to calibrate and validate the model using observations and reanalysis data.
- **Demonstrate Capabilities:** Yearly milestone simulations and a 50 year, fully-coupled capstone simulation.

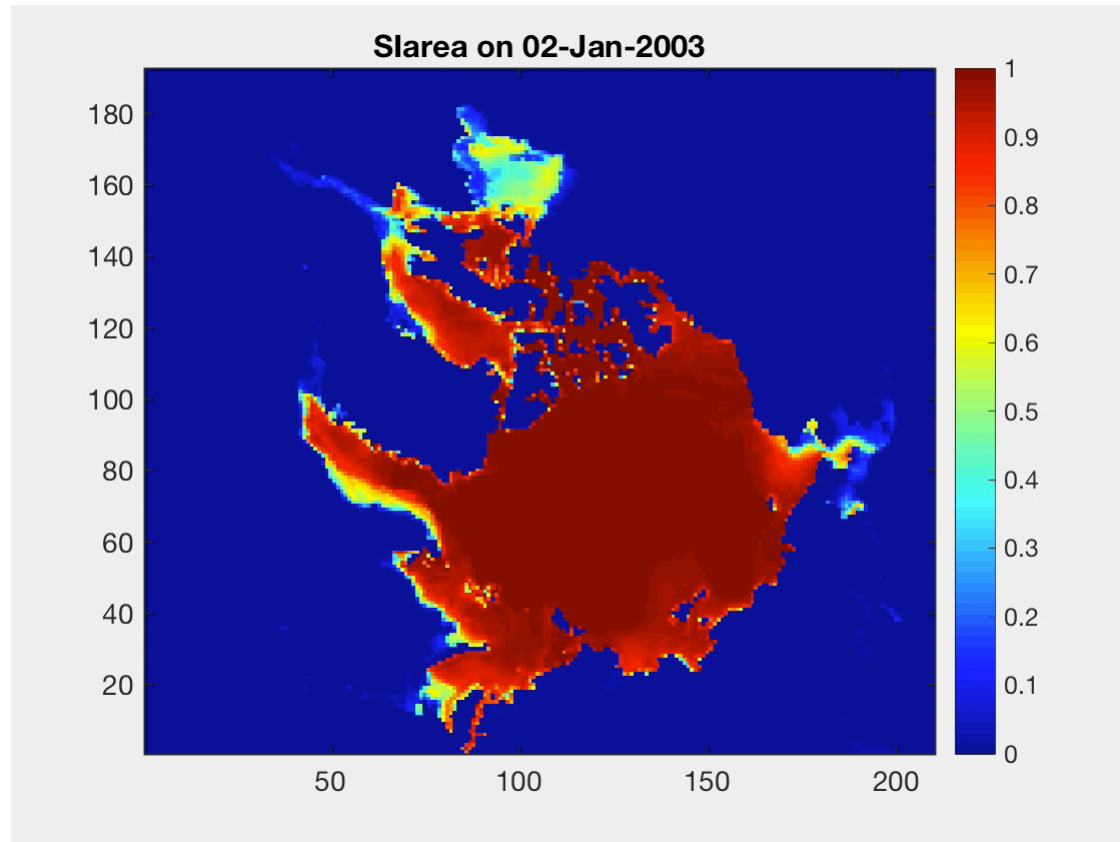
Why Elastic-Decohesive Model?

- Explicit representation of leads in sea ice
- Intact ice modeled as elastic
- Leads modeled as displacement discontinuities
- Model predicts initiation of a lead and its orientation
- Traction is reduced with lead opening until a complete fracture forms.

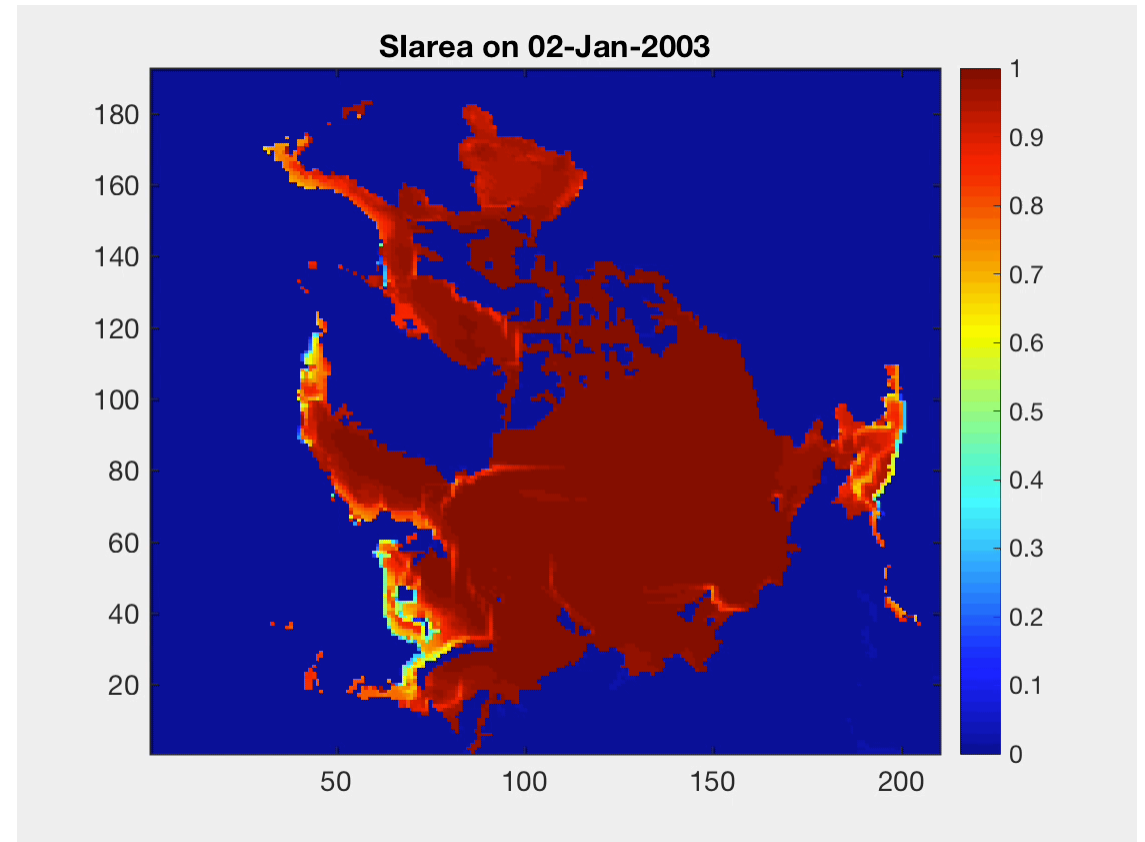


Arctic Simulation

MITgcm ~36km grid (cubed sphere) JRA-25 atmosphere

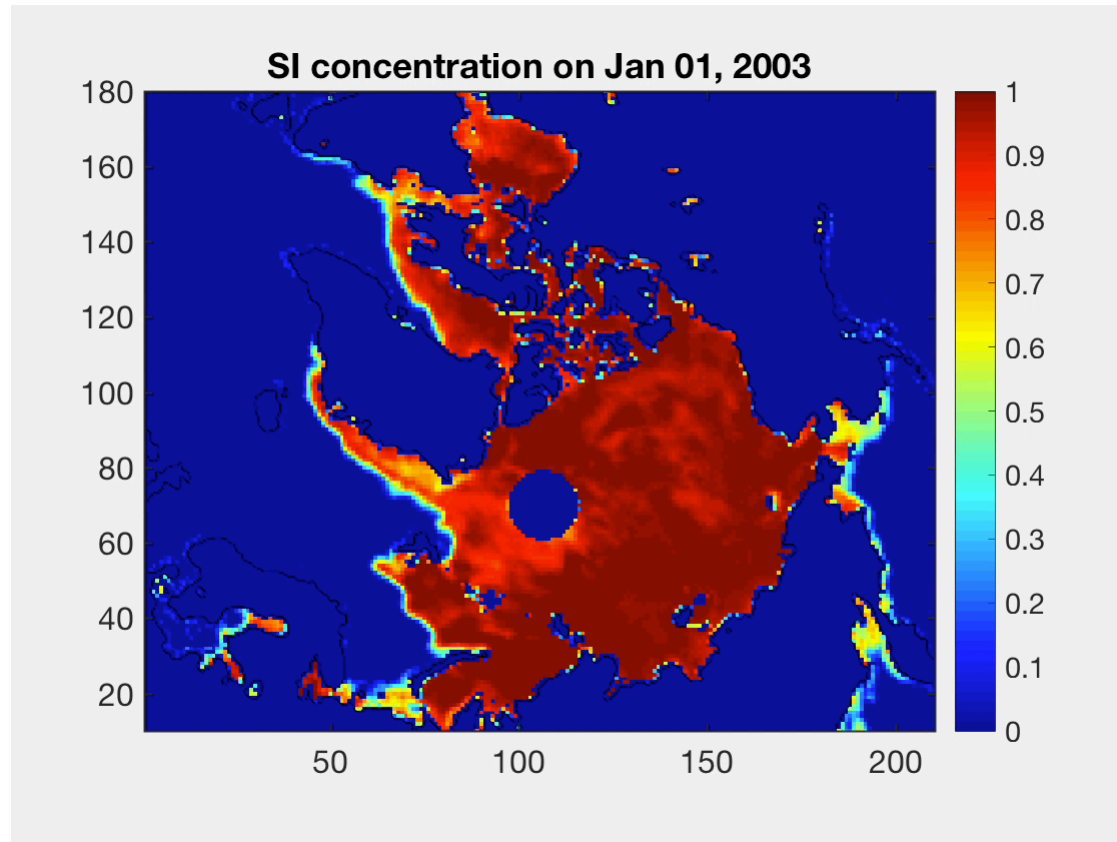


EVP

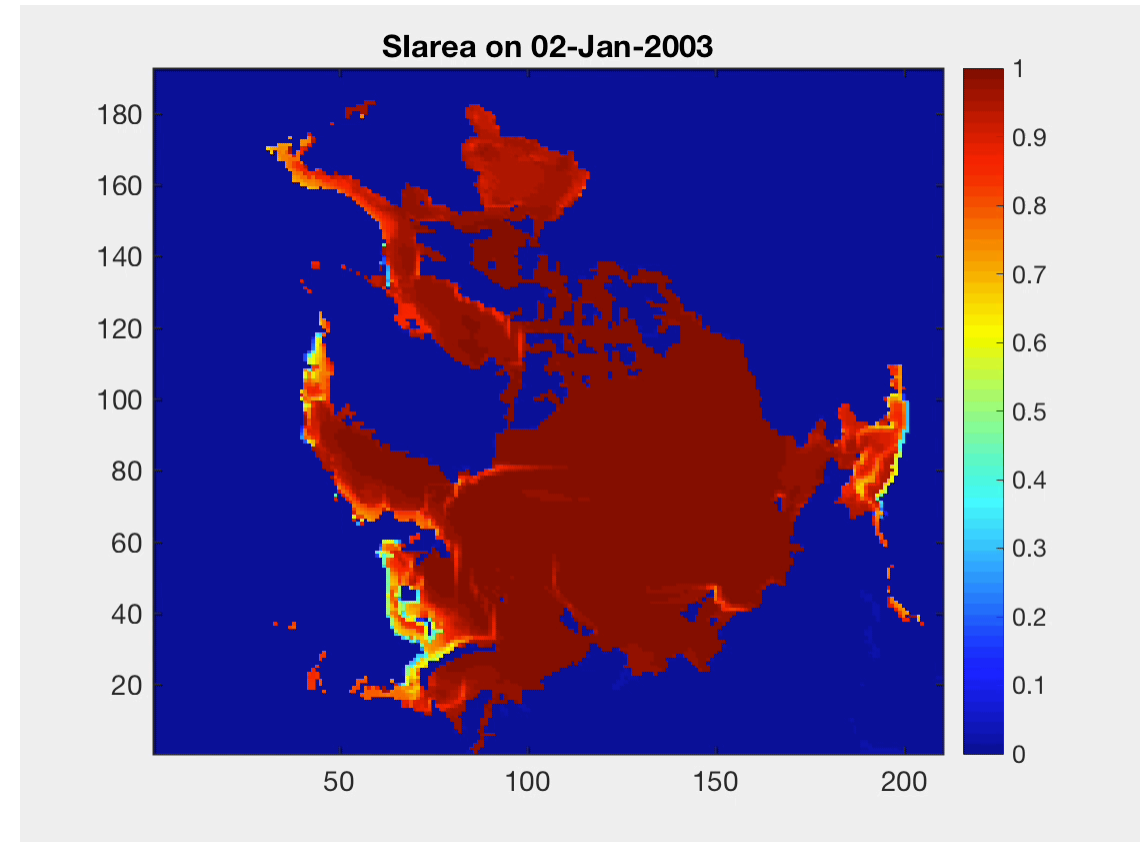


E-D

Nimbus 7



observation



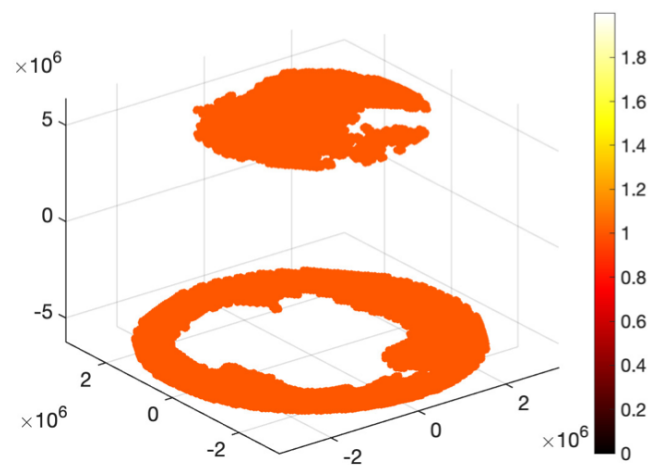
simulation

Why MPM?

- Dual description of ice: material points (Lagrangian) and mesh (Eulerian)
- Material points have all ice state and dynamics variables
- Advection performed by moving material points in the computed flow (including state variables for column physics and BCG)
- Flow is computed on the MPAS mesh
- Information is transferred between material points and the mesh by interpolation (only changes are interpolated keeping numerical dissipation relatively small)
- Lagrangian description useful for constitutive models with history dependence

MPM

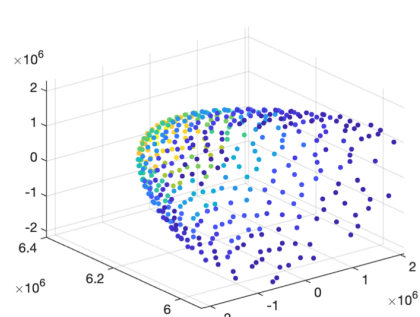
Initialization



Sea ice initial configuration using material points

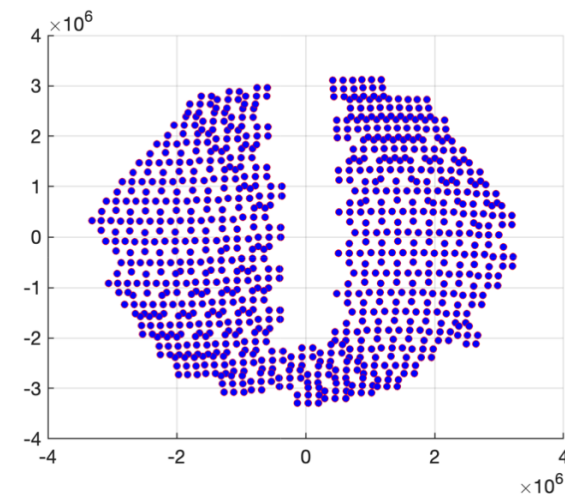
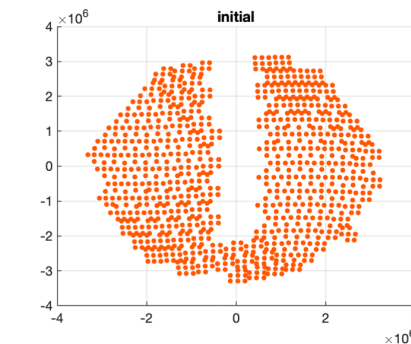
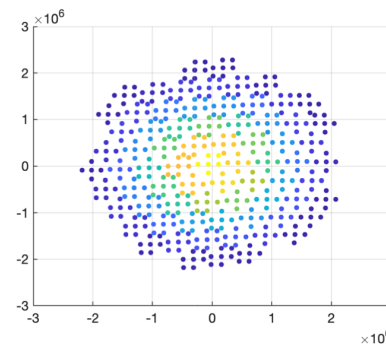
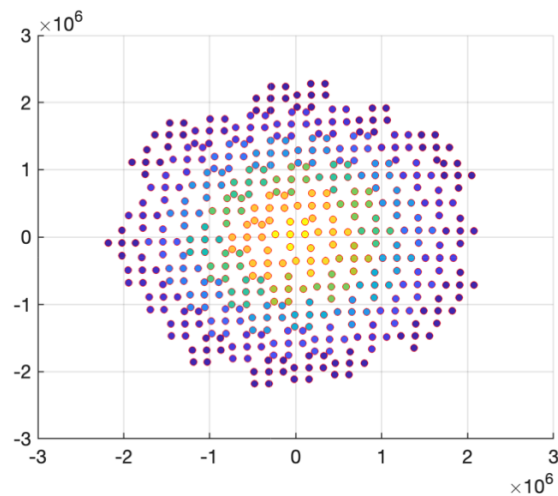
Advection test

Initial config



Velocity $(u_0 \cos \varphi, 0)$ where $u_0 = 2 \pi R / 120$ days

final config

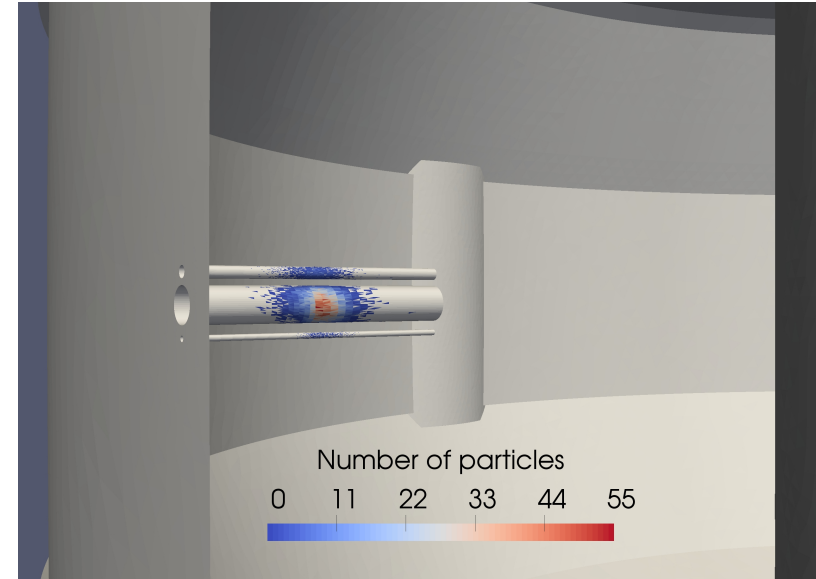
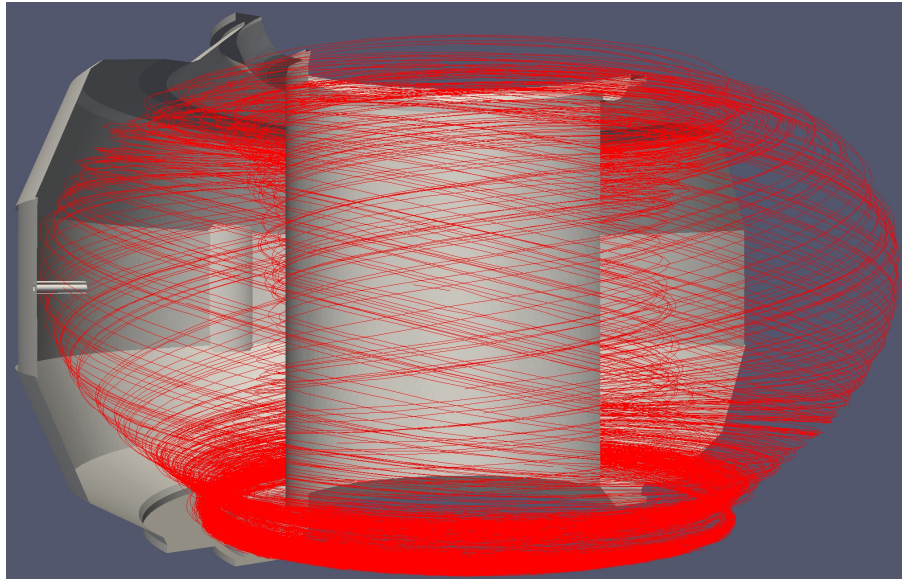
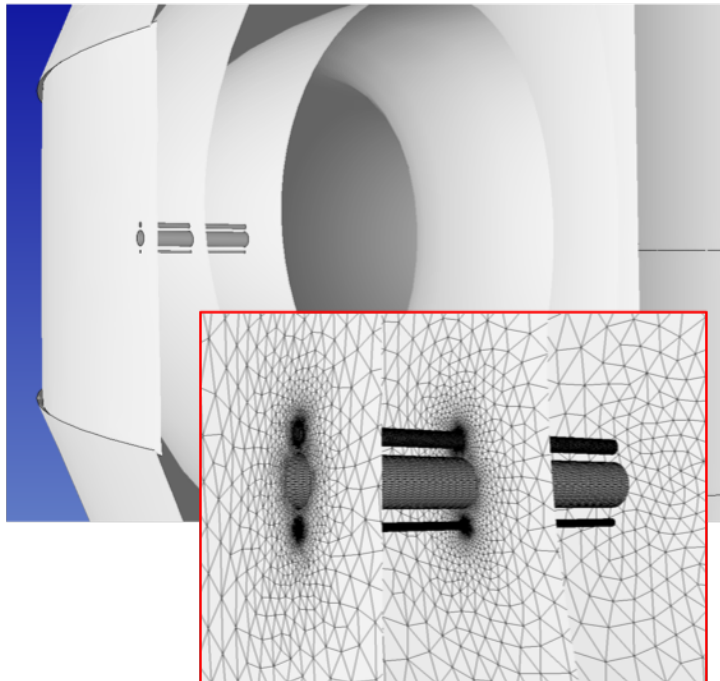


Why PUMIPic?

- PUMIPic is a GPU-enabled library that supports particle-mesh interactions for problems involving complex geometry and unstructured meshes on multi-GPU parallel computers.
- PUMIPic supports a wide range of GPU-performant data structures and is currently used by a variety of applications (e.g., fusion plasma and ice modeling over 4 FES and 2 BER SciDAC partnerships).
- PUMIPic runs on Frontier (AMD GPUs), Perlmutter (NVIDIA GPUs), and porting to Aurora (Intel GPUs) is underway. Good weak scaling was demonstrated on the full Summit system (NVIDIA GPUs) on 24,576 GPUs over 4096 nodes.
- For integration MPAS-Seaice, the polyMPO library has been built on top of PUMIPic and it supports MPAS Voronoi/polygonal meshes and relevant MPM operations including the mesh-to-MP and MP-to-mesh operations.
- polyMPO includes MLS function reconstruction on MPAS meshes, mesh-to-MP interpolation using Wachspress basis functions, and MP relocation within the MPAS mesh. It also supports Fortran interfaces to control MPM operations using `iso_c_binding`.

PUMIPic Library for GPU Acceleration

A PUMIPic-based example of the GITRm code for a particle-tracking simulation on GPUs for impurity transport in a fusion tokamak device involving 3D complex geometry with local features (probes), a highly graded unstructured mesh, and hundreds of millions of particles.



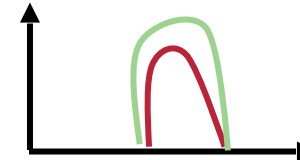
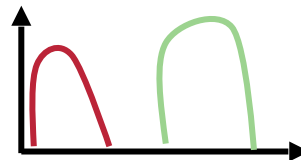
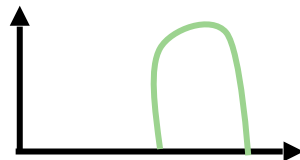
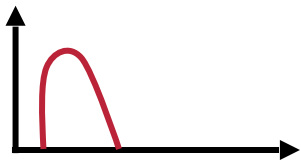
Why New Metrics?

- A Euclidean norm is not appropriate if fractures are misaligned or misshapen



Idea: Can we warp one image into the other?

Metric: Size of the warp + difference after warp



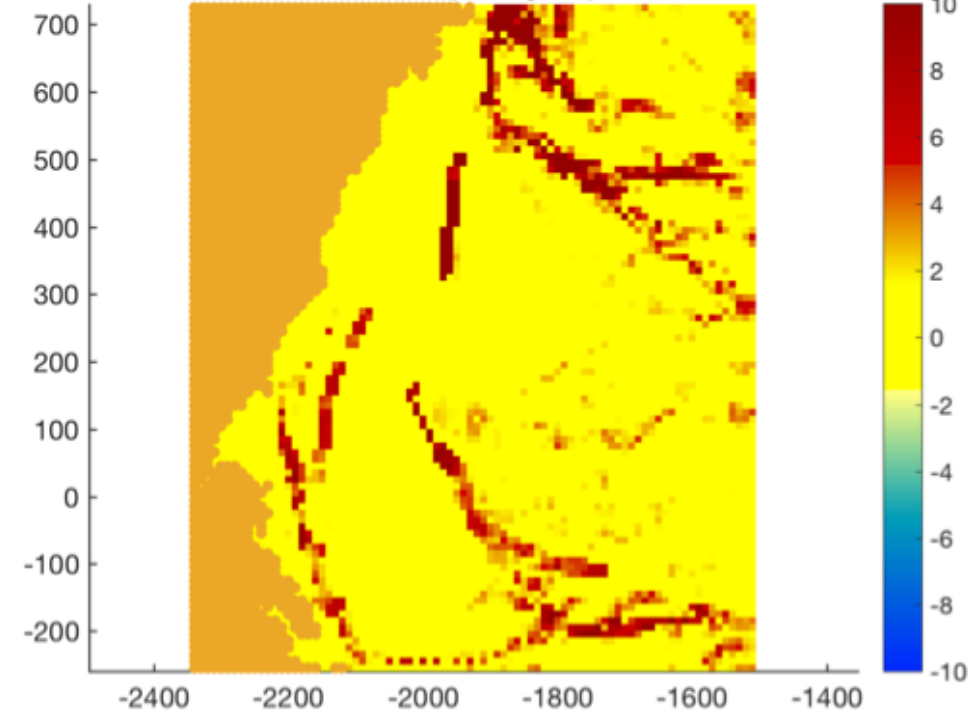
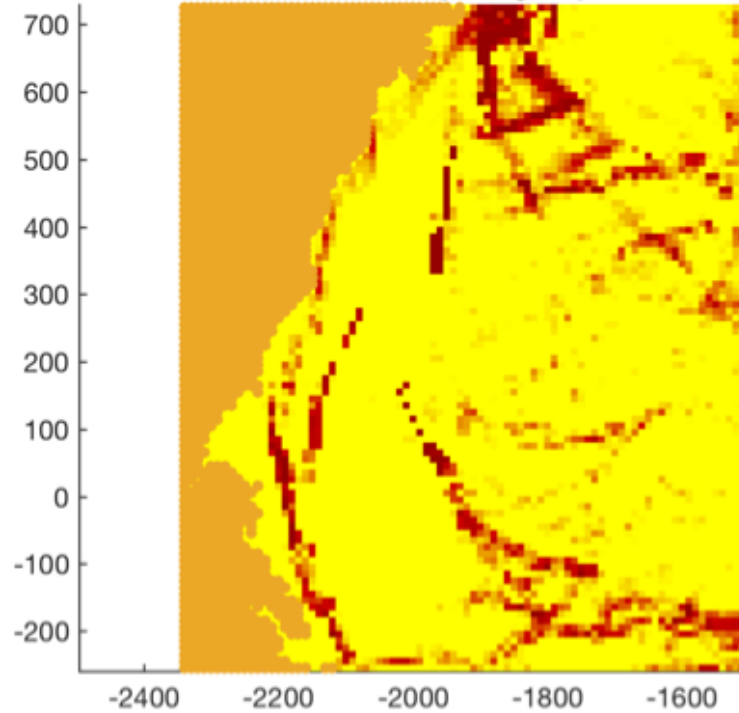
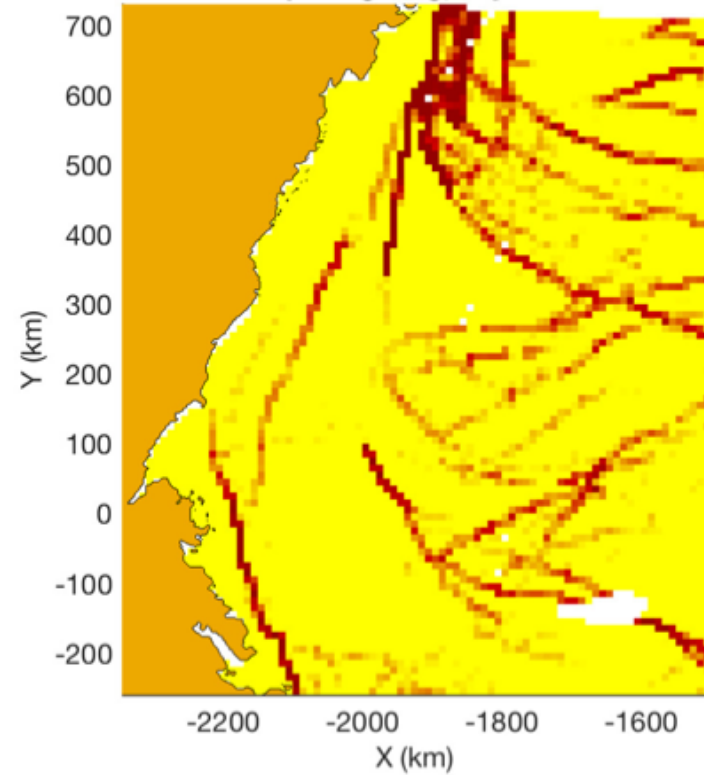
phase error + amplitude error

Calibration using RGPS data

RGPS Opening Mag, days:51.6-65.7

MPM cellOpening, day 65

MPM cellOpening, day 65



Expected Impact

- Improve the physical description of sea ice in E3SM using the elastic-decohesive model.
- Improve the representation of small scale sea ice deformation features and coupling fluxes generated by them.
- Utilize GPU accelerators in the sea ice component of E3SM through modifications to the PUMIPic library.
- Develop metrics for analyzing spatiotemporal sea ice data in general, and leads, in particular, for sea ice model validation and parameter calibration.

References

MPM

Sulsky, D., Schreyer, H., Peterson, K., Coon, M. and Kwok, R. (2007) Using the material-point method to model sea ice dynamics. *Journal of Geophysical Research*, 112, C02S90.

Sulsky, D. and Peterson, K. (2011) Toward a new elastic-decohesive model of Arctic sea ice. *Physica D*, 240, 1674–1683.

Sulsky, D. and Gong, M. (2016) Improving the material-point method. In *Innovative Numerical Approaches for Multi-Field and Multi-Scale Problems*, 217–240. Springer.

PUMIPic

Diamond, G., Smith, C.W., Zhang, C., Yoon, E., Shephard, M.S. (2021) PUMIPic: A mesh-based approach to unstructured mesh Particle-In-Cell on GPUs, *J. Parallel and Distributed Computing*, Volume 157, 1. GitHub: <https://github.com/SCOREC/pumi-pic>.

Elastic-Decohesive Model

Schreyer, H., Monday, L., Sulsky, D., Coon, M. and Kwok, R. (2006) Elastic-decohesive constitutive model for sea ice. *Journal of Geophysical Research*, 111, C11S26.

Tran, H. D., Sulsky, D. L. and Schreyer, H. L. (2015) An anisotropic elastic-decohesive constitutive relation for sea ice. *Int. J. Numer. Anal. Meth. Geomechan.*, 39, 988–1013.

Image Warping Metrics

Guan, Y., Sampson, C., Tucker, J. D., Chang, W., Mondal, A., Haran, M. and Sulsky, D. (2019) Computer model calibration based on image warping metrics: An application for sea ice deformation. *Journal of Agricultural, Biological and Environmental Statistics*, 24, 444–463.

Upston, J., Sulsky, D., Tucker, J.D., Guan, Y. (2023) CIEL*Ch color map for visualization and analysis of sea ice motion, *Journal of Computational and Applied Mathematics*, doi: <https://doi.org/10.1016/j.cam.2023.115126>.

