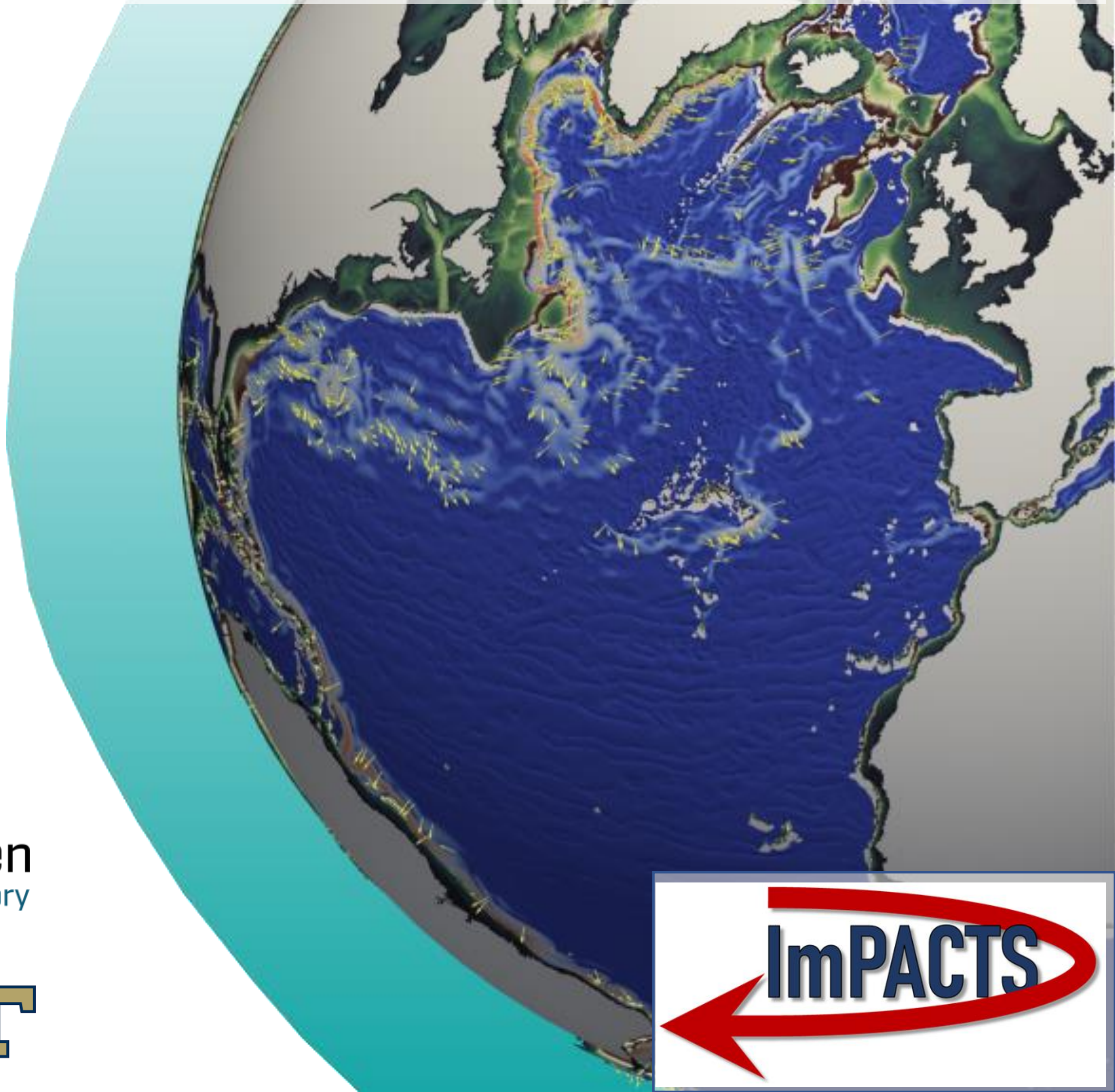
Improving Projections of AMOC and its Collapse Through Advanced Simulations (ImPACTS)



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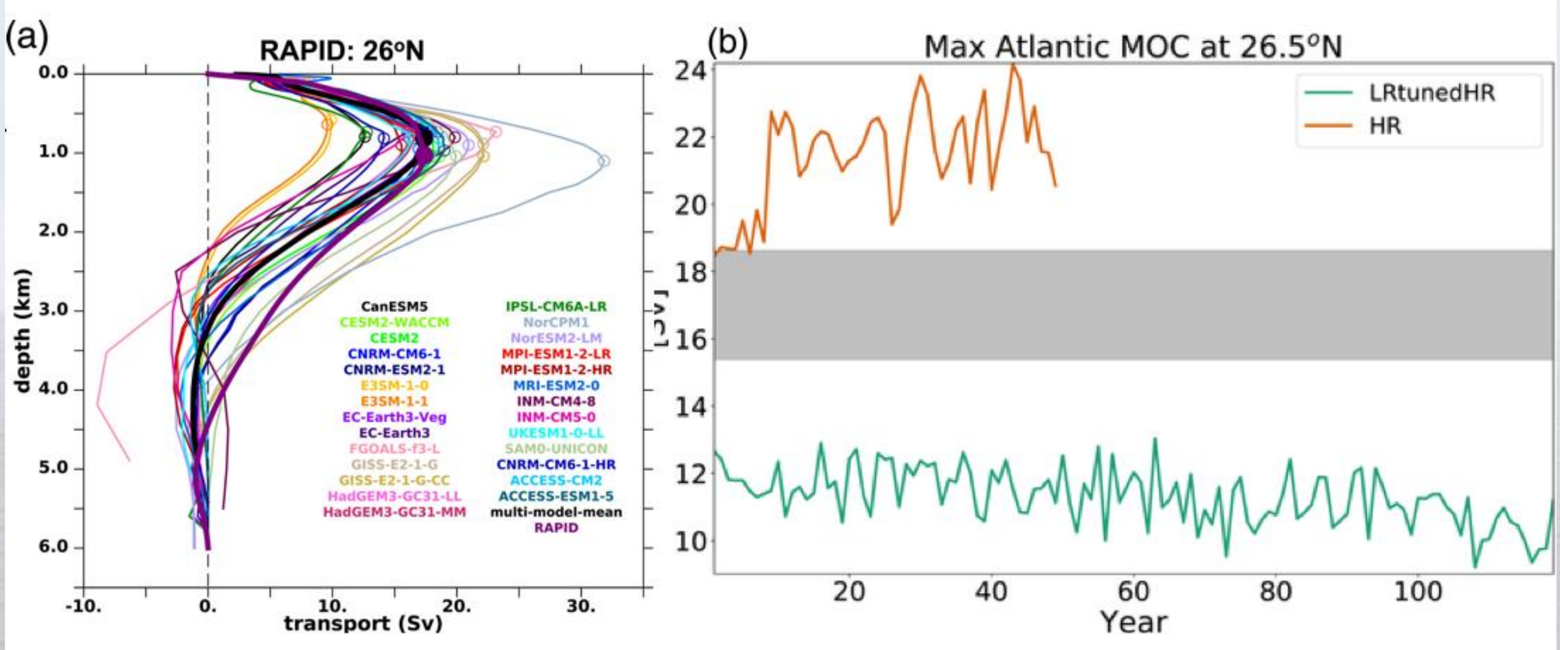
Collaborating Institutions

Los Alamos National Laboratory · Argonne National Laboratory · Oak Ridge National Laboratory · Brookhaven National Laboratory · NCAR · Scripps Institution of Oceanography · Texas, The University of Texas at Austin · Ohio State · GT

ImPACTS

Project Overview

- The Atlantic Meridional Overturning Circulation (AMOC) is a well known E3SM bias at non-eddy resolving resolutions



- A major goal of the ImPACTS project is to advance our understanding of AMOC to improve its representation in models like E3SM

Project Goals

- Understand the weak AMOC simulated by E3SM and improve the representation.
  - Leverage traditional oceanographic analyses in addition to advanced AI analysis (e.g. NN based model adjoint)
  - Collaborating directly with E3SM
- Improve analysis capability of ocean models
  - Improve in situ diagnostics, contribute to common analyses frameworks (e.g. METRIC), create novel algorithms to make lagrangian particle tracking possible for long term, high resolution configurations
- Assess AMOC stability at coarse and eddy resolving resolution
  - Advance spin up capabilities with AI methods
  - Improve model performance (GPU refactorization, new time stepping)

North Atlantic water mass transformation contributions to AMOC in eddy-parameterized and eddy-permitting simulations

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Objective

To better understand the **Atlantic Meridional Overturning Circulation (AMOC)** in E3SM at different resolutions by investigating surface temperature and salinity driven **water mass transformation (WMT)**

Water mass transformation

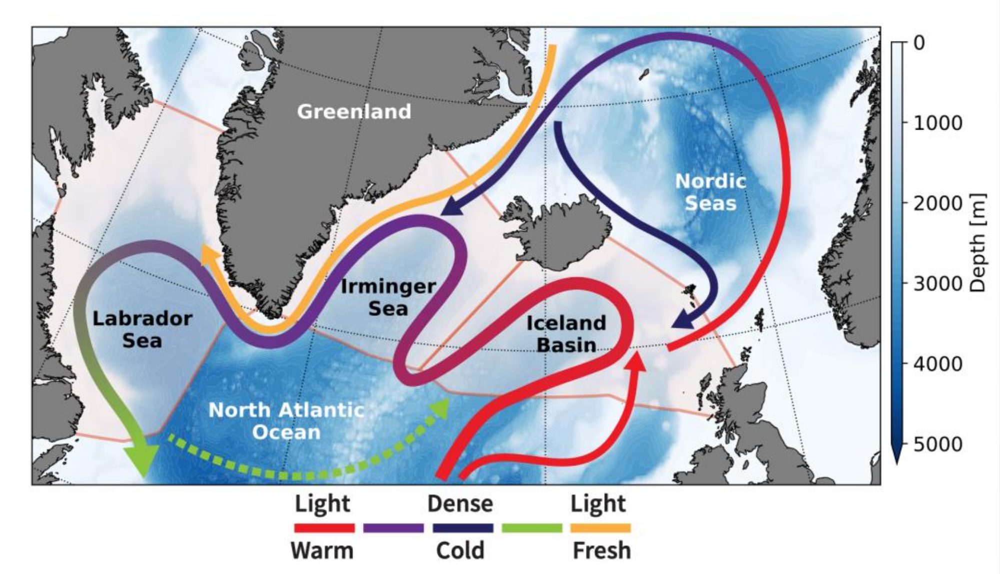
Consider some ocean surface property λ

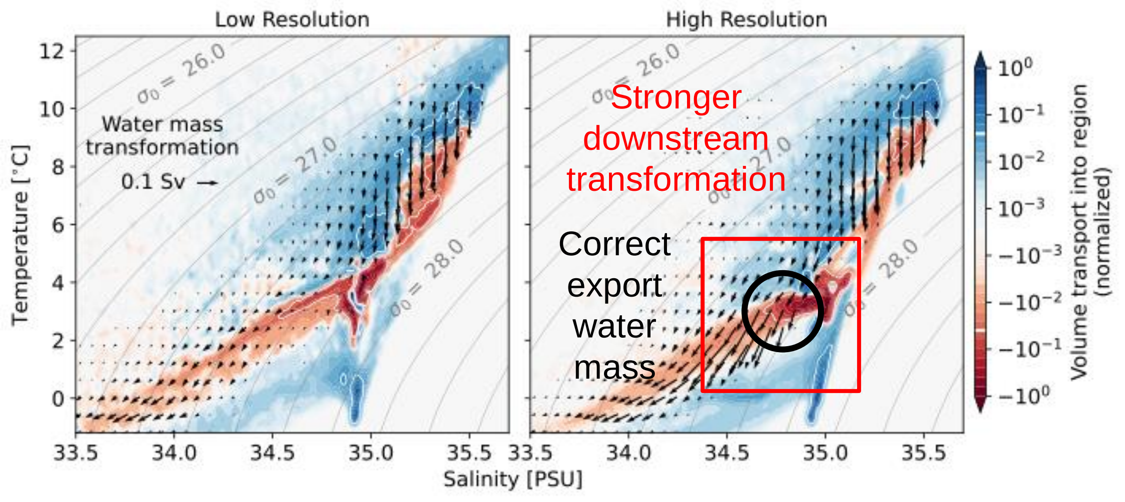
$$WMT(\lambda) = \frac{1}{\Delta\lambda} \iint [\ \Phi_{\lambda'}(x,y) \ \times \ \Pi(\lambda, \lambda'(x,y))\ ]\ dx\, dy$$

Surface flux of λ — Binning function

Simulations

- **E3SM** forced ocean-sea ice only (MPAS Ocean + MPAS Seaice, CORE-II 1948-2009)
  - **Low resolution** 30-60 km, Gent-McWilliams eddy parameterization
  - **High resolution** 6-18 km, eddy permitting/resolving





Mid-depth isopycnal, V , (U,V) and AMOC in observations and models

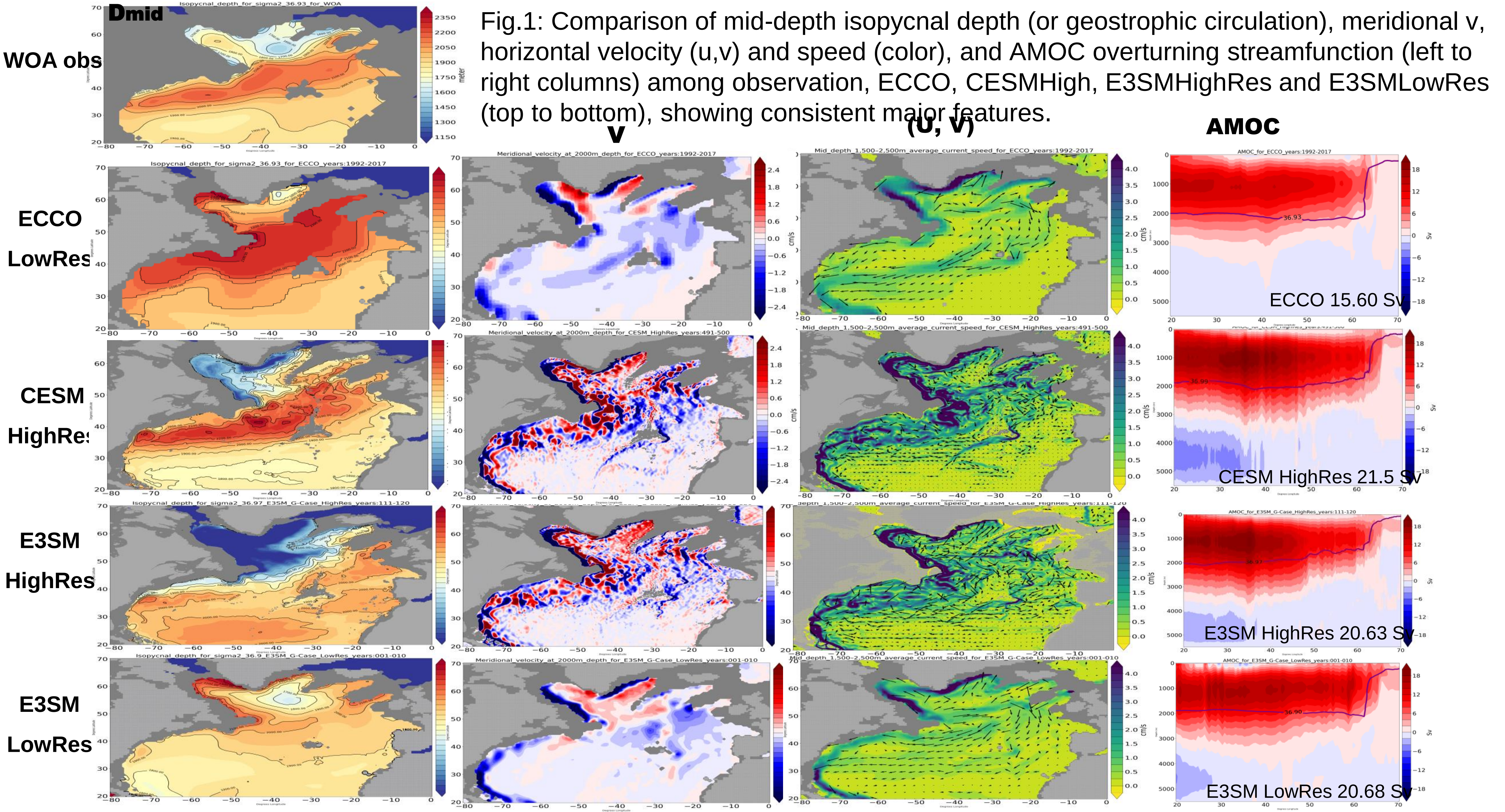


Fig.1: Comparison of mid-depth isopycnal depth (or geostrophic circulation), meridional v, horizontal velocity (u,v) and speed (color), and AMOC overturning streamfunction (left to right columns) among observation, ECCO, CESMHigh, E3SMHighRes and E3SMLowRes (top to bottom), showing consistent major features.

Explainable AI for Deep Climate Models

A Preliminary Study for Understanding Deep Neural Networks in their Applications to Climate Prediction

Scientific Achievement

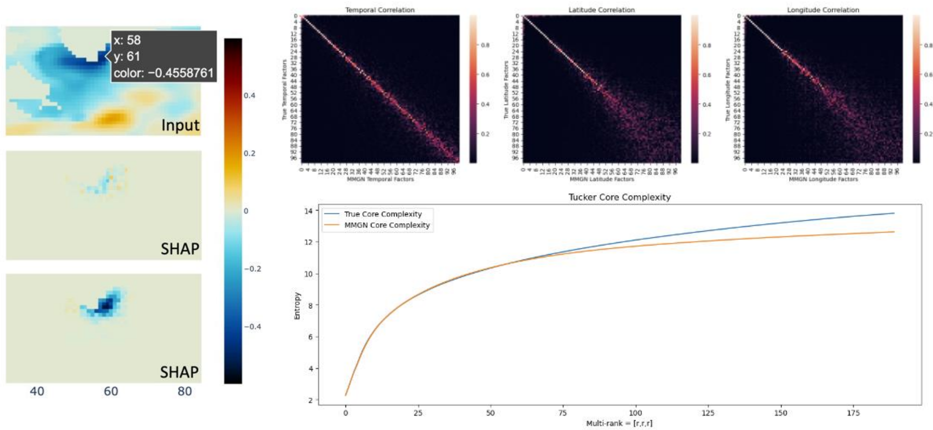
We present a study using a number of post-hoc explanation methods to enhance the transparency and understanding of the deep neural networks developed for the global or oceanic surface temperature reconstruction and prediction.

Significance and Impact

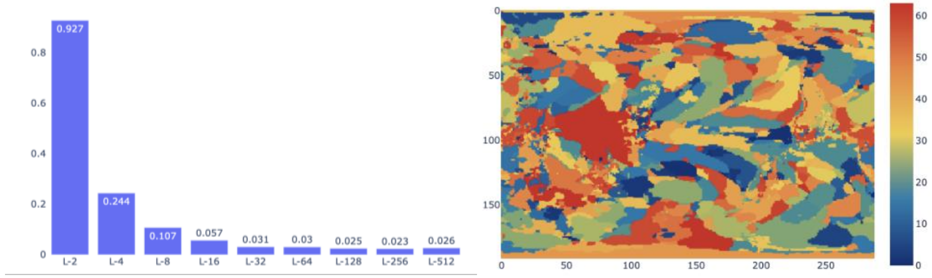
We demonstrate that Explainable AI (XAI) algorithms are effective and useful to bridge the knowledge gap between model developers and domain experts and assist the latter to gain confidence when adopting deep learning approaches.

Technical Approach

- Compared four feature importance methods as a spatial-temporal explanator highlighting the input regions and contributive months to the output location.
- Adopted a few dimension reduction methods (embedding, clustering, correlation analysis, tensor factorizations) to understand and compare latent spaces learned by the neural networks.
- Demonstrated the contextual information incorporated in the latent representations and their impact on the model performance.



Left: The heatmaps generated by a feature importance method (SHAP) highlighting the input regions of two different previous months (in row two and row three) contributing to the prediction of the output location.
Right: The correlation plots comparing the tensor decomposition in three directions (temporal, latitude, and longitude) of the latent space and the original data space.



Left: The correspondence of the learned latent representations and the original data showing that a larger latent size incorporating more contextual information.
Right: The ablation result indicating spatial linkage of temporal index.

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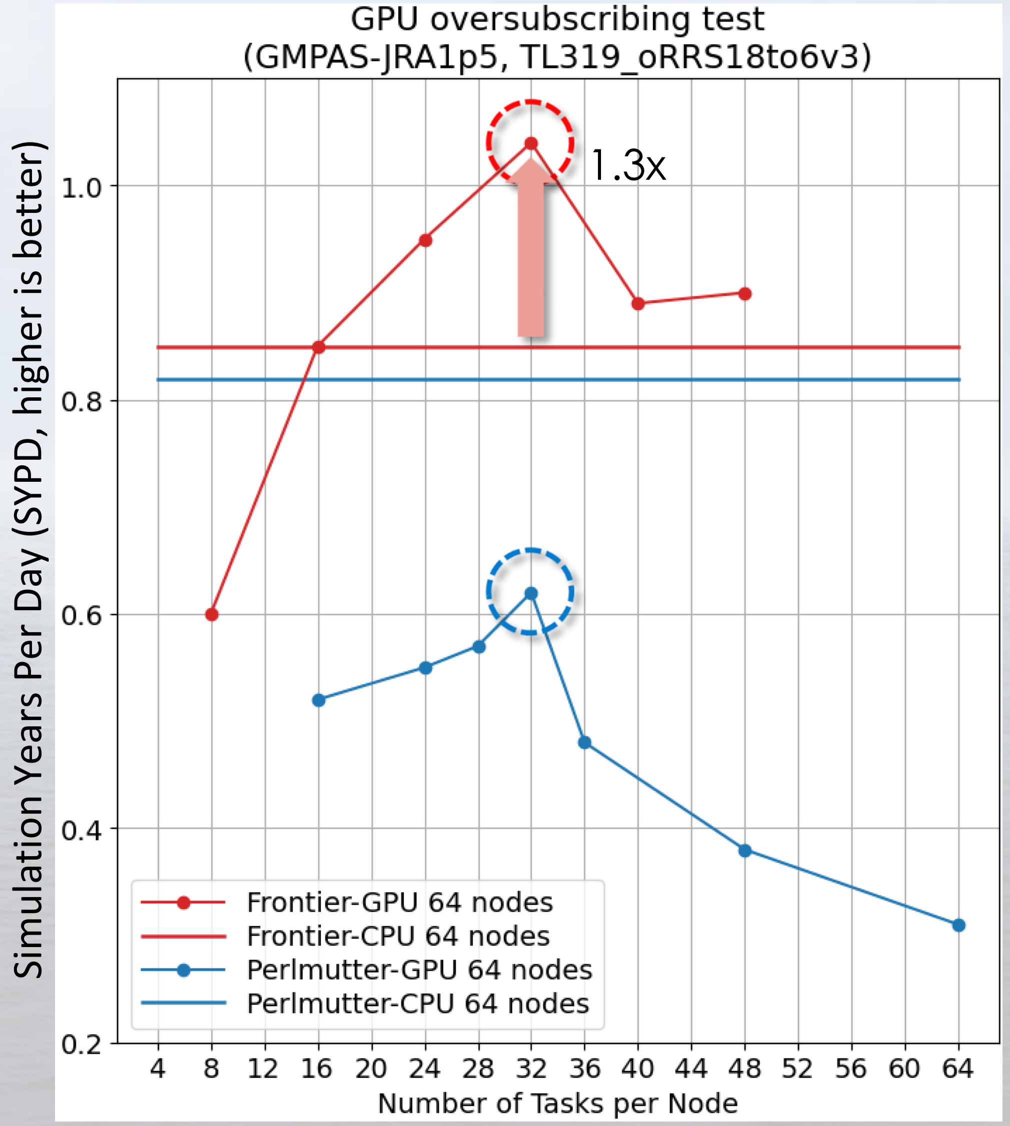
W. Xu, D. F. DeSantis, X. Luo, A. Parmar, K. Tan, B. T. Nadiga, Y. Ren, and S. Yoo, "Studying the Impact of Latent Representations in Implicit Neural Networks for Scientific Continuous Field Reconstruction," AAAI co-held XAI4Sci workshop, Feb. 2024.

Brookhaven National Laboratory

High-Resolution Ocean: Performance

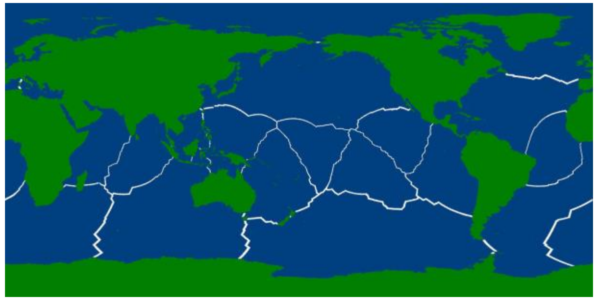
- GPU oversubscribing (multiple ranks/GPU)
  - Case: GMPAS-JRA1p5 (active ocean & sea-ice)
  - Resolution: RRS18to6 (18 km to 6 km)
- 1.1 SYPD on Frontier GPU
  - 4 CPU cores share 1 GPU (32 MPI tasks per node)
  - GPU performance exceeds CPU performance by oversubscribing GPUs (~1.3x).
- 0.62 SYPD on Perlmutter GPU
  - 8 CPU cores share 1 GPU (32 MPI tasks per node)
  - GPU performance is poorer than CPU.



Particle Thrust Year 2 Progress

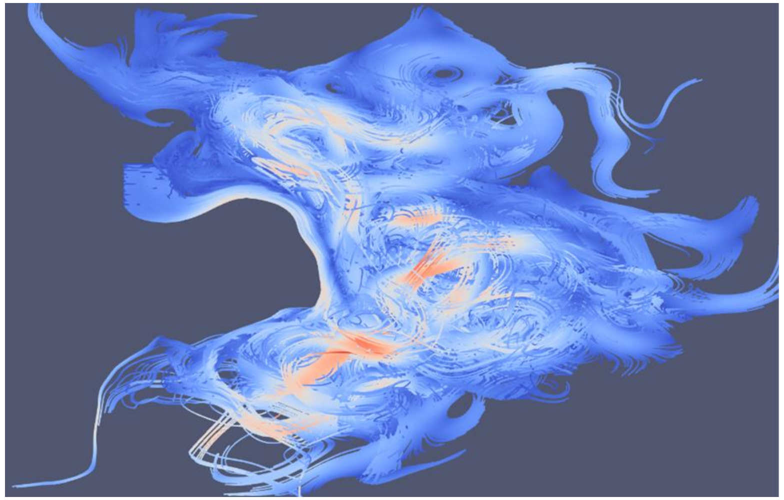
GPU Acceleration (Guo)

- Designed efficient data structures for cell locating and interpolation with MPAS-Ocean meshes on GPU
- Implemented high-accuracy integration that couples horizontal/vertical advection with RK4, optimized for GPUs
- Experimented high-resolution grid (RSS6to18) on one single GPU on Perlmutter



Distributed Parallelism (Shen)

- Designed domain partitioning for distributed particle tracing
- Implemented Streamed data I/O for time-varying data
- Supported sub-domain particle tracing for distributed workflow later



In Situ Workflow (Peterka and Yildz)

- OSUFlow Spack build with LowFive, Wilkins, NetCDF4, and HDF5
- Integrating in situ data transport layers (LowFive data transport library and Wilkins workflow management) with MPAS-O
- Experimenting coupling with the GPU particle tracing

The Ohio State University

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Near term deliverables

New capability for E3SM

- Increased GPU coverage
- Bug fixes in salinity restoring and vertical mixing
- New analysis (Fov and WMT)

Upcoming deliverables to E3SM

- Diffusive overflow parameterization (Fall 2024)
- Estuary box model (Fall to winter 2024)

Upcoming Goals

New simulations

- Begin simulations of AMOC stability at high resolution in E3SM and CESM
- Conduct and analyze transient simulations with CESM and E3SM to understand initial salinity drift in E3SM

ML/AI and Adjoints

- Identify useful, stable and non-oscillatory objective functions for the adjoint computation.
- Exploit the advances in energy-based/diffusion/neural operator models in the latent space for accurate spatial-temporal forecasts for longer time horizons.
- Use TF techniques to discover dominant spatio-temporal modes in the system
- Use scalable causal inference is beneficiary to identify and understand direct and indirect causal pathways of AMOC
- Explainable AI (xAI) approaches will be developed to increase transparency, guide development, and build trust in developed models, especially for domain users

Software

- Release first version of `Moka.jl` (a lower order MPAS-Ocean written in Julia) package following the redesign of the software infrastructure and infer parametric sensitivities through automatic differentiation