Study for Exascale Advances in a High-resolution Ocean using ROMS Coupled to E3SM (SEAHORÇE)

BER & ASCR Scidac 5 project

SEAHORÇE

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U.S. DEPARTMENT OF ENERGY | Office of Science

Project objectives

The **Study for Exascale Advances in a High-resolution Ocean using ROMS Coupled to E3SM** (SEAHORÇE) SciDAC5 project will:

Focus on ***improved representations*** *of small-scale coastal and open-ocean processes* — such as river plumes, coastal fronts, and meso- and submesoscale eddy processes — in the context of global ESM,

Design a scientific and technical ***framework for two-way coupling*** between ROMS and MPAS-O for optional, flexible, efficient, and robust dynamical up- and downscaling, and

Create ROMS-X, a GPU-enabled port of ROMS that will exploit the latest DOE exascale HPC architectures.

Dynamics Across Scales with MPAS-O

O(30km) 'ESM-LR' config. (not shown)
Missing dynamic evolution of loop current/eddies.

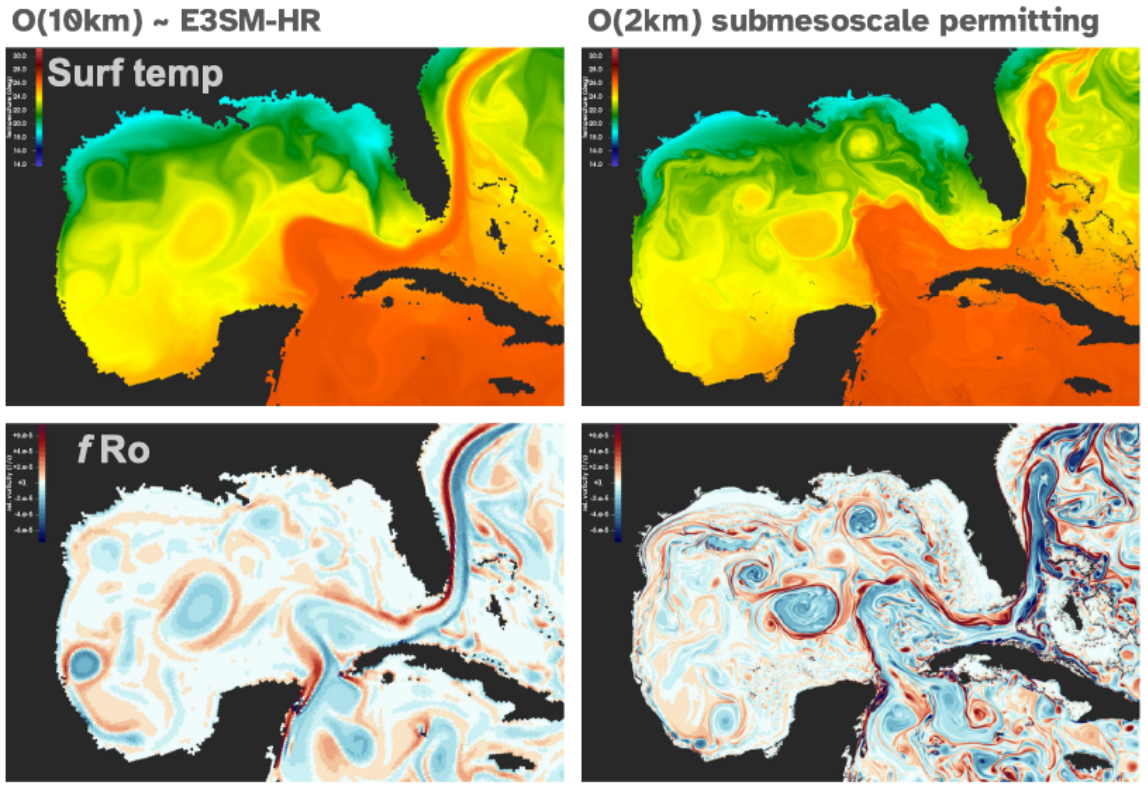
O(10km) 'E3SM-HR' config.
Eddy features present, but weak

O(2km) config.
Sharper fronts, and instabilities forming within the fronts, approaching submesoscale*

*Submesoscale is a dynamical scaling that depends on stratification and flow conditions,

submesoscale:	Ro~1, Ri~1
mesoscale:	Ro<<1, Ri>>1

or, *anisotropic energetic instabilities*



Dynamics Across Scales with MPAS-O

Submesoscale-permitting simulations with MPAS-Ocean positions us at forefront of contemporary O(1-5km) 'very high-resolution' ocean modeling efforts worldwide — but...

...these simulations are expensive!

- O(2km) represent highest resolution (baroclinic) MPAS-O simulation to-date.
- Current throughput: 96 simulated-days-per-day using 12,000 cores (NERSC HPC).
- Short, 5 year model spin-up requires 3 weeks wall clock.
- Are submesoscale dynamics 'well-enough' resolved at O(2km) resolution? No...
- Expect ***x4-x8 slowdown*** to achieve O(1km) resolution.
- Typical ROMS applications employ O(100m) resolution to capture submesoscale effects.

There are limits to how far we can refine resolution with MPAS-O, however, ***E3SM-HR (18-6km) efficiently spans the mesoscale-permitting space for global climate modeling, allowing meaningful coupling to 'coastal' or submesoscale models.***

A ***targeted, temporary, stealth nesting/coupling*** approach is reasonable considering

- Scientific questions may be limited to a particular domain (e.g., ICoM, GLM, InteRFACE)
- Smaller scale process have shorter spin-ups – a year is sufficient for most continental shelves
- Many small scale processes do not influence larger scales, so nesting will often be OK

Relevance for E3SM

A hierarchical approach using a nested/coupled ROMS in MPAS-O allows:

- Downscaling for actionable projections

  Better project climate signals in coastal regions, e.g., marine heat waves, and nutrient and carbon cycling in river plumes.

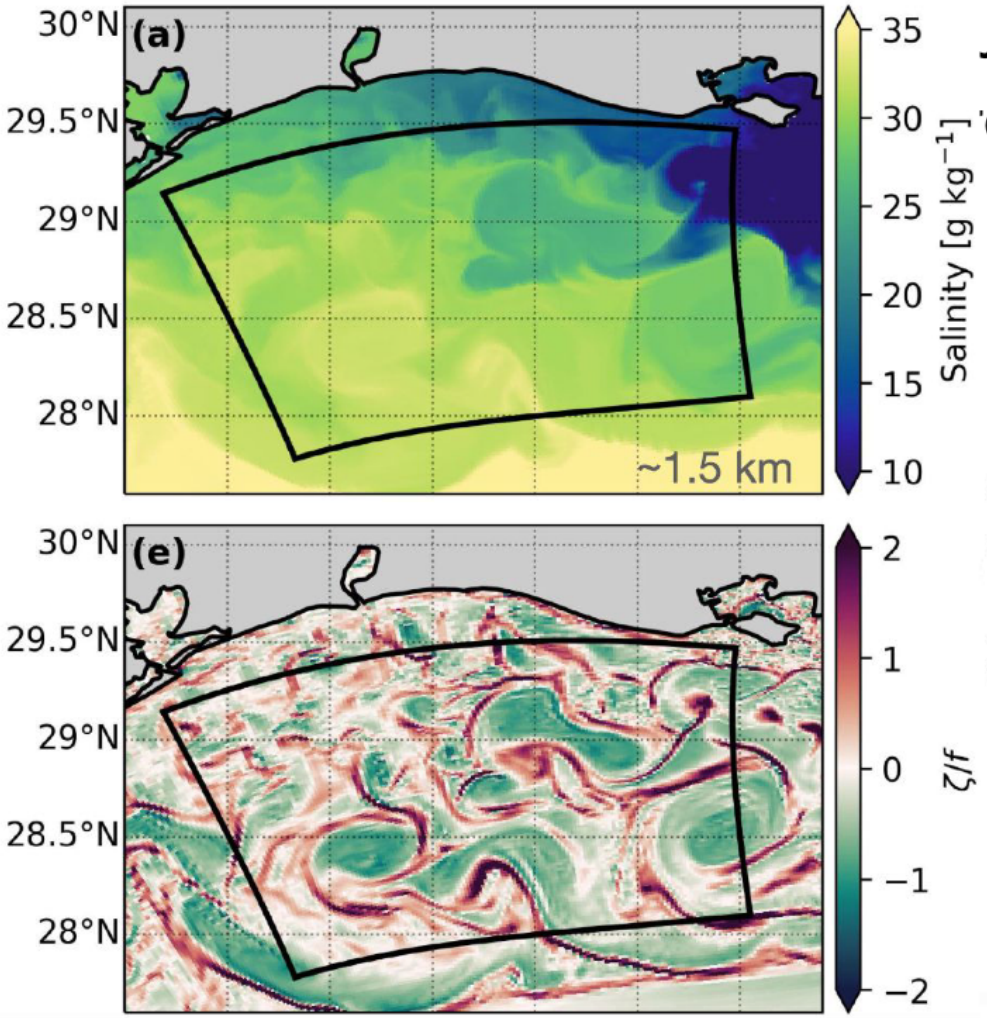
- Better process understanding

  E.g., biases in surface temperatures could be due to mis- or under-represented ocean processes; local refinement can help identify the sources of these biases.

- More efficient simulations

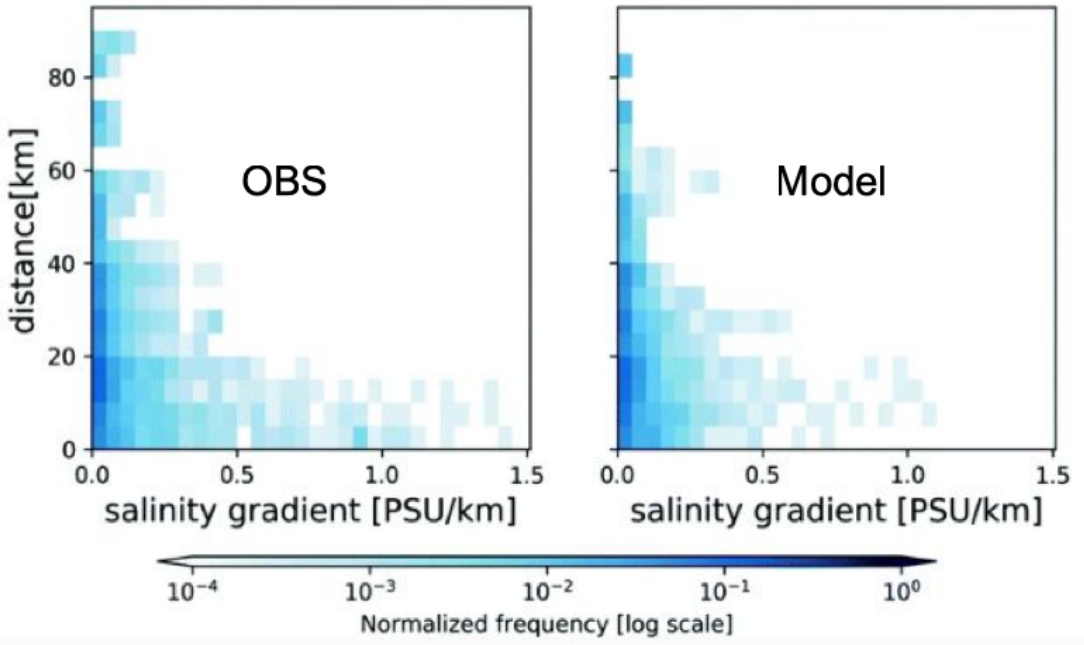
  A O(10km) E3SM run with targeted, temporarily nested grid refinement will allow for more efficient simulations, compared to a single refined MPAS-O grid due to long oceanic spin-up times.

  ROMS-X will allow us to continue this approach with GPU enabled E3SM.



Schlichting et al, (*JAMES*, 2023)

-1 km ROMS simulation is able to reproduce key submesoscale features.



Kobashi and Hetland (*Ocean Dyn.*, 2020)

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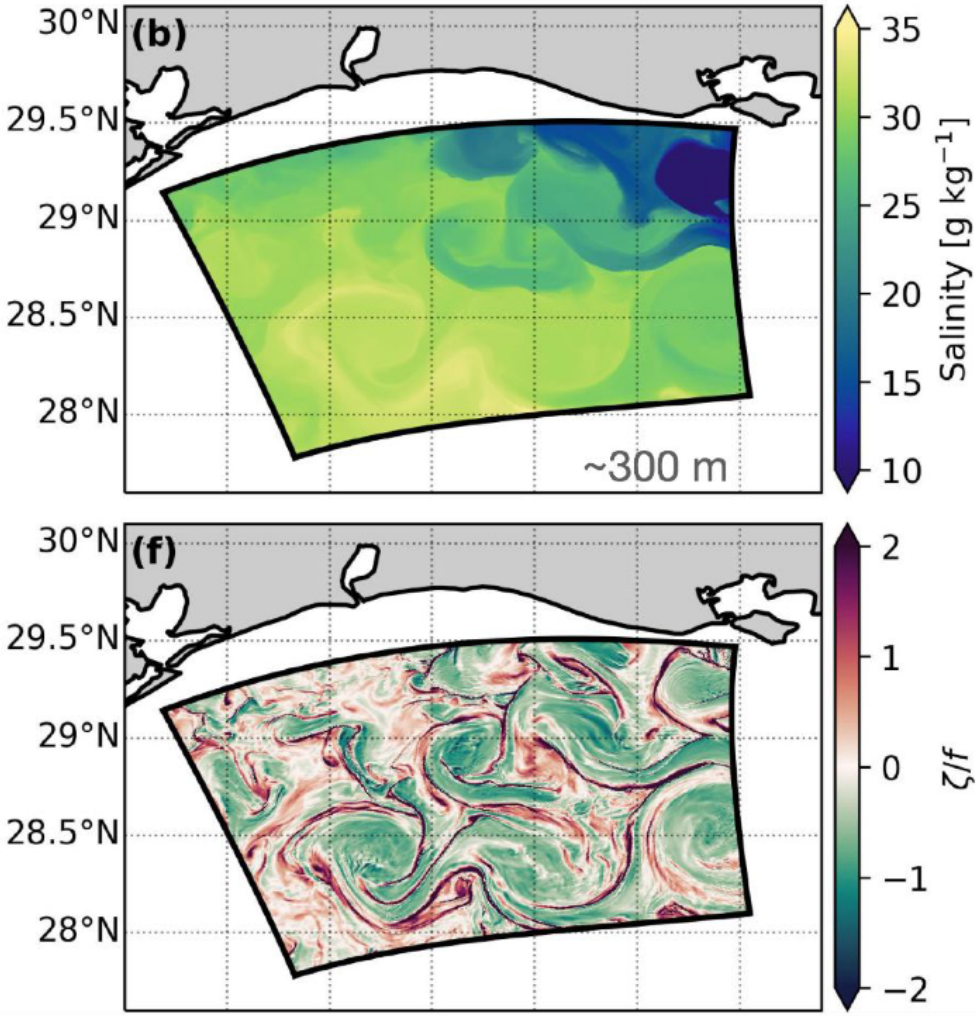
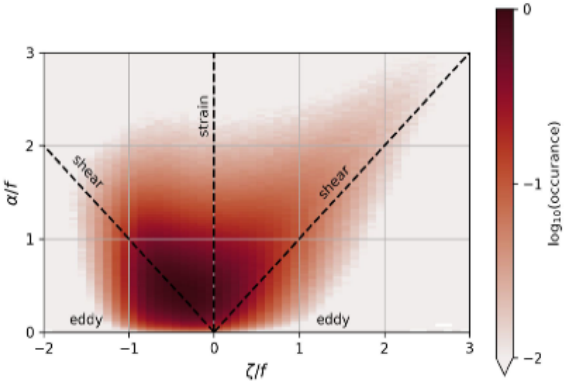
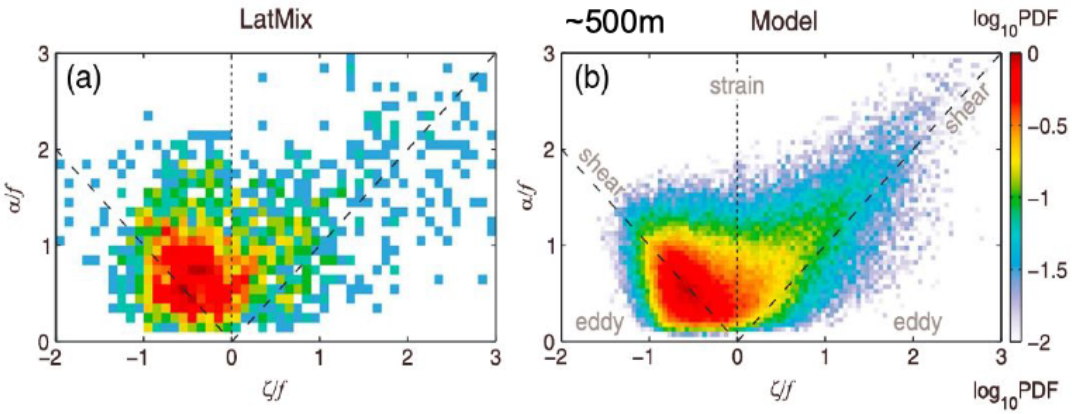


Schlichting et al, (*JAMES*, 2023)

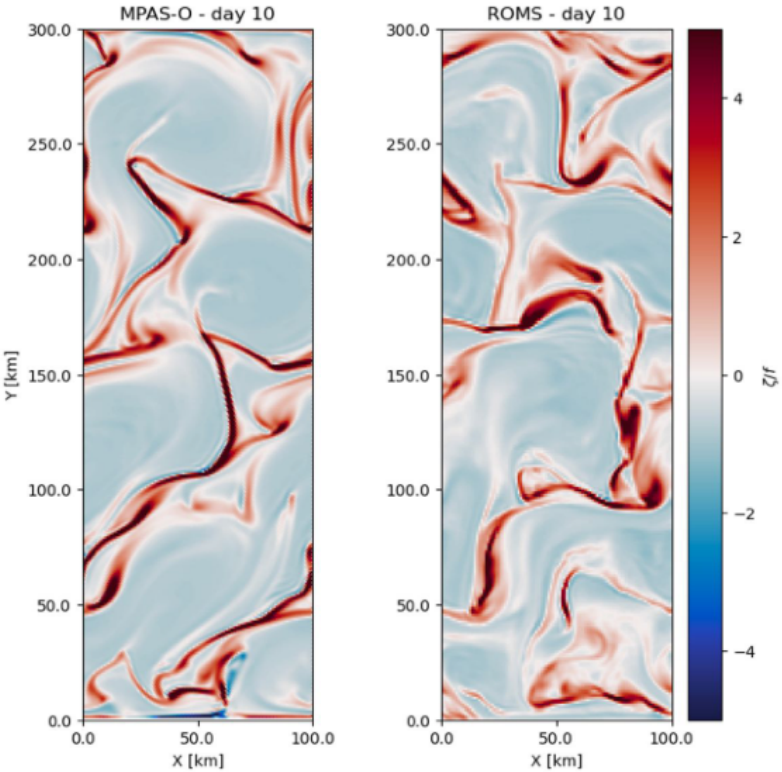


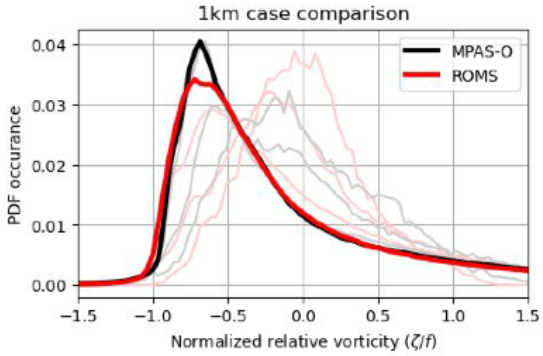


Shcherbina et al, (*GRL*, 2013)

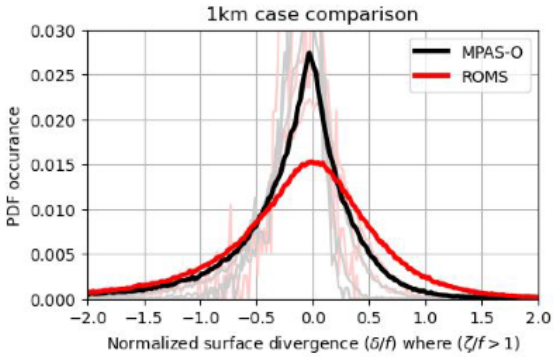
MPAS-O/ROMS comparisons

Idealized domain baroclinic instability in a channel



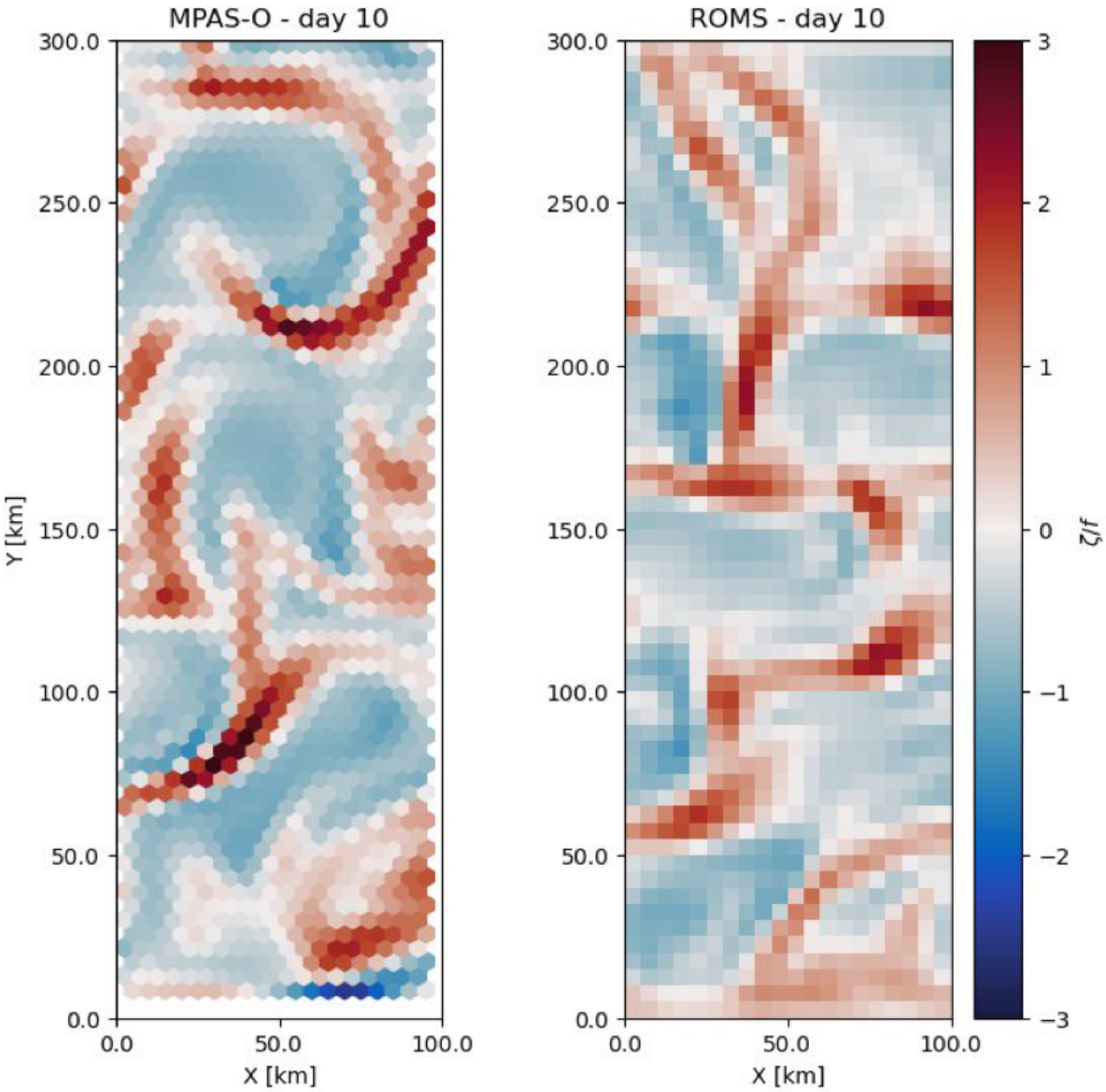


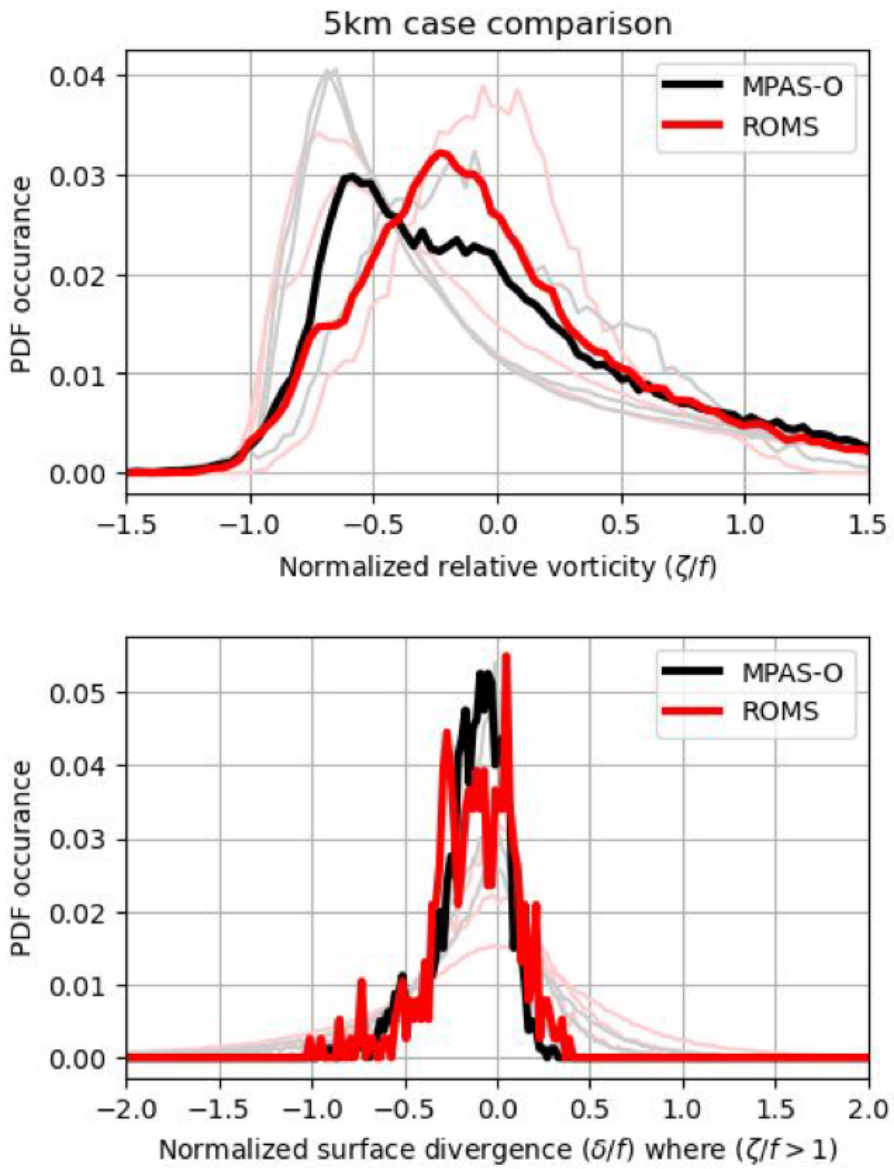
Both models have similar surface vorticity structure, especially in the vicinity of the strong cyclonic (ζ/f>1) flow at the fronts.



ROMS has slightly stronger convergence and divergence in regions of strong cyclonic flow (ζ/f>1) indicating frotogenetic dynamics within each model differs slightly.

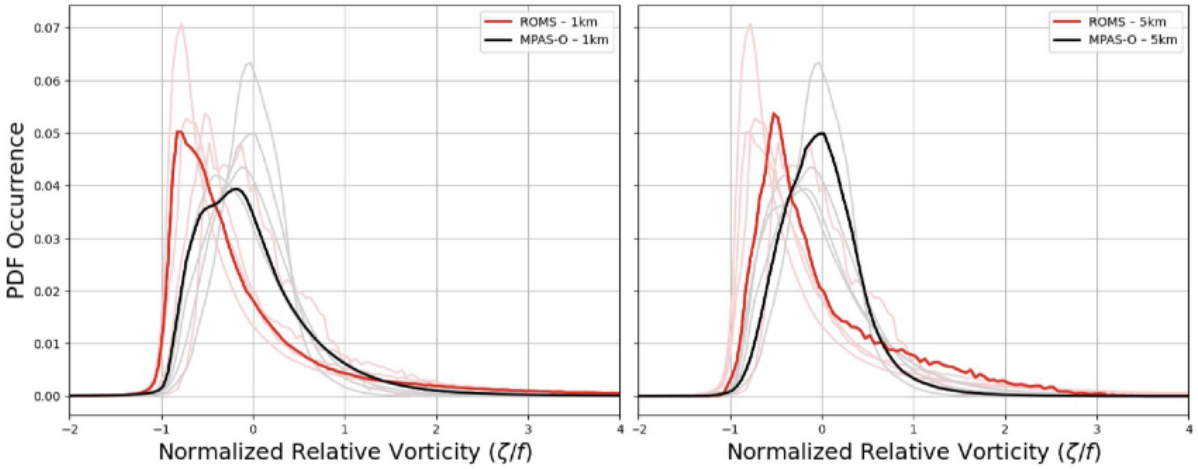
Both MPAS-O and ROMS show qualitatively similar flow characteristics in vorticity and other properties, suggesting a similar effective resolution of dynamical properties.


MPAS-O - day 10
ROMS - day 10
Y [km]
X [km]
X [km]
ζ/f
0.0
50.0
100.0
150.0
200.0
250.0
300.0
−3
−2
−1
0
1
2
3

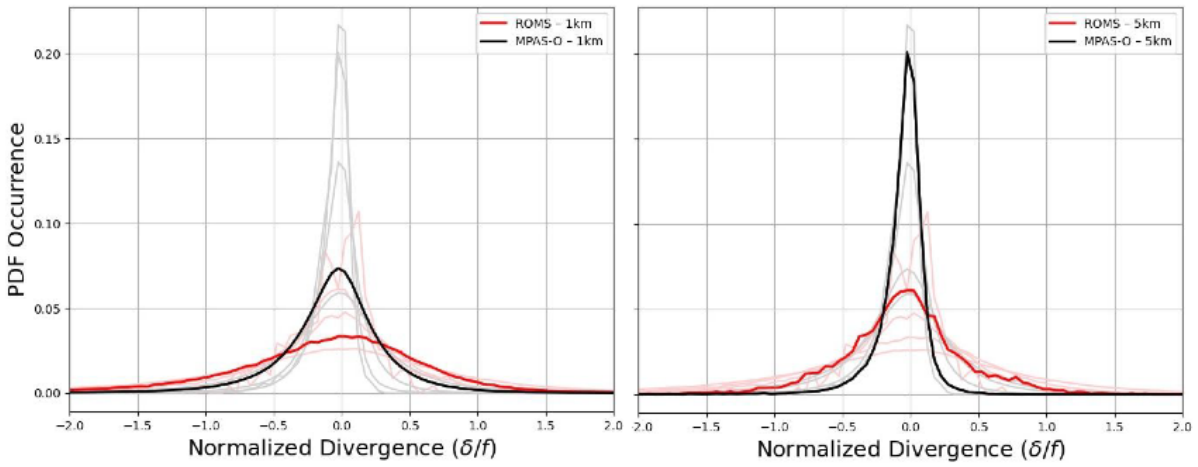

5km case comparison
MPAS-O
ROMS
PDF occurance
Normalized relative vorticity (ζ/f)
Normalized surface divergence (δ/f) where (ζ/f > 1)
0.00
0.01
0.02
0.03
0.04
0.05
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

1 km **5 km**

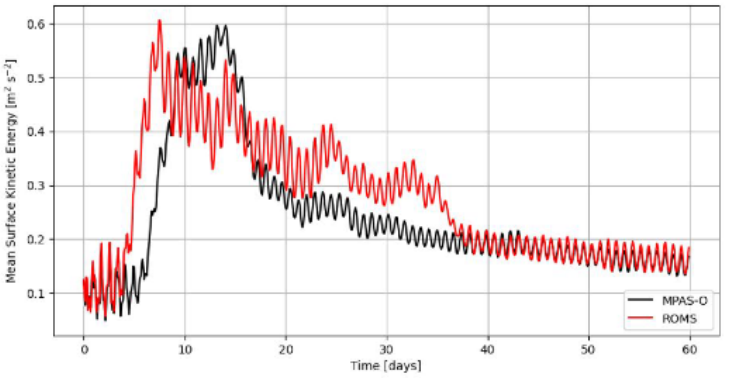
ζ/f



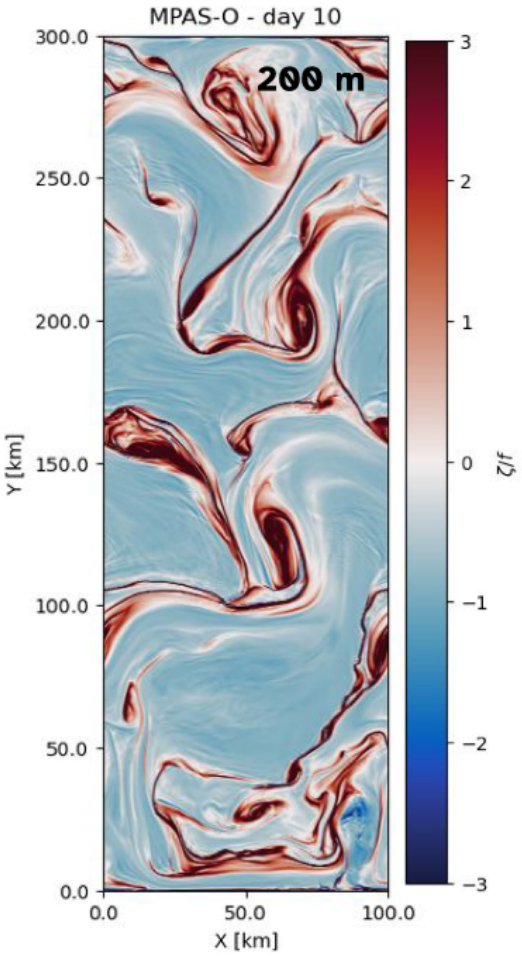
δ/f



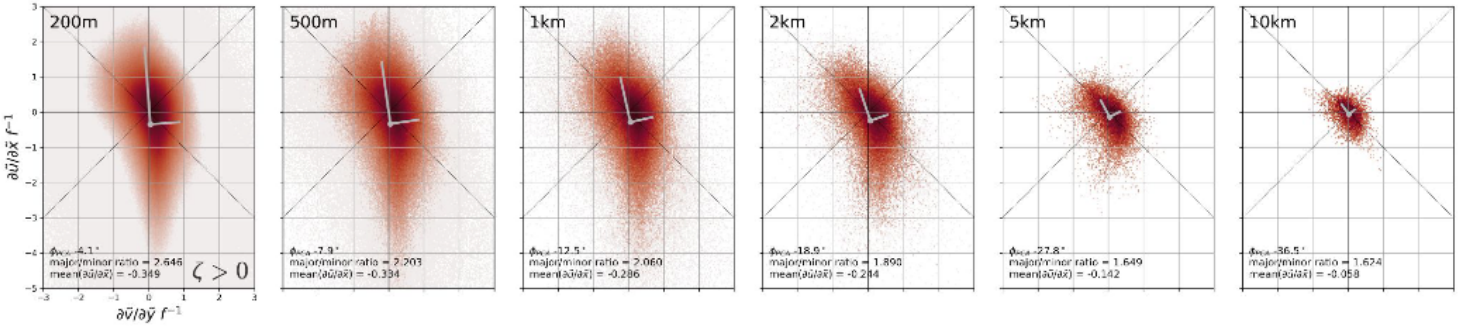
Newer results, where the parameters are more closely aligned between the two configurations shows that the models have diverged slightly in ζ/f distributions, but are more similar in EKE evolution.



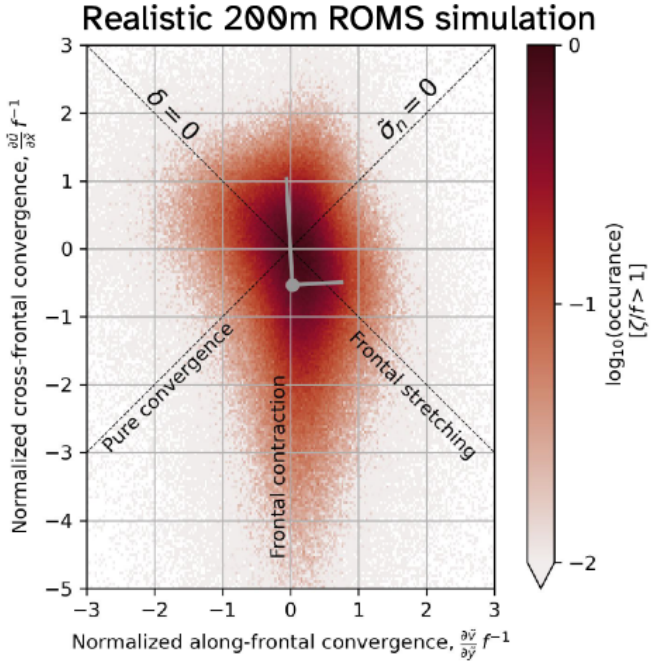
Next steps



Idealized ROMS simulations



Realistic 200m ROMS simulation

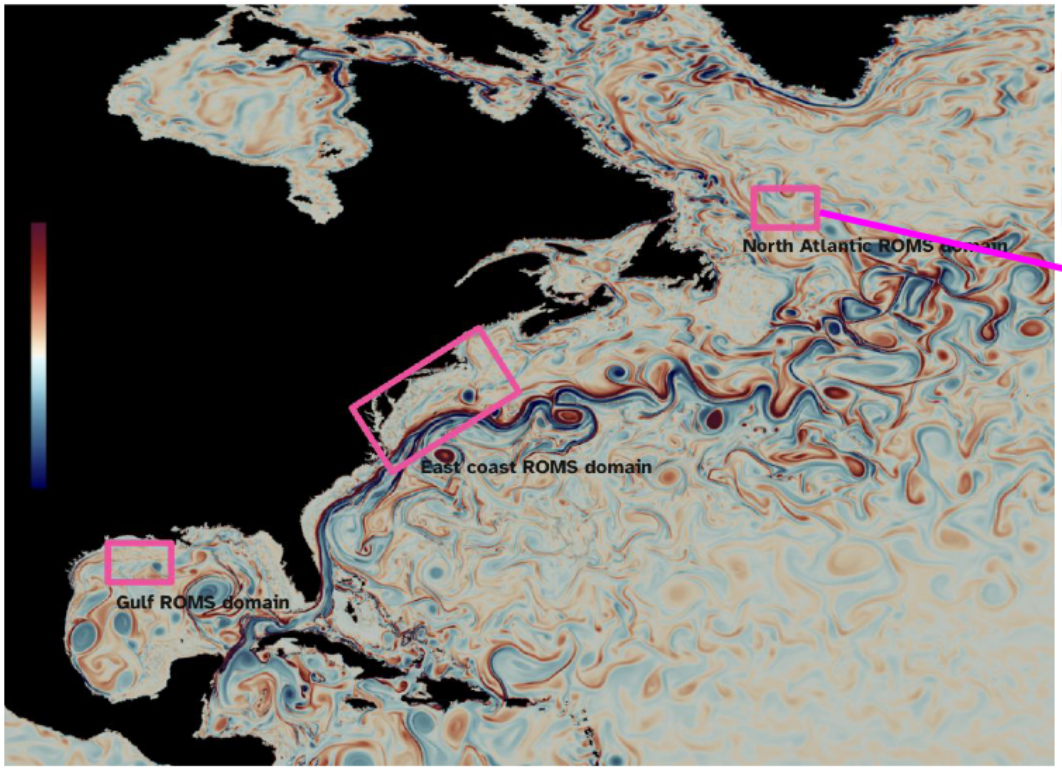


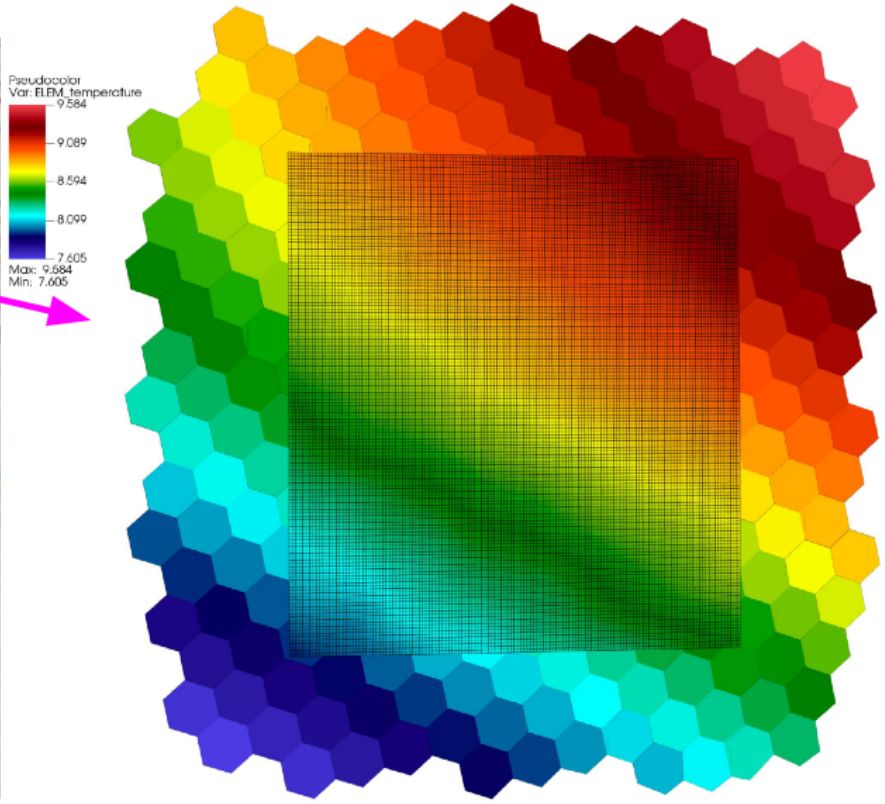
We have a framework to compare frontal processes at different resolutions

Model results suggest the same meso- to sub-mescoscale transition seen in the Loop Current region in the 2km MPAS-O run, at smaller spatial scales.

MOAB interpolates MPAS-O state variables to a ROMS grid

Planned subdomains

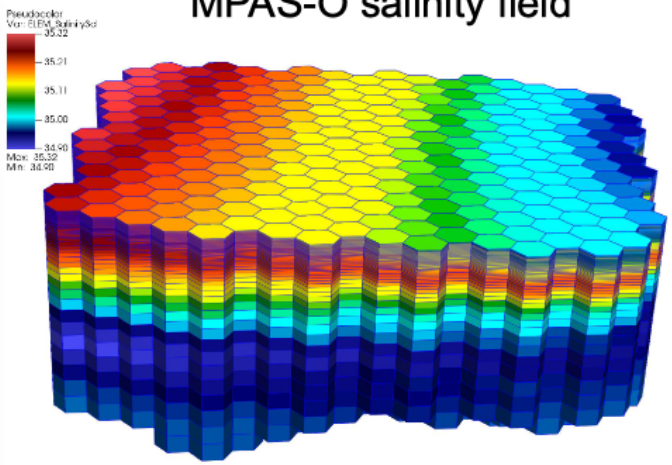




The ROMS domain is based on the NISKINE ONR project model domain

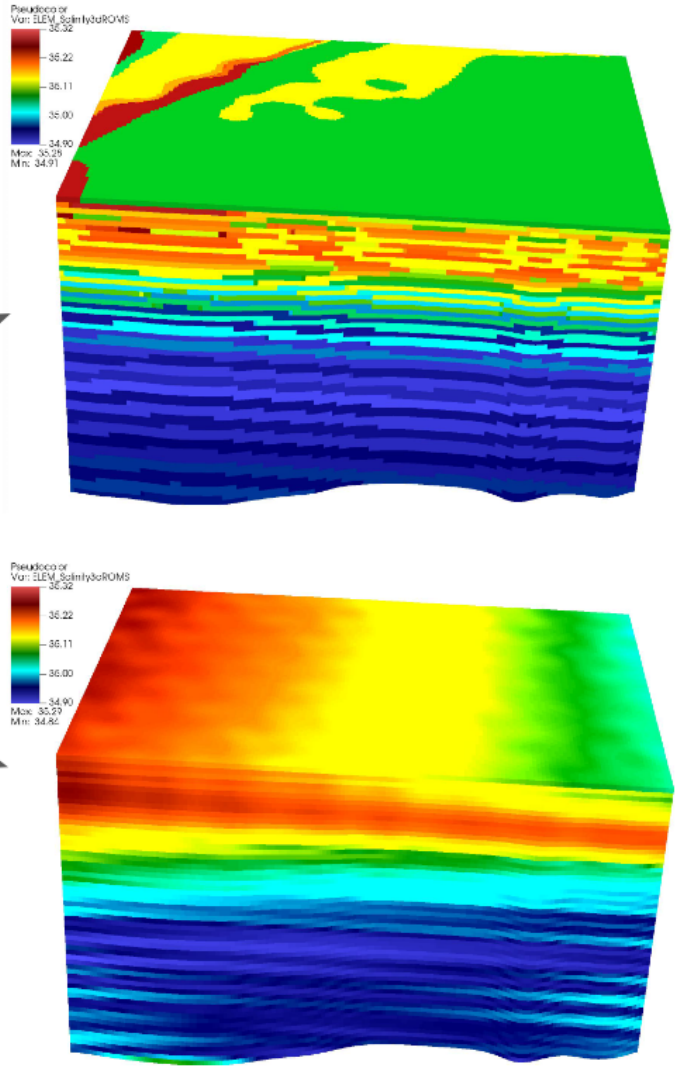
Remapping from MPAS-O to ROMS grids in the E3SM coupler MOAB.

MPAS-O salinity field



Natural neighbor interpolation

Cubic B-spline interpolation



Interpolated ROMS salinity fields

Cubic B-spline interpolation from MPAS-O to ROMS meshes reconstruct the field data more smoothly, with asymptotically third order accuracy.

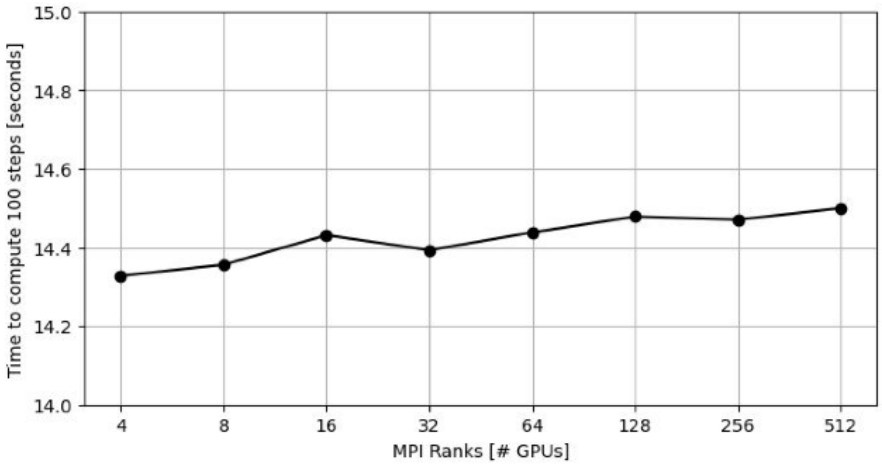
Locally conservative methods imprint the parent grid

ROMS-X development

ROMS-X is a new code built on the AMReX software framework, and can currently run with MPI + CUDA or HIP for NVIDIA/AMD GPUs.

Currently, ROMS-X has much of the base functionality of ROMS, implementing the same equations of motion for momentum and tracer evolution.

Preliminary ROMS-X weak scaling results for a modified upwelling problem on NVIDIA A100s of Perlmutter (graph below) are promising. (Perfect weak scaling would be a horizontal line)



ROMS-X is being carefully designed and implemented to perform robustly when coupled with other codes, and will replace ROMS in the coupler development work soon.

E3SM pull requests

- New ‘free-slip’ momentum boundary conditions have been implemented for MPAS-O, expanding our capability to model interactions with coastlines: https://github.com/E3SM-Ocean-Discussion/E3SM/pull/49

- An optimization of time-stepping coefficients for MPAS-O has been achieved, reducing the numerical dissipation associated with the split barotropic-baroclinic integration scheme to reduce the damping of surface gravity waves. This work is a collaboration with the ICoM project: https://github.com/E3SM-Ocean-Discussion/E3SM/pull/48

- An idealized channel configuration has been developed, and will be added to the COMPASS environment, providing an idealized test case to study fronts and submesoscale processes.

- E3SM-MOAB coupler draft pull request being prepared to merge the first version of the MOAB coupler into E3SM that can work alongside the current MCT coupler.

Conclusions

Initial comparisons between MPAS-O and ROMS indicate both models have roughly have the same effective resolution, and are capable of accurately simulating submesoscale processes.

Third-order cubic B spline interpolation methods seem promising, and we are exploring alternatives to deal with extrapolation in regions of strong bathymetry.

ROMS-X is running with a minimal, but functional dynamical core. We have engaged other groups as beta-testers, to help prioritize development.