Element-based Galerkin Methods in Geophysical Fluid Dynamics Modeling

NAHOMCon, June 17, 2024
Dartmouth College

Frank Giraldo, Distinguished Professor and Chair

Department of Applied Mathematics

Naval Postgraduate School

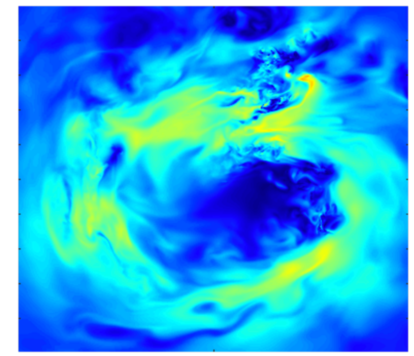
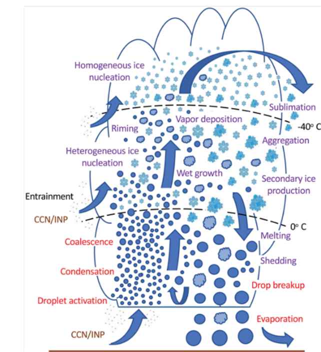
Monterey CA 93943

fxgirald@nps.edu

http://frankgiraldo.wix.com/mysite

Motivation

Resolution Scale

	$\mathcal{O}$(10~100 km)	$\mathcal{O}$ (1 km)	$\mathcal{O}$(100 m)	$\mathcal{O}$(<100 m)
	Global Circulation	**Cloud-scale Process**	**LES**	**Precipitation microphysics**
				
	Wikipedia	phys.org	Guimond et al.	Morrison et al. JAMES
Standard Simulation	**Resolved**	**Parameterized**		
Multiscale Simulation	**Resolved** (coarse grid)	**Resolved** (local fine grids)	**Parameterized**	

- Global Circulation Model (GCM) resolution approaching scales $\Delta h = \mathcal{O}(1\,km)$ and $\Delta v = \mathcal{O}(100\,m)$
- Vertical direction is special in that most "physics" occurs in this direction (i.e., moist processes such as the formation of clouds and precipitation of rain)
- **Will show results for GCM, CRM, and LES**

Acknowledgements

- **NUMA Model(s)**
  - Funded by ONR, NSF, DARPA, AFOSR
  - Collaborators: Soonpil Kang, Kiran Jadhav, FXG (NPS); Jim Kelly (NRL-DC); Felipe Alves (Un Reddy (LLNL), Yassine Tissaoui, Simone Marras (NJIT); Steve Guimond (Hampton Univ)
  - U.S. Navy's NEPTUNE dynamics based on NUMA. Both NUMA and NEPTUNE are space-weather capable.
  - NUMA is part of the Nvidia SDK Testing Analysis suite that is run nightly across various hardware and compilers.
  - https://frankgiraldo.wixsite.com/mysite/numa
  - https://frankgiraldo.wixsite.com/mysite/xnuma
- **NUMO Model(s)**
  - Funded by DOE, ONR
  - Collaborators: Yao Gahounzo, Michal Kopera (Boise State); Wieslaw. Maslowski, FXG (NPS);
  - NUMO is an incompressible NS solver used for studying the effects of ice-ocean interactions at, e.g., fjords.
  - h-NUMO is a multi-layer SWE equation developed by Yao Gahounzo (PhD thesis at Boise State Univ.).
  - https://frankgiraldo.wixsite.com/mysite/numo
  - https://github.com/ygahounzo/h-NUMO

Governing Equations

Atmospheric Equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\right) = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla P + \nabla \phi + 2\boldsymbol{\Omega} \times \mathbf{u} = 0$$

$$\frac{\partial E}{\partial t} + \mathbf{u} \cdot \nabla E + \delta(\gamma - 1) E \nabla \cdot \mathbf{u} = 0$$

$$P = (1 - \delta) P_A \left(\frac{\rho R \theta}{P_A}\right)^{\gamma} + \delta(\gamma - 1)\rho e$$

Ocean Equations:

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho_0} \nabla P + \frac{\rho}{\rho_0} g \mathbf{k} + 2\boldsymbol{\Omega} \times \mathbf{u} = 0$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \nabla \cdot \left(k_T \nabla T\right)$$

$$\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S = \nabla \cdot \left(k_S \nabla S\right)$$

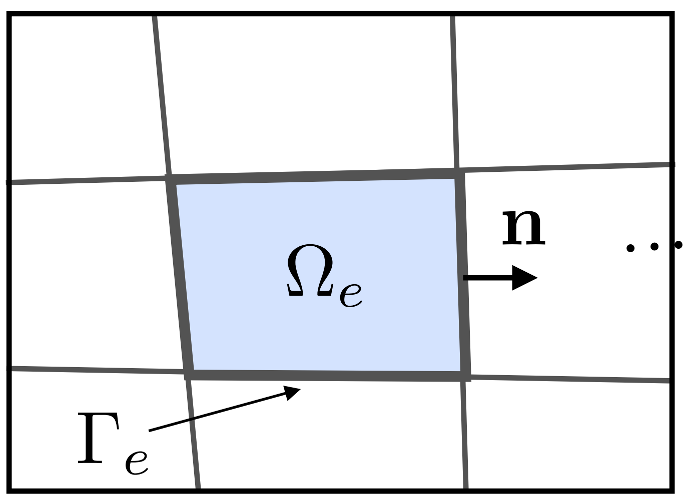
$$\rho = f(T, S)$$

- NUMA carries 4 different forms of compressible Euler/Navier-Stokes (non-hydrostatic) including conservation/balance law forms.
- NUMO carries Boussinesq incompressibble Navier-Stokes (non-hydrostatic) and h-NUMO is a hydrostatic version.

Element-based Galerkin Methods [1]

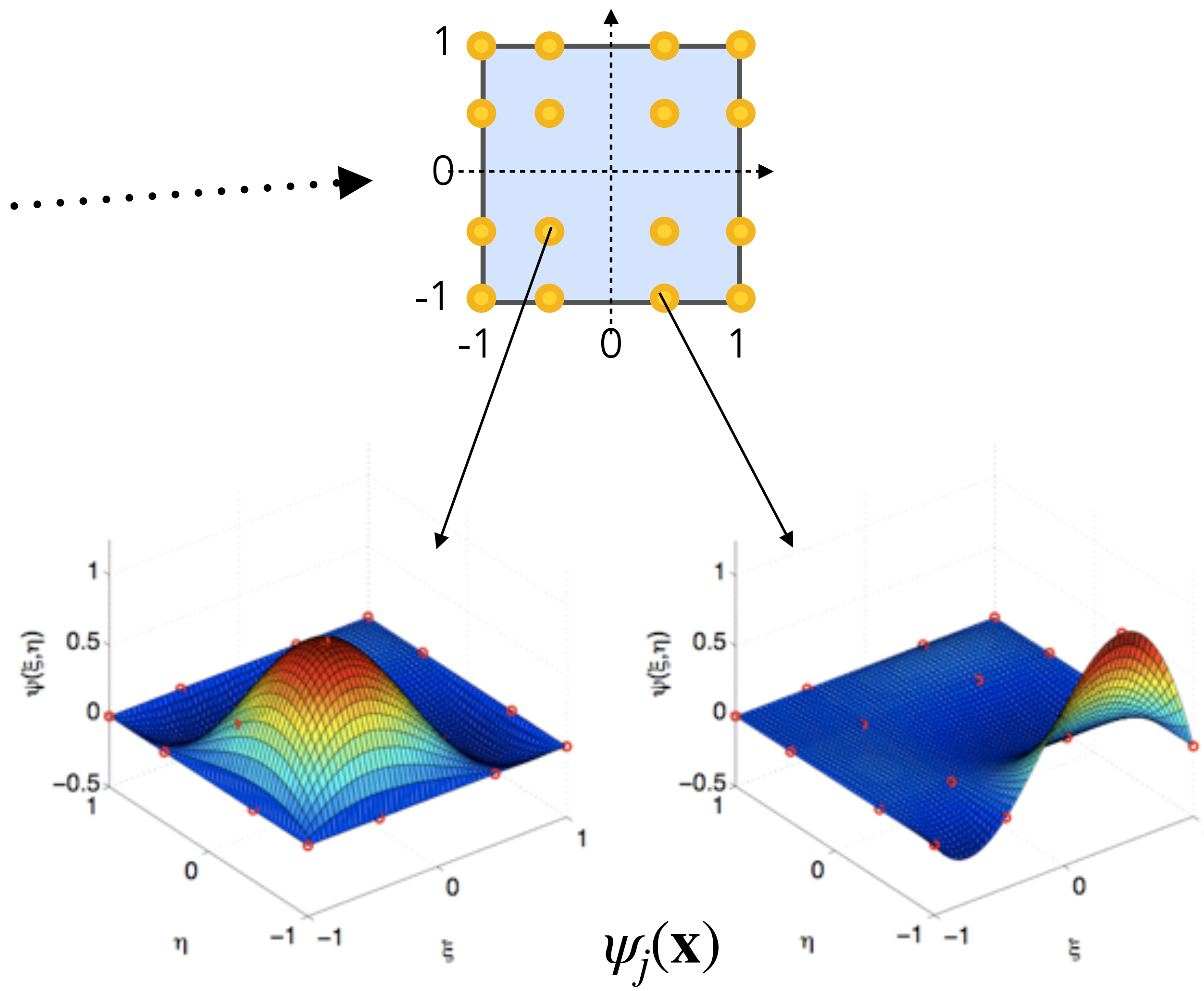
Domain decomposition

$$\Omega = \sum_{e=1}^{N_e} \Omega_e$$



Reference element

Legendre-Gauss-Lobatto points



Basis functions - Lagrange polynomials

Approximate local solution as:

$$q_N^{(e)}(\mathbf{x}, t) = \sum_{j=1}^{M_N} \psi_j(\mathbf{x}) q_j^{(e)}(t)$$

[1] F.X. Giraldo. An Introduction to Element-Based Galerkin Methods on Tensor-Product Bases: Analysis, Algorithms, and Applications, Springer Texts in Computational Science and Engineering, Series Volume 24, ISBN: 978-3-030-55068-4 (2020)

Element-based Galerkin Methods

Governing equation: $$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{q}) = S(\mathbf{q})$$

Approximate the **global** solution as: $$q_N^{(e)}(\mathbf{x},t) = \sum_{j=1}^{M_N} \psi_j(\mathbf{x}) q_j^{(e)}(t)$$

$$\mathbf{F}_N = \mathbf{F}(\mathbf{q}_N)$$
$$S_N = S(\mathbf{q}_N)$$

Define residual: $$R\left(q_N^{(e)}\right) \equiv \frac{\partial \mathbf{q}_\mathbf{N}^{(\mathbf{e})}}{\partial t} + \nabla \cdot \mathbf{F}_N^{(e)} - S_N^{(e)} = \epsilon$$

Problem statement:

test function

Find $\mathbf{q}_N \in \mathcal{S} \quad \forall \psi \in \mathcal{S}$ $$\begin{cases} \mathcal{S}_{CG} = \{\psi \in H^1(\Omega) : \psi \in P_N(\Omega_e)\ \forall \Omega_e\} \\ \mathcal{S}_{DG} = \{\psi \in L^2(\Omega) : \psi \in P_N(\Omega_e)\ \forall \Omega_e\} \end{cases}$$

such that $$\int_{\Omega_e} \psi_i R(\mathbf{q}_N) \mathrm{d}\Omega_e = 0$$

Element-based Galerkin Methods

Integral form:

$$\int_{\Omega_e} \psi_i R(\mathbf{q}_N^{(e)}) \mathrm{d}\Omega_e = 0$$

$$\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}_N^{(e)}}{\partial t} \mathrm{d}\Omega_e + \int_{\Omega_e} \psi_i \nabla \cdot \mathbf{F}_N^{(e)} \mathrm{d}\Omega_e - \int_{\Omega_e} \psi_i S_N^{(e)} \mathrm{d}\Omega_e = 0$$

Integration by parts: $\int_{\Omega_e} \psi_i \nabla \cdot \mathbf{F}_N^{(e)} \mathrm{d}\Omega_e = \int_{\Omega_e} \nabla \cdot (\psi_i \mathbf{F}_N^{(e)}) \mathrm{d}\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}_N^{(e)} \mathrm{d}\Omega_e = \int_{\Gamma_e} \mathbf{n} \cdot \psi_i \mathbf{F}_N^{(e)} \mathrm{d}\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}_N^{(e)} \mathrm{d}\Omega_e$

$$\boxed{\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}_N^{(e)}}{\partial t} \mathrm{d}\Omega_e + \underbrace{\int_{\Gamma_e} \mathbf{n} \cdot \psi_i \mathbf{F}_N^{(e)} \mathrm{d}\Gamma_e}_{\text{face integral}} \underbrace{- \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}_N^{(e)} \mathrm{d}\Omega_e - \int_{\Omega_e} \psi_i S_N^{(e)} \mathrm{d}\Omega_e}_{\text{volume integrals}} = 0}$$

Matrix form:

$$M_{ij}^{(e)} \frac{\mathrm{d}\mathbf{q}_j^{(e)}}{\mathrm{d}t} + \sum_{f=1}^{N_{faces}} \left(\mathbf{M}_{ij}^{(e,f)}\right)^T \mathbf{F}_j^{(e,f,*)} - \left(\tilde{\mathbf{D}}_{ij}^{(e)}\right)^T \mathbf{F}_{ij}^{(e)} - S_i^{(e)} = 0$$

$M_{ij}^{(e)} = \int_{\Omega_e} \psi_i \psi_j \mathrm{d}\Omega_e$ — mass matrix

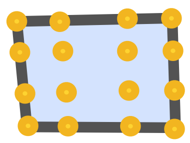
$\mathbf{M}_{ij}^{(e,f)} = \int_{\Gamma_e} \psi_i \psi_j \mathbf{n}^{(e,f)} \mathrm{d}\Gamma_e$ — face mass matrix

$\tilde{\mathbf{D}}_{ij}^{(e)} = \int_{\Omega_e} \nabla \psi_i \psi_j \mathrm{d}\Omega_e$ — differentiation matrix

Element-based Galerkin Methods

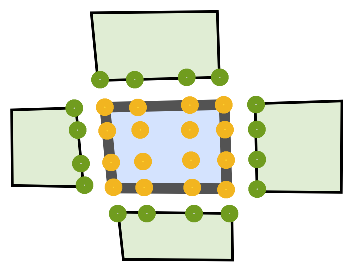
$$\boxed{\int_{\Omega_e} \psi_i \frac{\partial \mathbf{q}_N^{(e)}}{\partial t}\, d\Omega_e + \int_{\Gamma_e} \psi_i \mathbf{n} \cdot \mathbf{F}_N^{(*)}\, d\Gamma_e - \int_{\Omega_e} \nabla \psi_i \cdot \mathbf{F}_N^{(e)}\, d\Omega_e - \int_{\Omega_e} \psi_i \mathbf{S}_N^{(e)}\, d\Omega_e = \mathbf{0}}$$

1. Evaluate "volume" integrals on element interiors



$$R^{(e)} := \int_{\Omega_e} \nabla \psi_i \cdot F_N^{(e)}\, d\Omega_e + \int_{\Omega_e} \psi_i\, S_N^{(e)}\, d\Omega_e$$

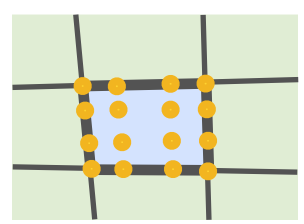
2. Evaluate flux integrals



$$R^{(e)} := R^{(e)} - \int_{\Gamma_e} \psi_i\, n \cdot F_N^{(*)}\, d\Gamma_e$$

CG: cancels at interior element edges

3. Direct Stiffness Summation



$$R = \bigwedge_{e=1}^{N_e} R^{(e)}$$

DG: matrices are block diagonal except for the flux matrix

4. Multiply by inverse global mass matrix and evolve time step

$$\frac{dq_i}{dt} = M_i^{-1} R_i$$

We rely on inexact integration so M is diagonal

- NUMA/NUMO carry CG and DG, xNUMA CG, and ATUM/h-NUMO DG

SBP methods

- An interesting area of research in EBG concerns SBP methods [**see MS01, MS03, MS05 for more recent developments in this area**]

- For conservation laws discretized as: $M_i \frac{d\mathbf{q}_i^{(e)}}{dt} + D_{ij} f_j^{(e)} = \mathbf{0}$ we rewrite as

$$M_i \frac{d\mathbf{q}_i^{(e)}}{dt} + \sum_{i=1}^{M_N} D_{ij} \circ \hat{f}_{ij}^{(e)} = \mathbf{0}$$

- with, e.g., the kinetic-energy-preserving flux [2] being $\hat{f}_{ij}^{(e)}(q, \mathbf{u}) = 2\{\{\mathbf{u}_i\}\}\{\{q_j\}\}$ and other options for entropy-stable flux [3]

- Will show the benefits of these methods in the Results section

[2] Souza et al. The flux-differencing DG applied to an idealized fully compressible nonhydrostatic dry atmosphere, JAMES 2023
[3] Waruszewski et al. Entropy Stable DG for Balance Laws in Non-Conservative Form: Applications to the Euler Equations with Gravity JCP (2022)

EBG GFD Models

Atmospheric Models

- NUMA* (NPS, USA)
- NEPTUNE (U.S. Navy's global NWP model)
- ATUM* (NPS, USA)
- KIM (South Korea)
- LFRic* (UK Met Office)
- CAM-SE (in CESM at NCAR, USA)
- EAM (in E3SM at DOE, USA)

Ocean Models

- NUMO* (BSU/NPS, USA)
- h-NUMO* (BSU, USA)
- SLIM3D* (UCL, Belgium)
- Fluidity (Imperial College, UK)
- RiCOM (NIWAR, NZ)
- SCHISM (VIMS, USA)

*use EBG in all 3 directions. *use high-order EBG (P>1)

Results

1. Baroclinic Instability on the Sphere (NUMA, GCM scale)

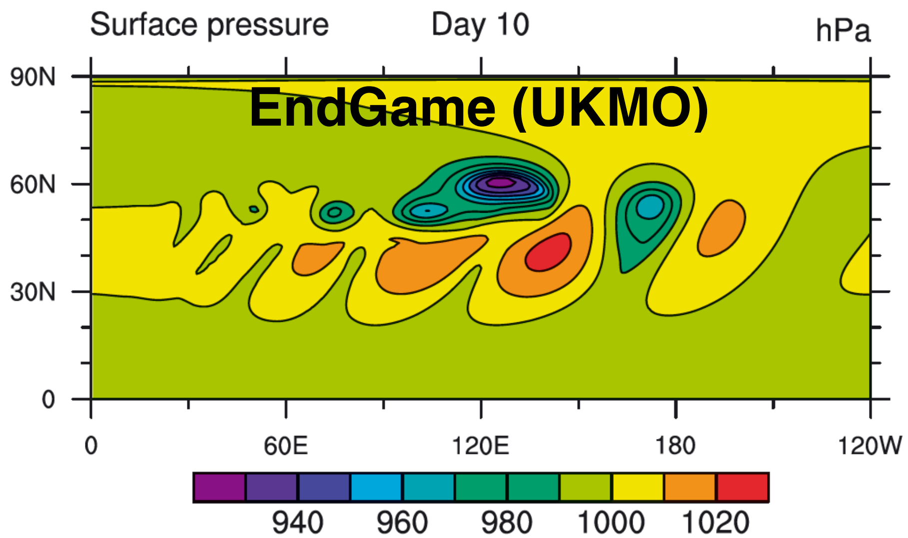
2. Tropical Cyclone Simulations to better understand rapid intensification (NUMA, CRM/LES scales)

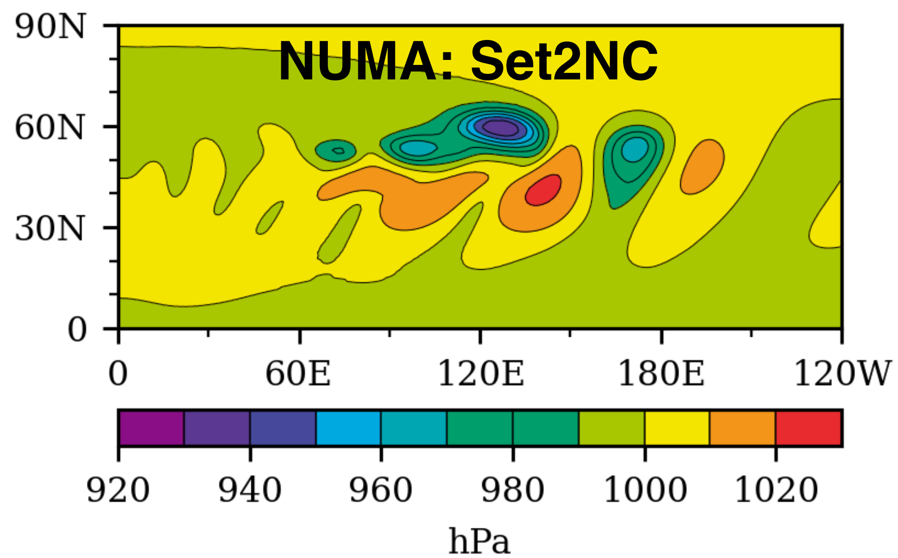
3. Density Current with Salinity (NUMO, LES scale)

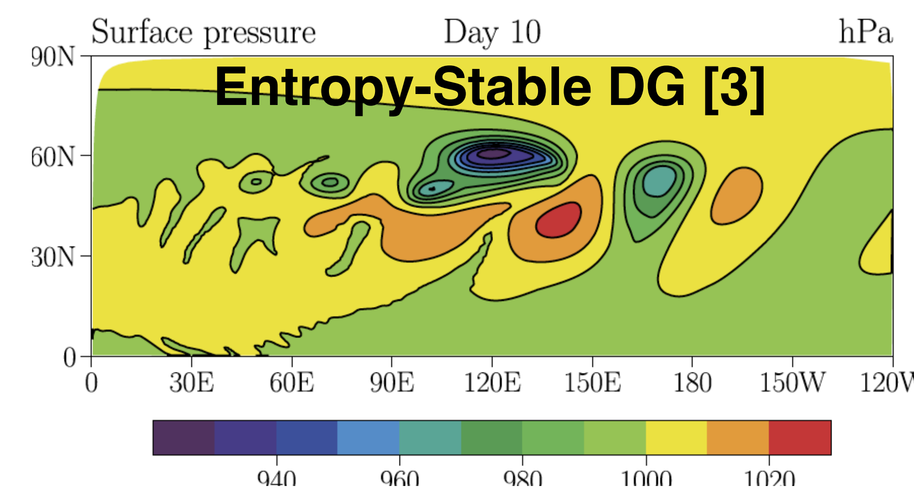
4. Double Gyre (h-NUMO, GCM scale)

Result 1: Baroclinic Instability (GCM scale) [4]

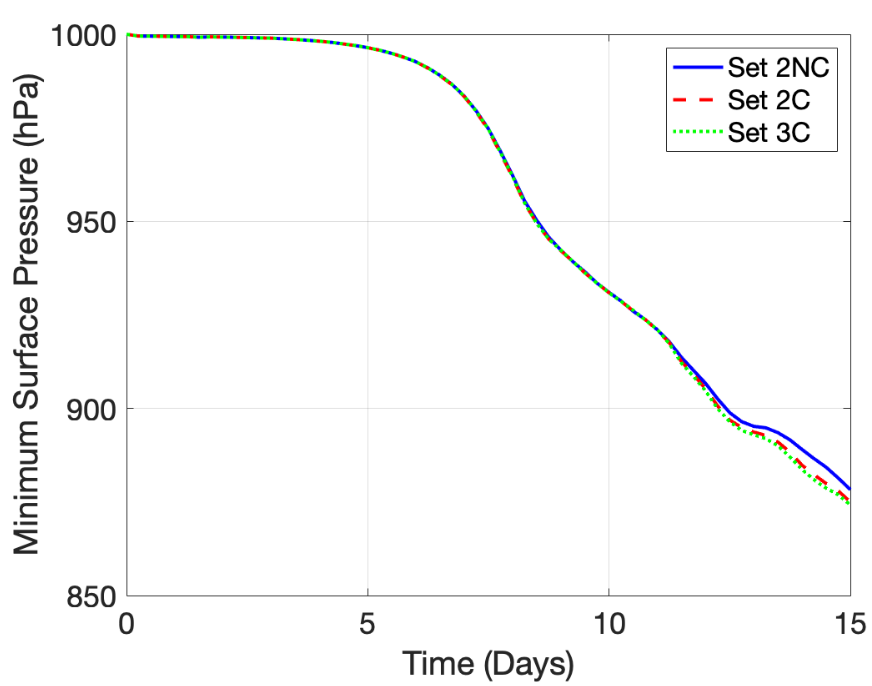
Baroclinic Instability on the sphere for 10-day forecast simulation with Grid Resolution: $\Delta h = 100\ km$ and $\Delta v = 1\ km$. ES-DG uses no viscosity (conserves total energy exactly) and remains stable for all time

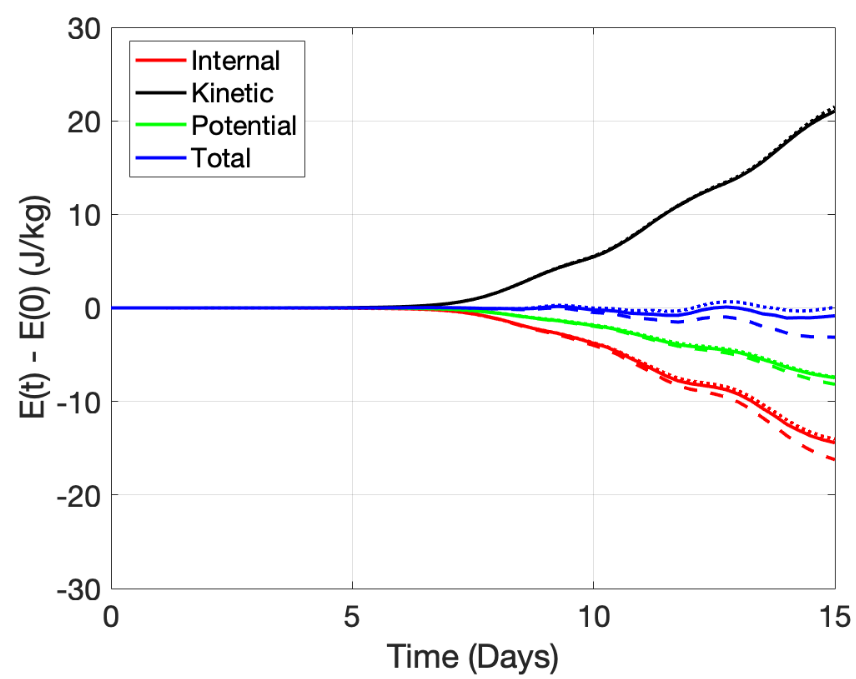


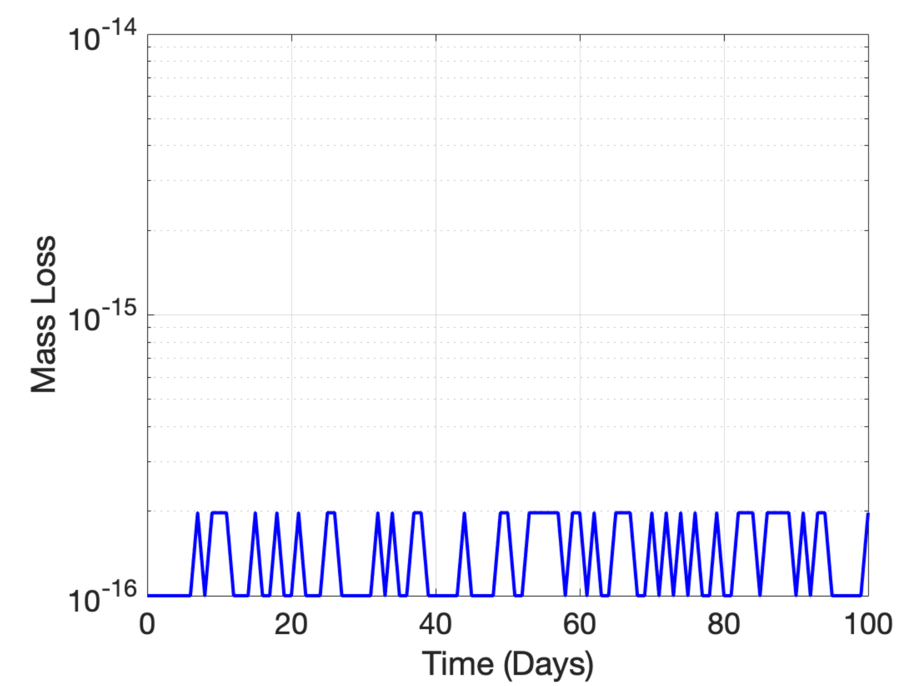




All NUMA equation sets give similar results. Mass conservation is imperative.

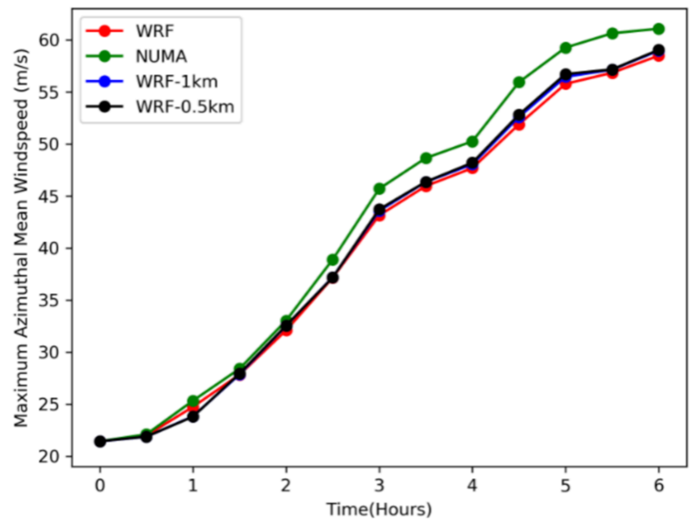


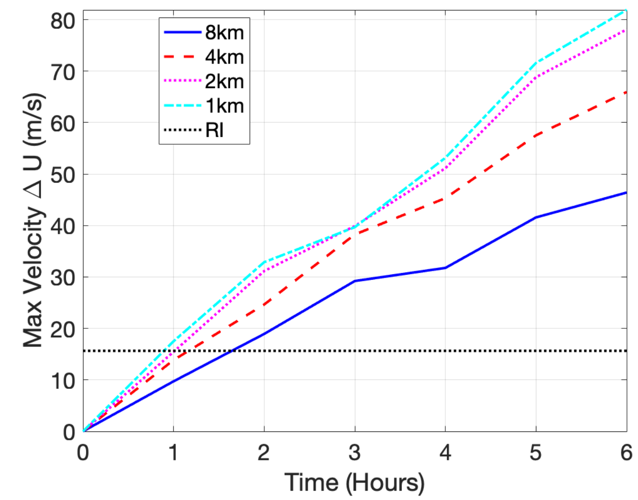




Result 2: Tropical Cyclone (CRM scale)

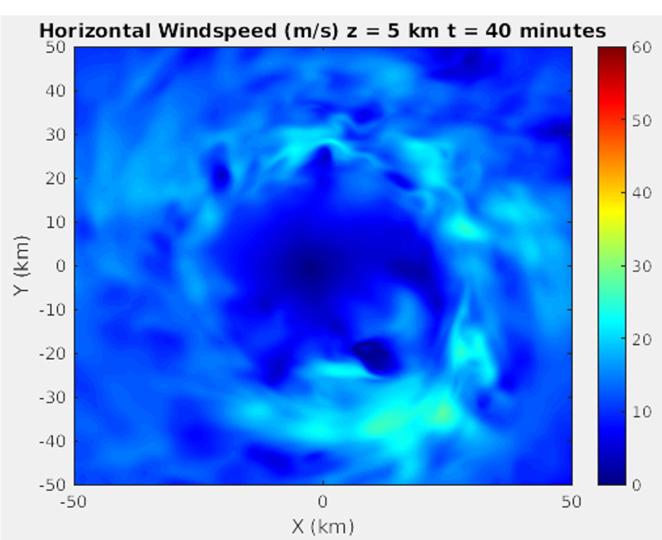
Tropical Cyclone Rapid Intensification (RI) (where max wind velocities exceed 30 mph within 24-hour period) is important to understand extreme weather. Here is a sample plot from [5] where we show our model vs the U.S. National Hurricane Center model. RI requires running with minimal dissipation and high resolution.

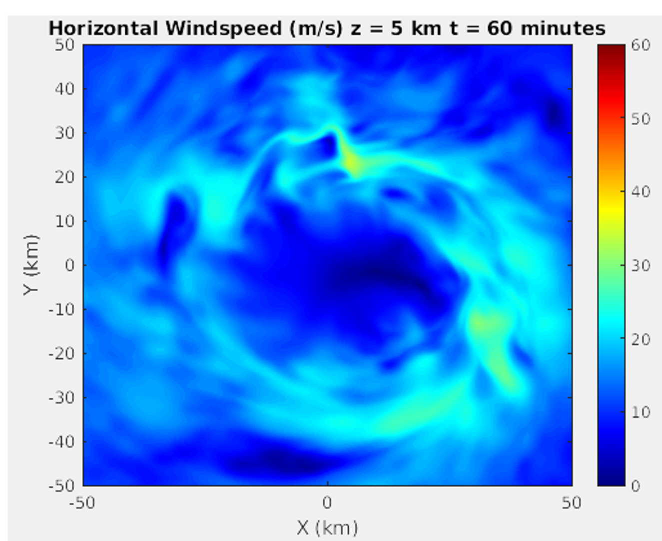


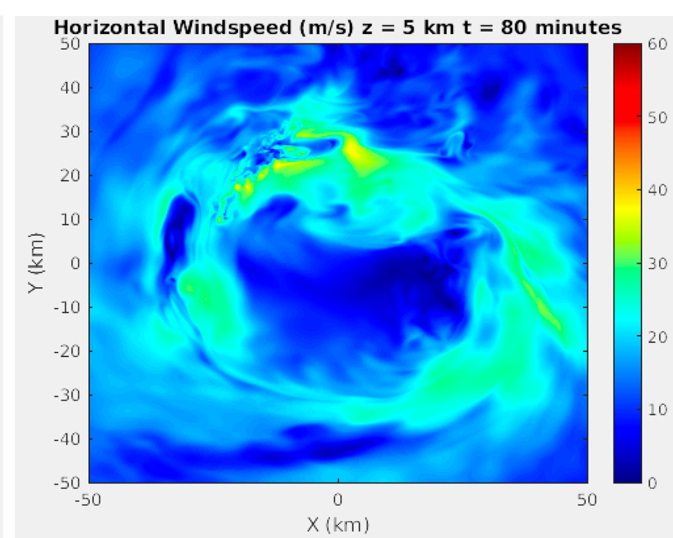


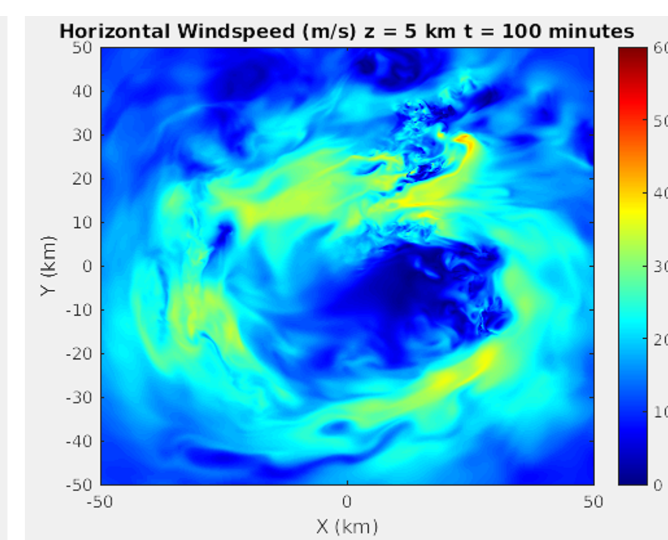
To properly capture RI requires LES models at $\Delta x = \mathcal{O}(100\,m)$. Running a CRM at this resolution is still too expensive (cannot be done on a regular basis). Our simulations in [5] were run at $\Delta x = \mathcal{O}(2\,km)$ (with 80 million DoF, cost is 1 simulation hour/wallclock hour on 5000 AMD Epyc cores). LES requires 32 billion DoF with Δt 20x smaller ($\mathcal{O}(10^4)$ more expensive). (The simulation shown below used 10 billion DoF (reduce the domain size); courtesy of Steve Guimond UMBC)

To make such simulations possible require leveraging: 1) multi-scale modeling frameworks (MMF), 2) dynamic adaptive mesh refinement, 3) new time-integration and preconditioning strategies, and 4) HPC.



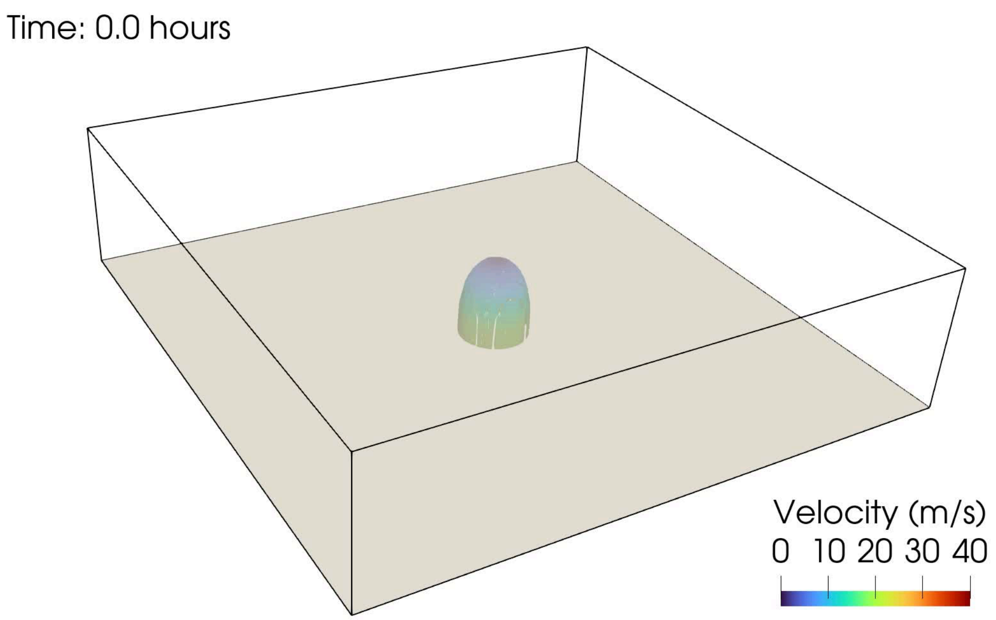


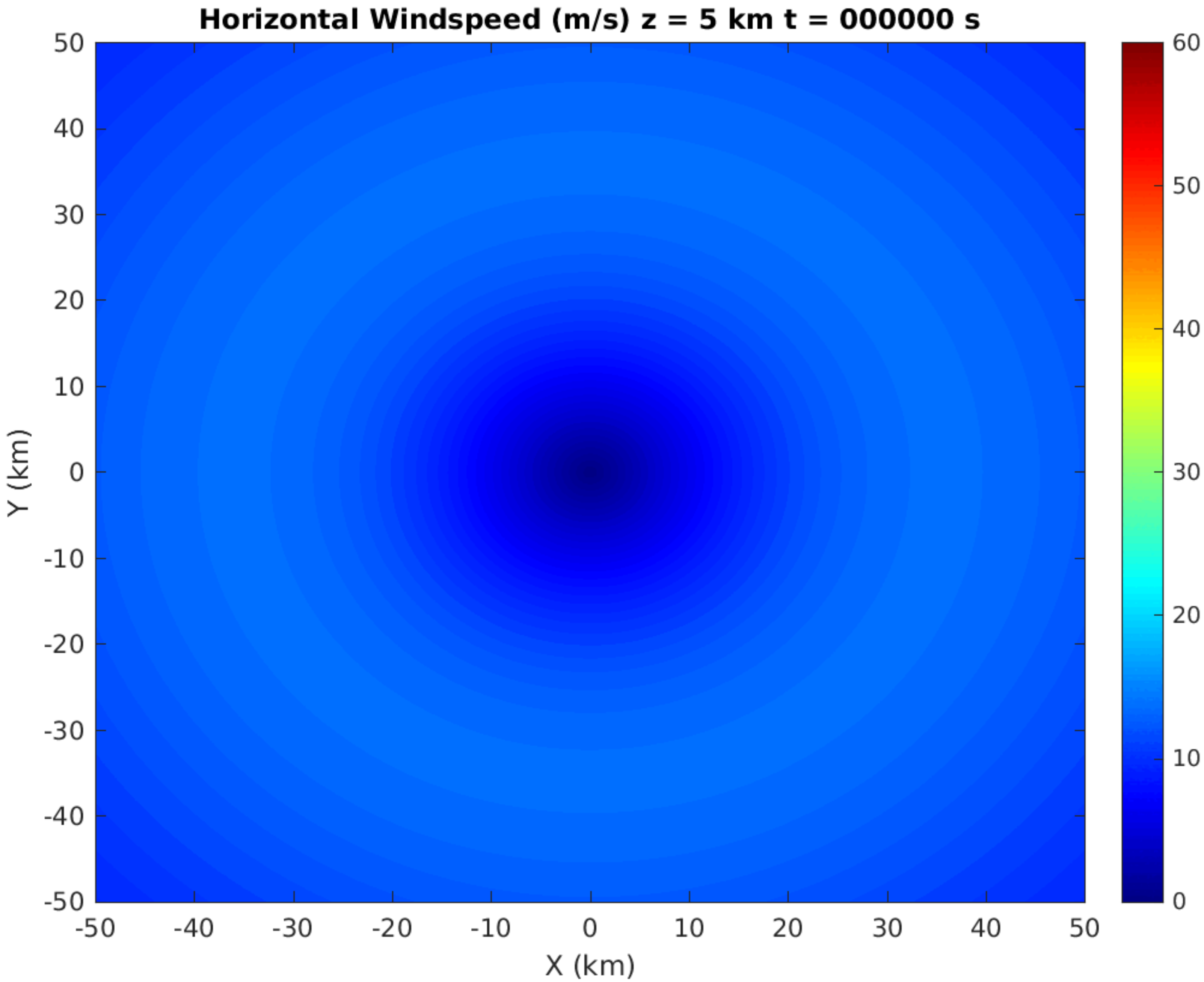




[5] Hasan et al., The effects of numerical dissipation on hurricane rapid intensification with observational heating, JAMES Vol 14 Issue 8 (2022)

Result 2: NUMA Tropical Cyclone (LES scale) [6]





The eye-wall of Hurricane Guillermo undergoing RI. Real data consists of 4D observational latent heat forcing derived from airborne radar. Model resolution is $\Delta x = \Delta y = \mathcal{O}(60\, m)$ and $\Delta z = \mathcal{O}(100\, m)$, on 9000 AMD Epyc cores); courtesy of Steve Guimond, Hampton University)

Result 3: Density Current (LES-scale) [7]

$Ra = 5 \times 10^6$ $Sc = 1$

$\nu_h = 1.17\ m^2/s$

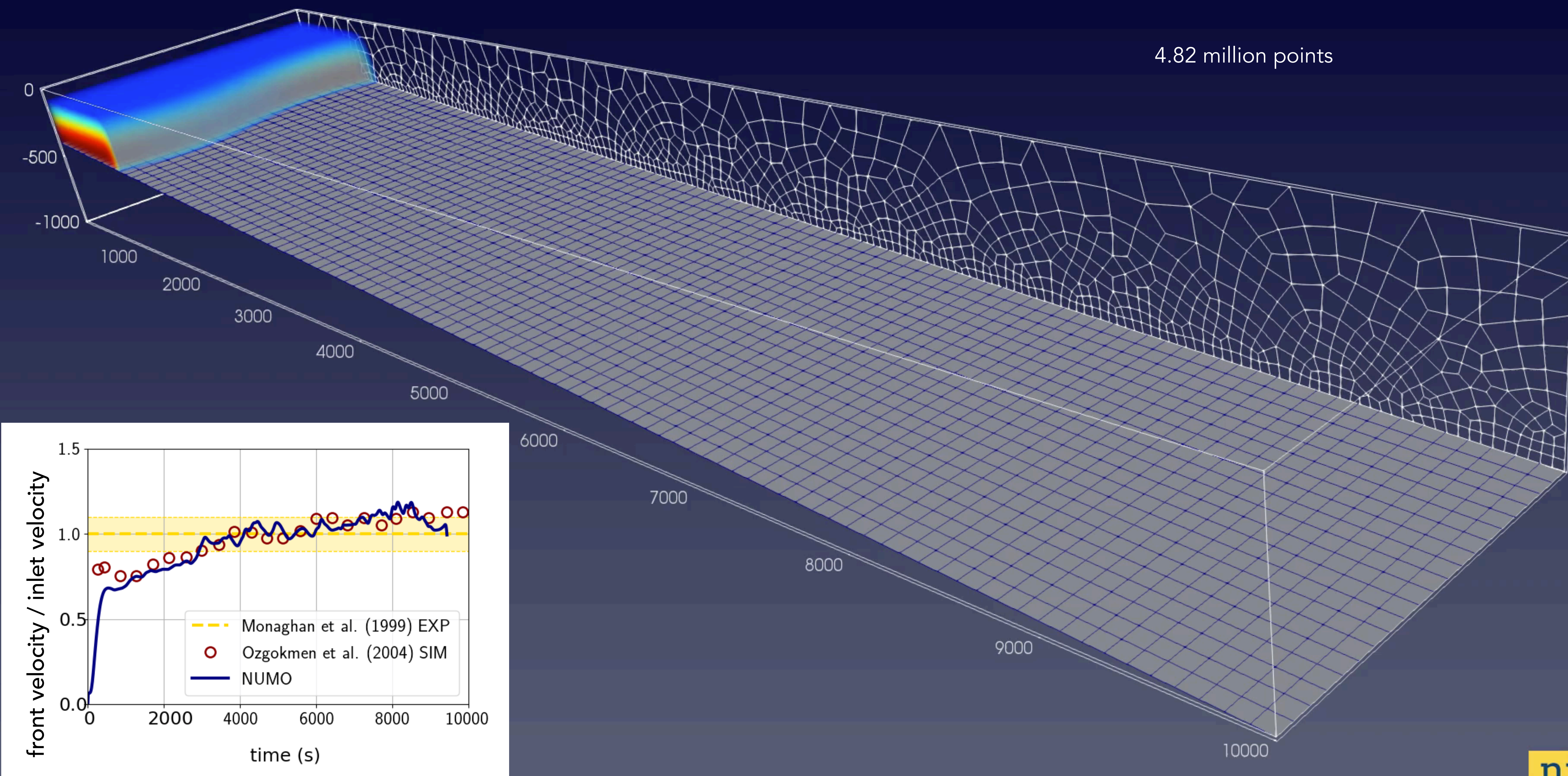
$\nu_v = 2.34 \times 10^{-2}\ m^2/s$

$\Delta x, \Delta y = 6 - 25\ m$

$\Delta z = 25m$
38,560 elements

4.82 million points

t = 10.0s

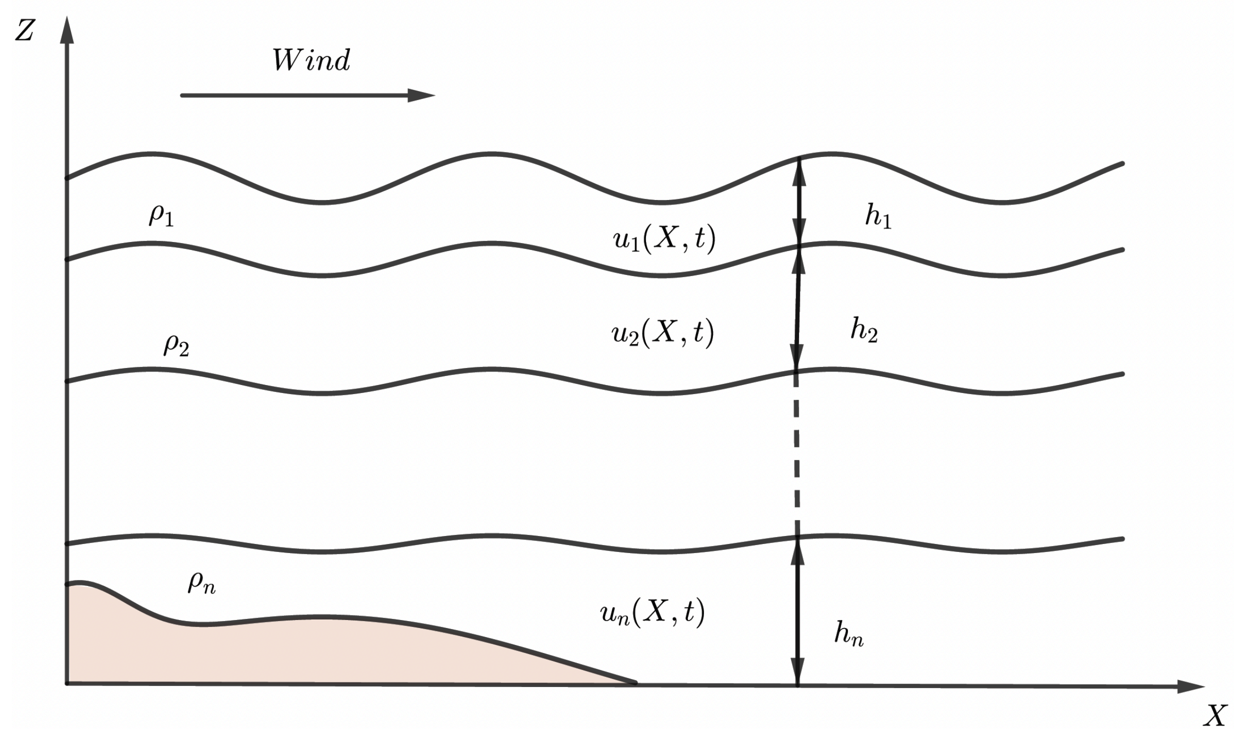


numo

[7] Kopera et al., Non-hydrostatic Unified Model of the Ocean (NUMO) with application to ice/ocean interaction modeling, Int. J. Geomathematics 2023

Result 4: Double-Gyre (GCM scale) [8]

- Multi-layered shallow water equations
- Hydrostatic
- Isopycnal coordinates (layers of constant density
- Equations are solved for Δp_k and $\mathbf{U}_k$



$$
\begin{aligned}
\frac{\partial \Delta p_k}{\partial t} + \nabla \cdot \mathbf{U}_k &= 0, \\
\frac{\partial \mathbf{U}_k}{\partial t} + \nabla \cdot \left(\frac{\mathbf{U}_k \otimes \mathbf{U}_k}{\Delta p_k} + H_k \mathbf{I} \right) + f \mathbf{k} \times \mathbf{U}_k &= g \left(p_{k-1} \nabla z_{k-1} - p_k \nabla z_k \right) \\
&\quad + g \Delta \tau_k + \nabla \cdot (\nu \Delta p_k \nabla \mathbf{u}_k),
\end{aligned}
$$

$\Delta p_k = p_k - p_{k-1}$ is the layer pressure

$\mathbf{U}_k = \mathbf{u}_k \Delta p_k$ is the layer momentum

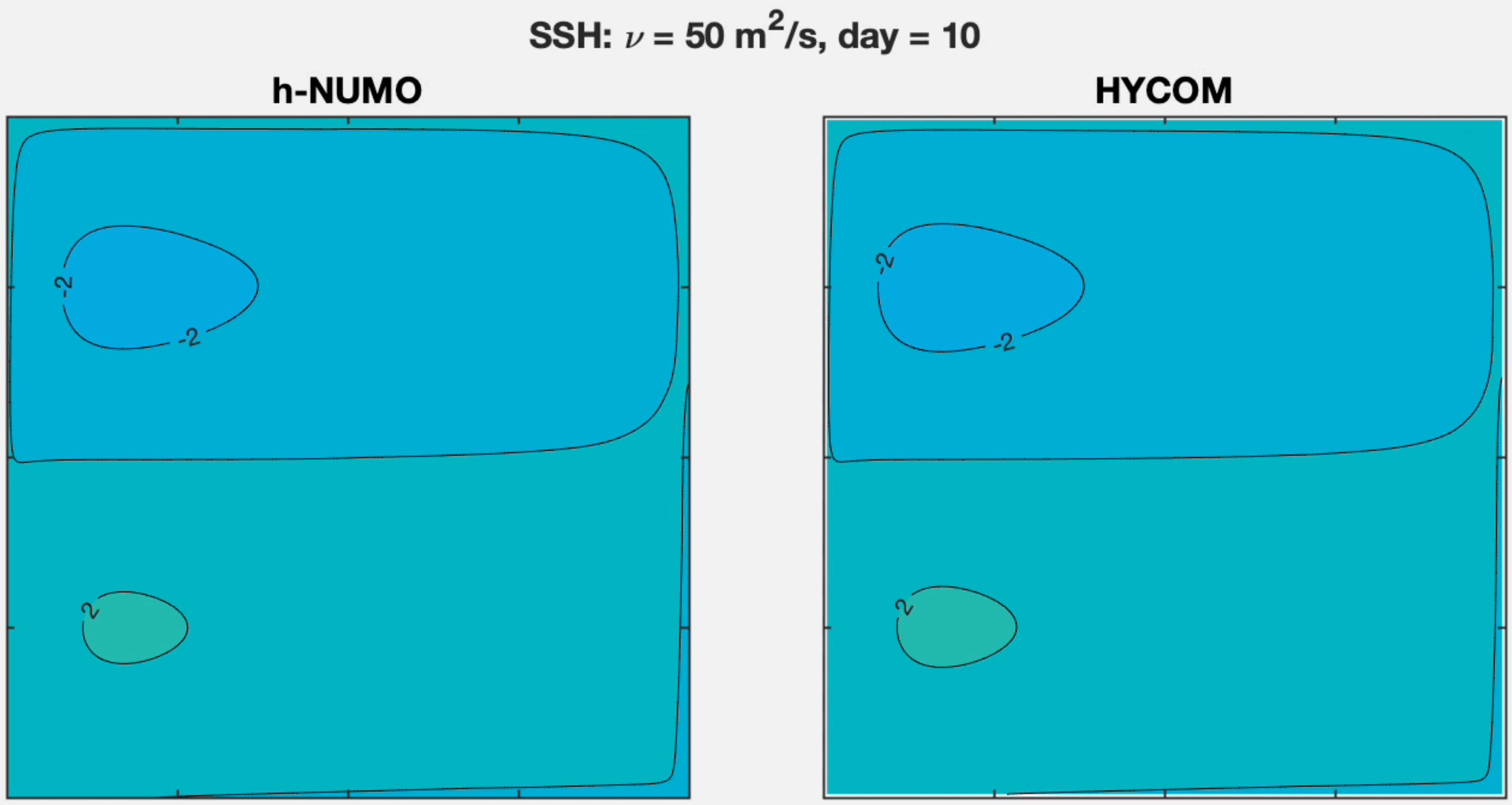
$H_k(x, y, t) = g \int_{z_k}^{z_{k-1}} P(x, y, z, t) dz$

$\Delta \tau_k$ is the shear stress

[8] Yao Gahounzo, Multi-scale ocean modeling using the discontinuous Galerkin method (PhD Dissertation, Boise State University) 2024

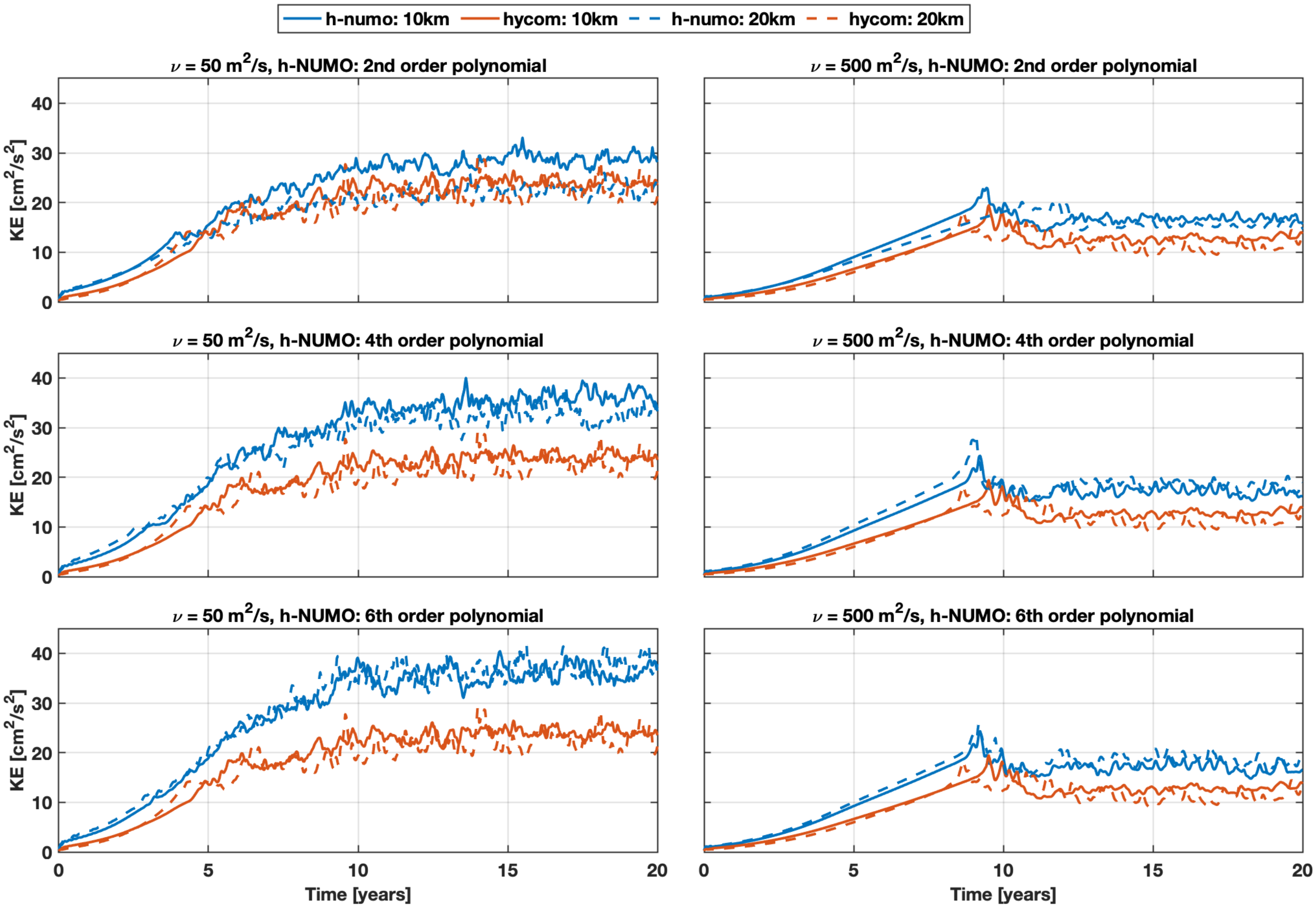
Result 4: Double-Gyre (GCM scale)

- Comparison between h-NUMO and HYCOM; HYCOM is the U.S. Navy's operational global ocean model
- 2 layers using at $\Delta x = 10\,km$ resolution integrated for 20 years with $\nu = 50\,m^2/s$
- xy-slice showing sea surface height



[8] Yao Gahounzo, Multi-scale ocean modeling using the discontinuous Galerkin method (PhD Dissertation, Boise State University) 2024

Result 4: Double-Gyre (GCM scale)



h-NUMO shows higher KE for the same resolution and viscosity

[8] Yao Gahounzo, Multi-scale ocean modeling using the discontinuous Galerkin method (PhD Dissertation, Boise State University) 2024

Closing Remarks

- **Element-based Galerkin Methods**
  - The minimal inherent dissipation of EBG/high-order methods offers the possibility of making advances in better understanding of important weather/ocean dynamics (e.g., TC RI in atmosphere and more accurate kinetic energy in the ocean).
  - Some (i.e., continuous Galerkin) are entirely non-dissipative and need help to maintain stability. Others (i.e., discontinuous Galerkin) have more mechanisms to introduce dissipation but still need some help. Entropy-Stable (ES) methods allow for mathematically rigorous construction of stable methods but have high complexity (5-10x more FLOPS) [**see MS01,MS03,MS05 today**]. Can we extend these to CG?
  - Efficiency continues to be the Achilles heel of these methods.

Closing Remarks

- **Future of Atmospheric Models**

  - As resolutions of GCMs approach cloud-resolving scales $\mathcal{O}(1\,km)$, many of the important processes are resolved explicitly (less reliance on parameterizations).

  - However, the LES scale $\mathcal{O}(100\,m)$ is quite out of reach at the moment.

  - To curtail the cost of LES-scale simulations requires using: (1) MMF (e.g., see [7]); (2) HPC particularly on GPUs [**see MS09 and Noel Chalmers' plenary Tuesday morning**]; and (3) Scientific Machine Learning/ROM [**see MS02, MS04, MS06, MS13**].

[7] Kang et al. , Multiscale modeling framework using element-based Galerkin methods for moist atmospheric limited-area simulations, Journal of Advances in Modeling Earth Systems 2024 (in review)

Closing Remarks

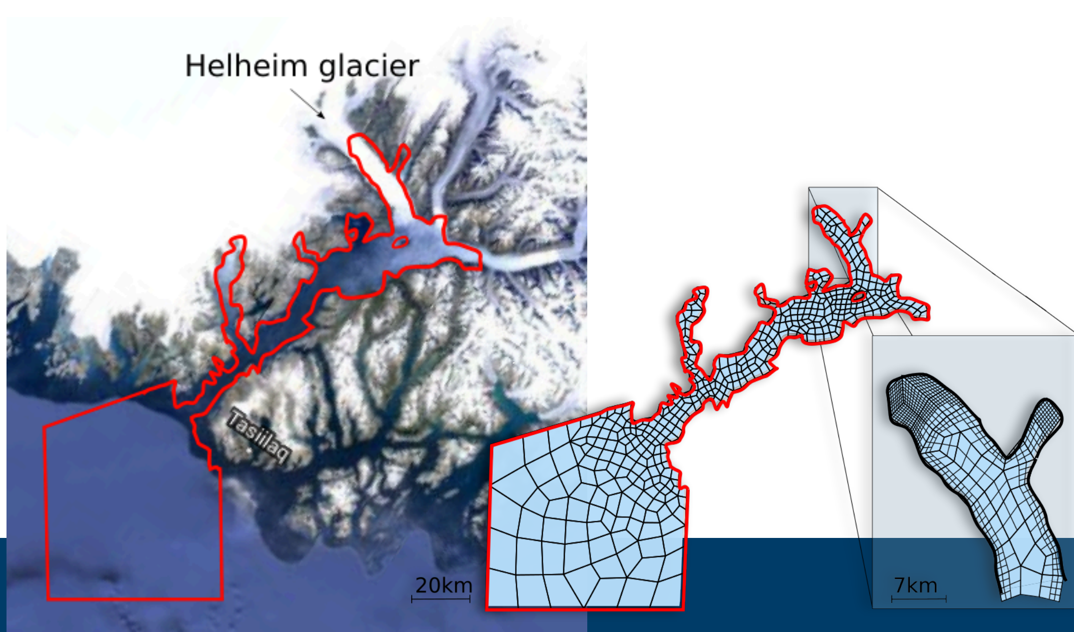
- **Future of Ocean Models**

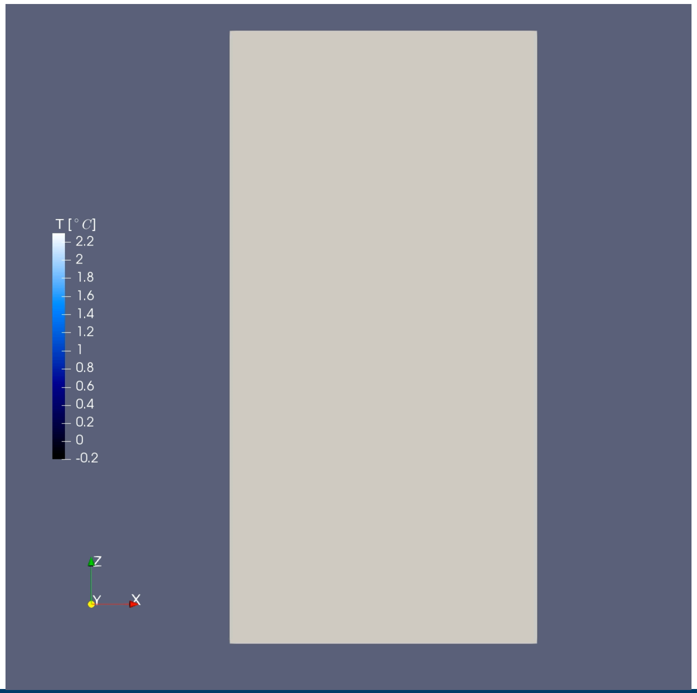
  - Recent MOU on Ocean Sciences between NPS and Stanford Doerr School of Sustainability provides an exciting opportunity to develop a new EBG ocean model to couple with NUMA/NEPTUNE.

  - Currently, all operational ocean models are hydrostatic (few exceptions). Is hydrostatic sufficient or do we need to switch to nonhydrostatic as the atmospheric community recently did?

  - SBP methods should play a key role in developing stable high-order ocean models.

  - In some ways, EBG may be more optimal for ocean models due to the need for unstructured grids (e.g., Greenland fjords).





Melting Ice at Ice/Ocean Interface [5]

Closing Remarks

- **Final Thoughts**

  - Did not discuss time-integration (TI) but much work to be done. A brief list includes: (1) Multi-rate methods [**see Carol Woodward's plenary on Wednesday**], (2) implicit methods for SBP [**see talks on SBP minis on this topic today**]. TI for GFD needs to consider the disparate spatial scales between the horizontal and vertical directions.

  - High-order methods are in very good shape and are competing with other methods for operational/industrial-type applications in terms of both stability and performance (e.g., 2024 Gordon Bell award to E3SM team)

  - NAHOMCon is a great venue for us to continue to share our experiences to improve HO methods - thanks to the organizers and participants and let's keep it going!