

# Convergence and performance aspects of physics-dynamics coupling in US-Department of Energy research

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U.S. DEPARTMENT OF  
**ENERGY**

Office  
of Science

Office of Biological  
and Environmental Research

# Department of Energy Research context

**DOE Earth system research includes field work and process research on atmosphere and terrestrial systems, and model development and analysis for the full coupled system, as well as interactions between human (energy) and earth systems.**

**Focus today on computational-mathematical aspects**

- **Energy Exascale Earth System Model**
- **DOE hardware**
- **Scientific Discovery through Advanced Computing (SciDAC)**
- **Highlights of relevant work from 11 current activities**

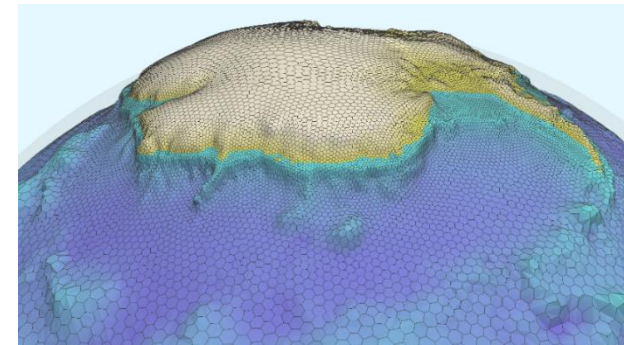
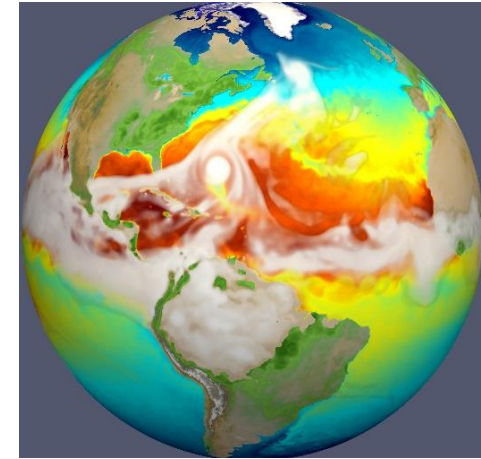
# Energy Exascale Earth System Model and project



E3SM is a DOE-Office of Science model project and model

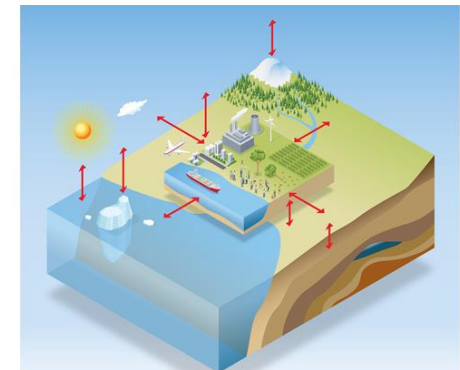
Unique features:

- Push to use DOE supercomputers and advanced software practice
- Focus is on high-resolution configuration (25km) and the coupled system
- DOE science and mission are central to the development priorities
- **Variable-resolution-mesh capabilities included in all components** (up to 10km atmos, 6km ocean, 500m ice-sheet); need for scale-aware treatments!



## Science Goals

- “Water cycle”: What factors govern precipitation and water cycle (land-atmosphere-ocean) now and in the future? How will freshwater supplies change?
- “Cryosphere-ocean”: What is likelihood of Antarctic-ice-sheet destabilization, regional sea-level changes and storm-surge?
- “Biogeochemistry”: What are the effects of nutrients and land-use on soil carbon reservoirs?



Two-way coupling (synchronous)

# Energy Exascale Earth System Model

## Programmatics:

- Version 1 was released in April, 2018: includes code, output, analysis tools
- The Project code is now Open-Development: <https://github.com/E3SM-Project/E3SM>
- New project website: <https://E3SM.org>
- Phase 2 of the project was reviewed May 14-16, 2018

## Simulation progress (v1):

- The lower resolution (100km) coupled system behaves well and many simulations are completed. Coupled biogeochemical simulations (with more processes and tracers) are nearly ready to begin.
- High-resolution (25 km) tuning nearly completed, production simulations imminent

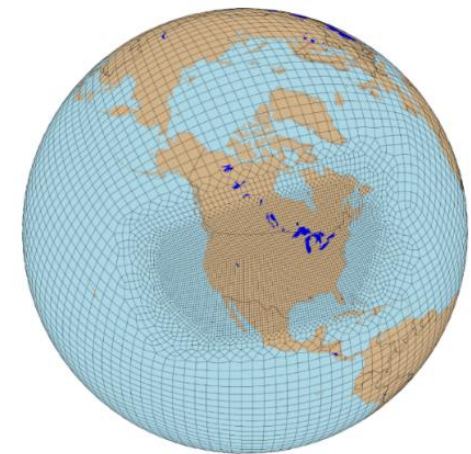
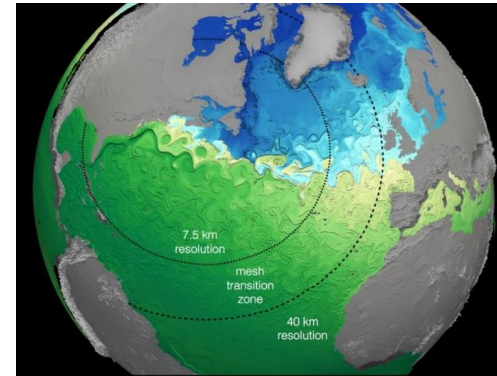
## Phase 2 high-level plans (v2-v3-v4)

- Regional refinement over North America, focus on Energy-relevant science (e.g. water management, land-use, crops)
- V3-v4 will ultimately target very high-resolution (3km) atmospheric version with simpler physics and strong scaling on DOE computers
- Ongoing work, with variable mesh around Antarctica, to determine AIS instabilities and SLR

## Community engagement

- Several new University and DOE-Laboratory projects, including SciDAC projects, will use E3SM. On-line training provided early this fall.

## SciDAC projects will contribute mainly to v4-v5



Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Oak Ridge National Laboratory	<b>Summit</b> - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband <b>IBM</b>	2,282,544	122,300	187,659	8,806
7	Oak Ridge National Laboratory	<b>Titan</b> - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x <b>Cray Inc.</b>	560,640	17,590	27,112	8,209
10	Lawrence Berkeley National Laboratory	<b>Cori</b> - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect <b>Cray Inc.</b>	622,336	14,014	27,881	3,939
17	Argonne National Laboratory	<b>Mira</b> - BlueGene/Q, Power BQC 16C 1.60GHz, Custom <b>IBM</b>	786,432	8,586	10,066	3,945
21	Argonne National Laboratory	<b>Theta</b> - Cray XC40, Intel Xeon Phi 7230 64C 1.3GHz, Aries interconnect <b>Cray Inc.</b>	280,320	6,921	11,661	--

<https://www.top500.org/list/2018/06/?page=1>

# Summit compared to Titan

## Coming in 2018: Summit will replace Titan as the OLCF's leadership supercomputer



- Many fewer nodes
- Much more powerful nodes
- Much more memory per node and total system memory
- Faster interconnect
- Much higher bandwidth between CPUs and GPUs
- Much larger and faster file system

Feature	Titan	Summit
Application Performance	Baseline	5-10x Titan
Number of Nodes	18,688	4,608
Node performance	1.4 TF	42 TF
Memory per Node	32 GB DDR3 + 6 GB GDDR5	512 GB DDR4 + 96 GB HBM2
NV memory per Node	0	1600 GB
Total System Memory	710 TB	>10 PB DDR4 + HBM2 + Non-volatile
System Interconnect	Gemini (6.4 GB/s)	Dual Rail EDR-IB (25 GB/s)
Interconnect Topology	3D Torus	Non-blocking Fat Tree
Bi-Section Bandwidth	112 TB/s	115.2 TB/s
Processors	1 AMD Opteron™ 1 NVIDIA Kepler™	2 IBM POWER9™ 6 NVIDIA Volta™
File System	32 PB, 1 TB/s, Lustre®	250 PB, 2.5 TB/s, GPFS™
Power Consumption	9 MW	13 MW

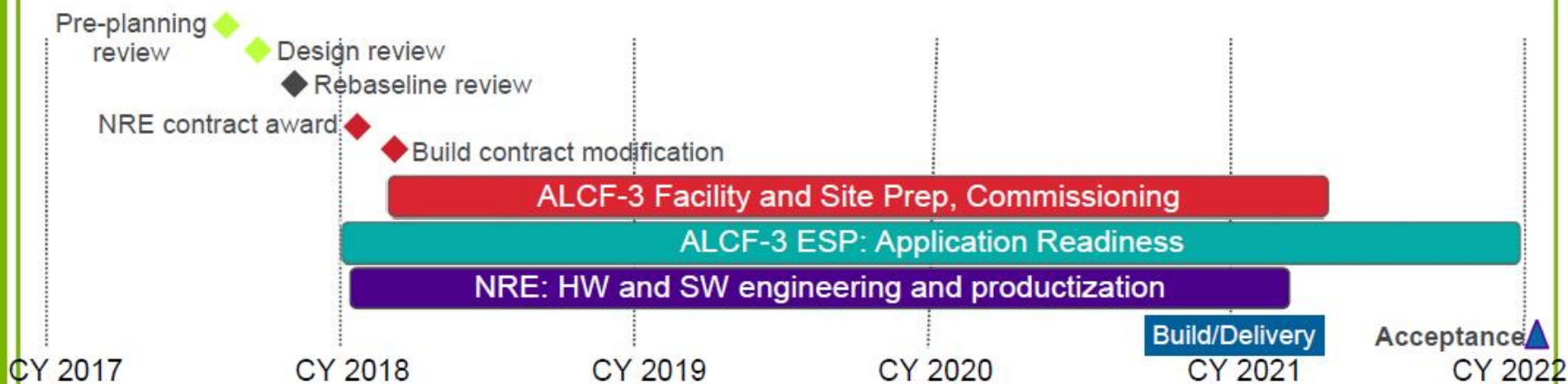
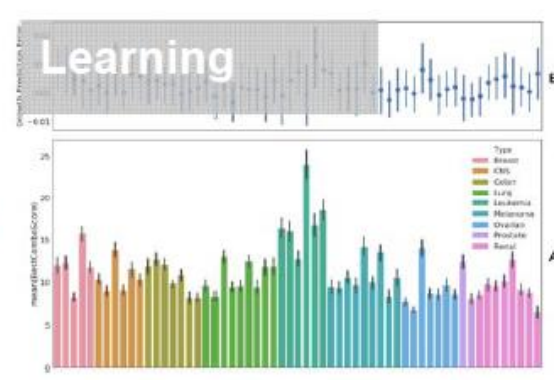
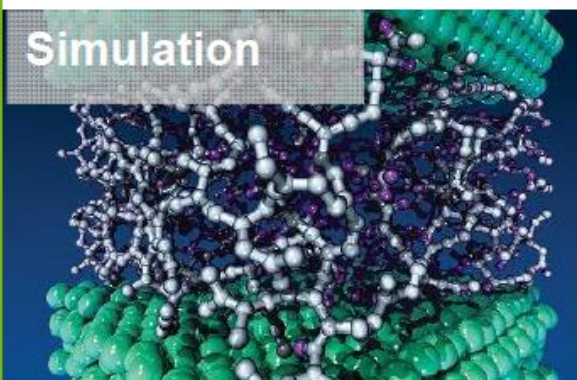
# ALCF 2021 EXASCALE SUPERCOMPUTER – A21

Intel/Cray Aurora supercomputer planned for 2018 shifted to 2021

Scaled up from **180 PF** to **over 1000 PF**



Support for three “pillars”



# Scientific Discovery through Advanced Computing (SciDAC)

SciDAC is a partnership between the Environmental (BER) and Computing Research Offices (ASCR) at DOE.

- All projects are co-funded and co-managed (Koch and Laviolette)
- Projects must be active collaborations between Earth system modelers and applied mathematicians or computer scientists to solve problems that require such an active collaboration
- Current SciDAC projects are working on problems that are important for the E3SM project to succeed in its aggressive computational objectives.
- Topics include new algorithm designs that improve model fidelity and performance, and other math/computer-science related methods to improve model fidelity, performance, and to reduce uncertainty.
- Currently there are 8 SciDAC projects, most of these will be featured here
- Two types of projects:
  - 2 Large 5-year projects that responded to specific topics
    - Tracing uncertainty in SLR to processes in ice-sheet – ocean system
    - Improving on coupling methods
  - 6 Smaller 2.5 year pilot projects to explore high-risk approaches, must improve coupled model efficiency



# 11 Projects

## **Improving numerics and solution convergence**

1. Wan (already presented)
2. Tang
3. Salinger

## **Improving computational performance through new solution methods**

4. Gunzburger
5. Taylor – tracers

## **Improving computational performance through splitting**

6. Caldwell/Donahue (already presented)

## **Improving computational performance through layout**

7. SCM – parallelizing – Evans
8. CANGA

## **Improving model accuracy by better resolving processes**

9. Ice sheets
10. Sea-ice
11. Ocean eddies

# 1. Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM, Hui Wan

## The Challenge

- Parameterizations often use simple time stepping and long step sizes
- Convergence can be significantly slower than 1<sup>st</sup>-order

## Approach

- Reduced models + formal analysis of truncation error
- Identify cause of problematic behavior, develop alternate methods

## First Results

- Identify parameterizations responsible for convergence problems
- Constructed simplified cloud parameterization coupled with dynamics that captures one difficult issue; restored 1<sup>st</sup>-order convergence by revising sequential splitting, highlighting impact of
  - Coupling between fast and slow processes
  - Singularity associated with division by zero

## Next steps

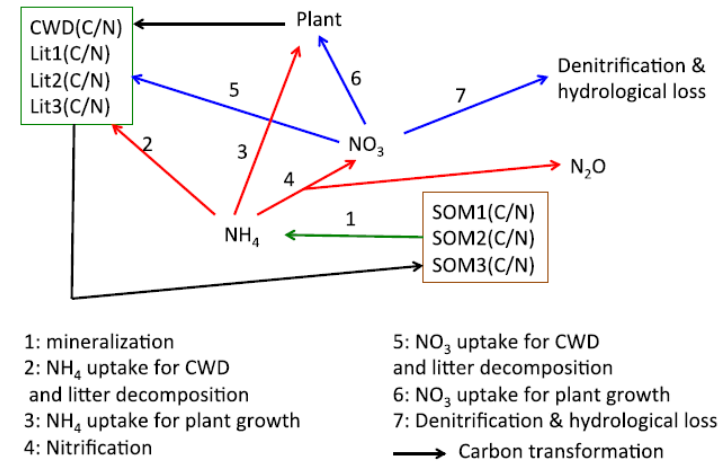
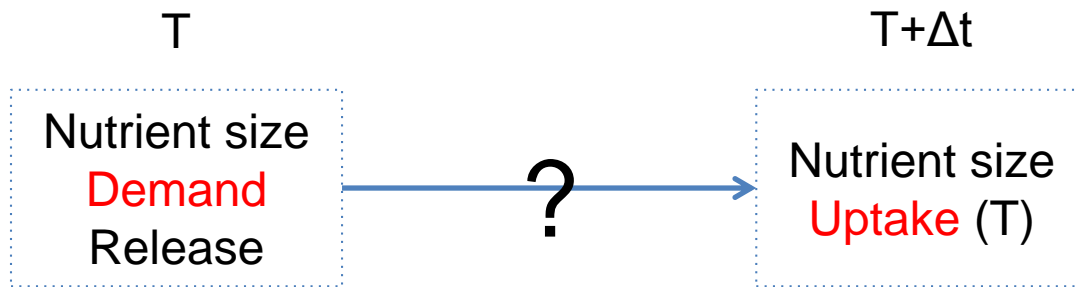
- Understand and improve convergence in E3SM's cloud and turbulence parameterizations
- Explore additional metrics for measuring solution accuracy

# 2. Land model biogeochemistry

## ELM/Nutrient coupling, J.Y. Tang and W. J. Riley

### The Challenge

Three common numerical coupling schemes of nitrogen uptake and mineralization processes affect simulated land carbon dynamics  
 Large uncertainty in turning **demand** into **uptake**



**Figure 1.** A schematic illustration of how plant and microbial processes compete for different soil mineral nitrogen species. Pathway 1 (green arrow) is the only nitrogen mobilizing process. The red and blue lines indicate immobilizing processes. In competing for soil mineral nitrogen, a demand flux is first computed for each immobilizing process. The total demand is then compared with available nitrogen to either satisfy all immobilizing demands or scale them down using the different coupling schemes described in the main text. A description of how the biogeochemistry of ELM is computed can be found in Oleson et al (2013).

### Approaches

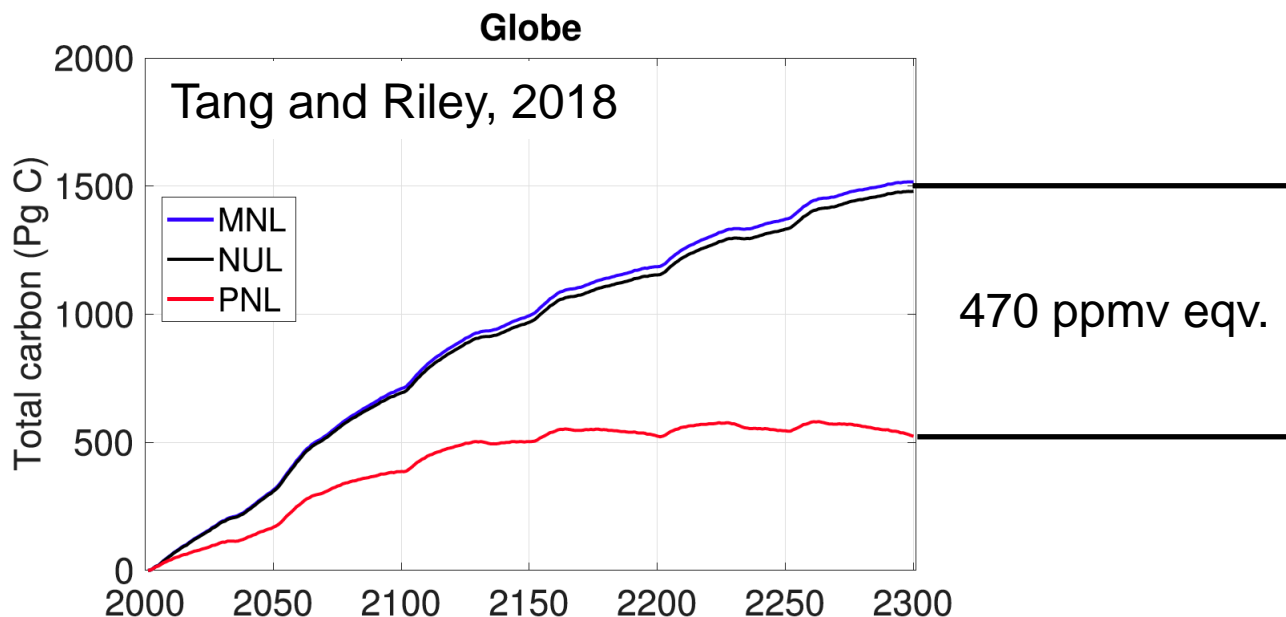
Three coupling methods explored with ELM

- MNL: Mineral Nitrogen based Limitation
- NUL: Net Uptake based limitation
- PNL: Proportional N uptake based Limitation, or “multi-substrate co-limiting algorithm”

## 2. ELM/nutrient coupling, cont'd

### Results

Divergence in long-term projections of carbon land sequestration is 75% of CIMP5 models for RCP4.5



### Next steps

- Revisit the nutrient uptake algorithms
- Evaluate various advanced numerical solvers

# 3. Verification

## software advancement project **Salinger et al**

### The Challenge

- To increase the trust in climate simulation and projection

### Approach

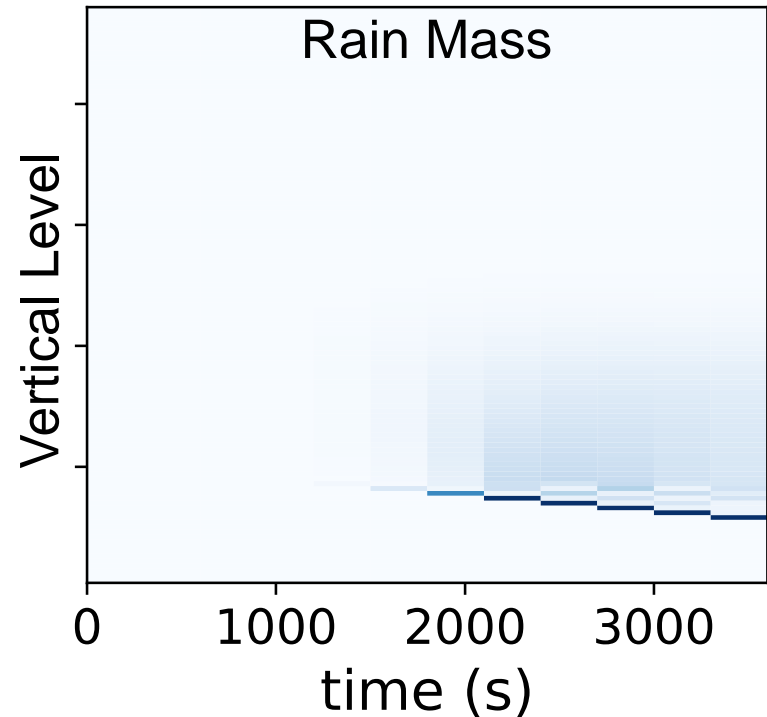
- Testing if implementation is correct:
  - Comparison against known solutions, model problems, other codes, asymptotic behavior
  - Order of convergence with respect to time step, grid spacing

### Results

- Several precipitation bugs were detected, improving skill of E3SM and CESM

### Next Steps

- Expand verification to be required for all new code features



Numerical artifact of substepping precipitation without recalculating falling speed led to unphysical results. Detected and fixed by verification effort.

Andy Salinger: [agsalin@sandia.gov](mailto:agsalin@sandia.gov)

# 3. Regression Testing for Scalable Code Development

## The Challenge

- To enable large, dispersed team to work in parallel while protecting trusted code.

## Approach

- Large test suites running automatically, overnight, on all main development and production machines
- New code must pass tests before being accepted onto “master” (*git workflow*)

## Results

- Code base is stable, and integration is keeping pace with development
- The E3SM team now knows:
  - “Any capability that you want to preserve must be protected by a test.”

### Machine | Suite | Fail | Pass

E3SM_Baseline			
Site	Build Name	Test	
		Fail	Pass
melvin	acme_developer_	0	40
melvin	acme_developer_	0	37 <sub>-3</sub>
sandiatoss3	acme_integration	56 <sup>+56</sup>	0 <sub>-56</sub>
sandiatoss3	acme_integration	58 <sup>+56</sup>	0 <sub>-56</sub>
E3SM_Machine			
Site	Build Name	Test	
		Fail	Pass
cetus	acme_developer_	2 <sub>-1</sub>	38 <sup>+1</sup> <sub>-1</sub>
edison	acme_developer_	0	41
cori-haswell	acme_developer_	1 <sup>+1</sup>	40 <sub>-1</sub>
cori-knl	acme_developer_	0	40 <sup>+1</sup> <sub>-2</sub>
titan	acme_developer_	3 <sup>+1</sup> <sub>-1</sub>	37 <sub>-1</sub>
mira	acme_hi_res_next	2	0
cori-knl	acme_hi_res_next	0	2
cetus	acme_integration	3	54
blues	acme_integration	2	57
bebop	acme_integration	5	53
anvil	acme_integration	4	54 <sub>-1</sub>
anvil	acme_prod_maste	0	1
edison	acme_prod_next	0	1
anvil	acme_prod_next	0	1
cori-knl	acme_prod_next	0	1
titan	acme_prod_next	0	1
E3SM_Custom			
Site	Build Name	Test	
		Fail	Pass
skybridge-login6	run_acme_script	0	1
skybridge-login5	run_acme_script	0	1

# 4. Ocean: Time-stepping for variable-resolution grids

PI's: M. Gunzburger (FSU) & L. Ju (USC)

FSU: S. Calandrini, K. Pieper, C. Sockwell; USC: P. Hoang, Z. Wang

## The Challenge

### Multiple scales in ocean models

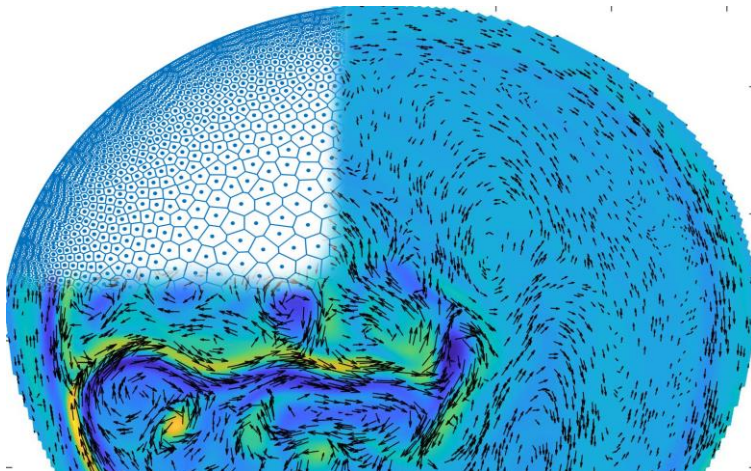
- different mesh resolutions (*local*)
- fast and slow dynamics (*global*)

### New time-stepping algorithms that have

- global time step not restricted by local CFL
- excellent conservation properties

### Multiresolution mesh generation

- physical fidelity and efficiency of algorithms



## Approach

### Exponential time differencing (ETD)

- global dynamics splitting: barotropic/baroclinic/advective
- long-term stability (decades) and fidelity

### Conservative, explicit local time stepping (LTS)

- spatially-dependent time step sizes
- high accuracy in selected regions
- naturally parallelizable with domain decomposition (DD)

### Insure conservation properties

- global mass conservation
- energy/enstrophy dynamics

## Next Steps

- development of LTS and ETD for more complicated ocean dynamics models and for tracer equations
- LTS for split-explicit method
- parallel, localized ETD: fully integrate ETD-DD-LTS approaches

Max Gunzburger: [mgunzburger@fsu.edu](mailto:mgunzburger@fsu.edu)

# 4. Ocean: Time-stepping for variable-resolution grids, cont'd

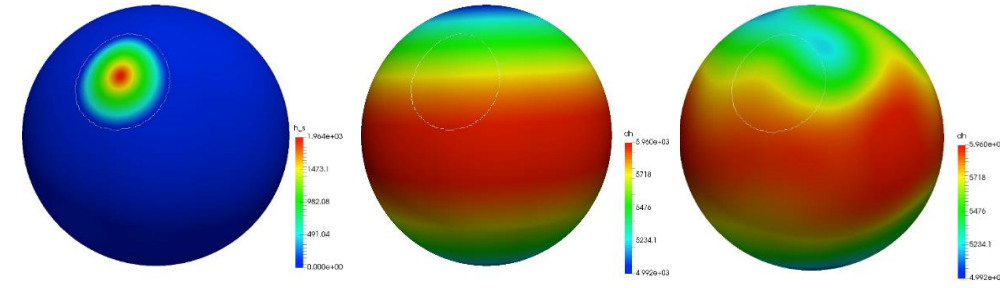
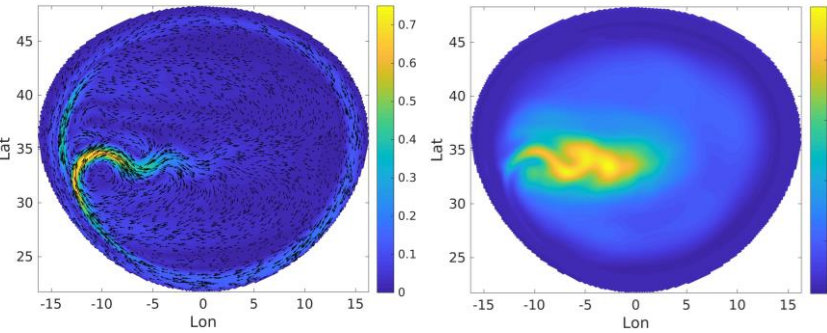
## ETD-Results: Three layer test case based on SOMA

Mid-latitude regional ocean with variable bathymetry (2.5 km to 100 m) over ten years

## LTS-Results: Shallow water equations (SWTC5)

Coarse cell area is approximately four times of the fine cell area (the circular region)

$$\Delta t_{coarse} = M \Delta t_{fine}$$



Bottom topography

Fluid height initially and after 15 days

Mean flow (surface velocity)

RMS of the sea surface height

- ETDwave: linear waves treated exponentially → No CFL
- B-ETDwave: only linear *barotropic* waves treated exponentially; more efficient.
- Efficiency increase with number of layers

$\Delta t_{coarse}$	Fluid thickness [CR]	Velocity [CR]
$0.5 \Delta t_{CFL}$	3.38e-06	2.20e-05
$0.25 \Delta t_{CFL}$	5.88e-07 [2.52]	3.27e-06 [2.75]
$0.125 \Delta t_{CFL}$	7.80e-08 [2.91]	4.20e-07 [2.96]
$0.0625 \Delta t_{CFL}$	1.24e-08 [2.85]	6.25e-08 [2.93]

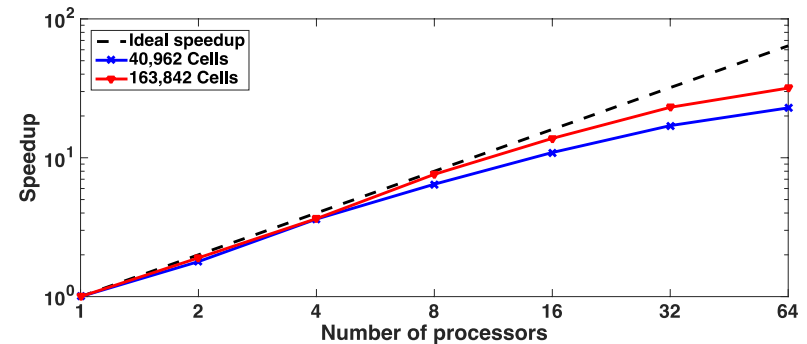
$M$	Fluid thickness	Velocity
1	1.69e-06	9.38e-06
2	6.76e-07	3.68e-06
4	5.95e-07	3.27e-06
8	5.88e-07	3.25e-06

Errors and convergence rates (CR) vs. time step size for the LTS scheme,  $M=4$ .

Errors with a fixed coarse time step size & varying  $M$

Method	$\Delta t / \Delta t_{CFL}$	SYPD	mean-flow (rel.)	SSH-RMS
RK4	3/4	0.911	0.054	0.054
ETD2wave	15	2.77	0.044	0.060
B-ETD2wave	7	4.61	0.037	0.071

Accuracy for statistical quantities and simulated years per day (SYPD) of different ETD methods



Parallel scalability of the third-order LTS algorithm,  $M=4$



# 5. New E3SM non-hydrostatic atmosphere dycore formulation based on Semi-Lagrangian transport

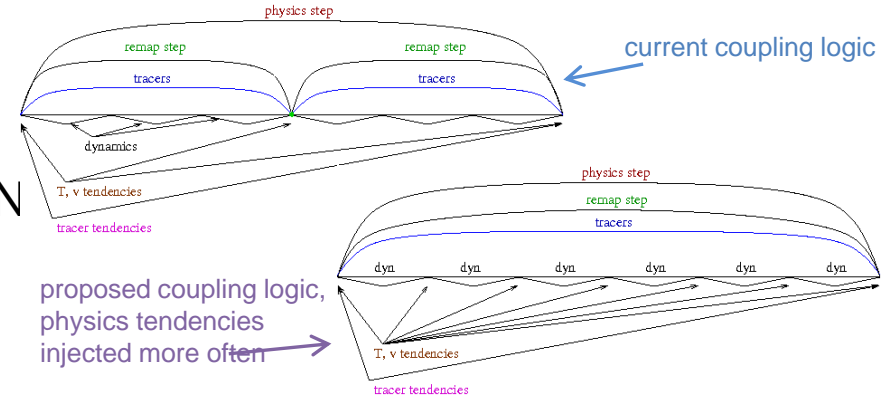
Tracer advection: very computationally expensive

New physics coupling logic in E3SM enables longer semi-Lagrangian tracer time steps

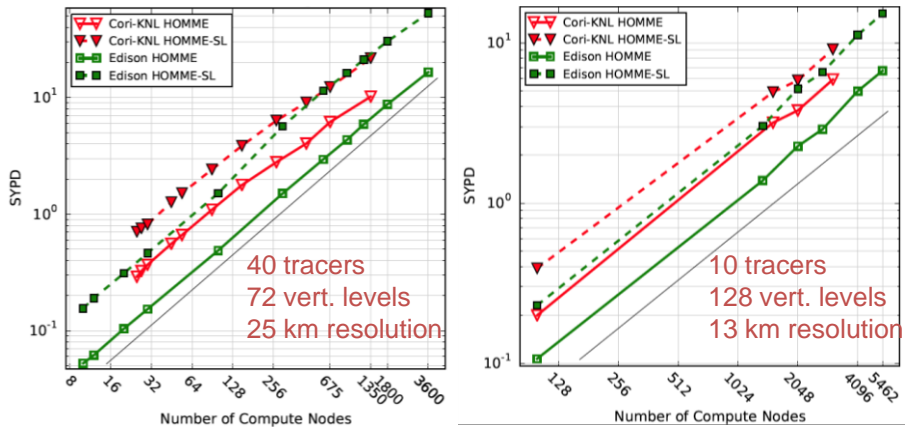
New semi-Lagrangian transport algorithm<sup>1,2</sup>: Speeds up dycore by 3.2x in E3SM v1 high-resolution configuration.

- Long time steps and compact data stencil (multimoment) lead to less communication
- Quasi-local mass conservation, shape preservation, tracer consistency obtained through new CEDR algorithm<sup>2</sup>.
- Requires single all-reduce per tracer time step

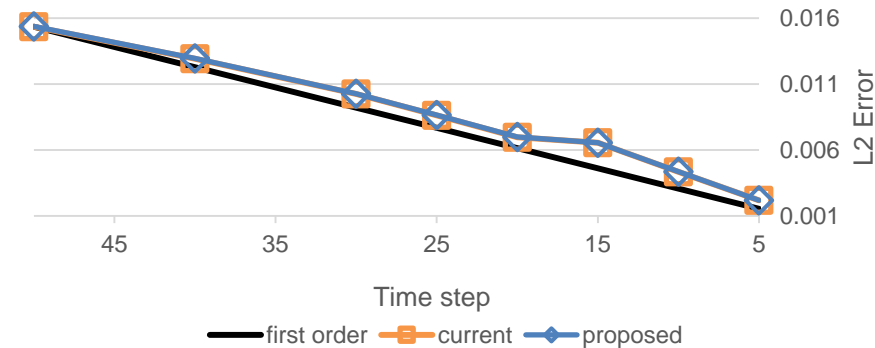
Old coupling logic limits tracer time step, does not take advantage of available frequent tendency injections



## Performance (dycore) for Edison and Cori-KN



Coupling logic being verified with idealized tropical cyclone test



More frequent tendency injections lead to smaller errors.

<sup>1</sup>P. A. Bosler, A. M. Bradley, M. A. Taylor, “Conservative multi-moment transport along characteristics for discontinuous Galerkin methods”, submitted to *SIAM J. Sci. Comput.*, 2018

<sup>2</sup>A. M. Bradley, P. A. Bosler, O. Guba, M. A. Taylor, and G. A. Barnett. “Communication-efficient property preservation in tracer transport,” submitted to *SIAM J. Sci. Comput.*, 2018.

Pete Bosler: [pabosle@sandia.gov](mailto:pabosle@sandia.gov)

# 6. Improving atmosphere model performance

A.S. Donahue and P.M. Caldwell

## The Challenge

- Improve the E3SM atmosphere model (EAM) performance through concurrent calculation of physics and dynamics.

## Results

- Parallel physics/dynamics coupling implemented in EAM.
- 40% better performance at highest core counts.
- More restrictive stability criteria for parallel-split that must be addressed before widespread adoption.

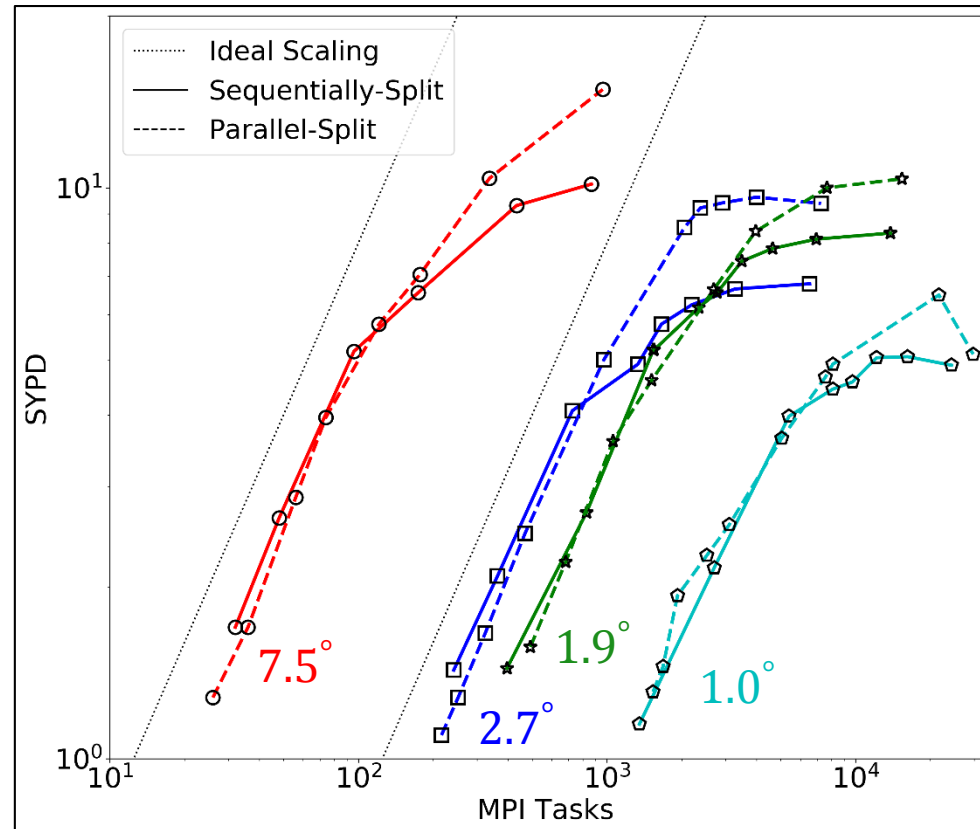


Figure: Summary of EAM performance results for four spectral element meshes. All simulations run using  $\Delta t = 300\text{sec}$ .

# 7. Optimization of sensor networks for improving climate model predictions **Dan Ricciuto**

## The Challenge

- Many ensembles of single column model runs needed to quantify model uncertainty and determine placement of sensor networks that will optimally reduce prediction uncertainty

## Approach

- Design an efficient simulation framework for a “network” of single-column coupled land-atmosphere model ensembles using point scale data
- Determine sources of model uncertainty from land and atmospheric physics
- Create an uncertainty quantification framework to optimize placement of new observations for uncertainty reduction in model predictions
- Propagate uncertainty with multi-fidelity approach: Multi-level Monte Carlo (MLMC) can be used to propagate uncertainties *in fully coupled mode* over a range of fidelity and resolution.

# 7. Address multitude of serial, single column model runs by using a multi-GPU computing system

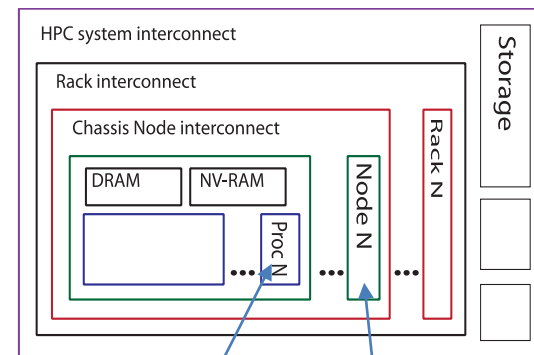
## Early Tasks

- Develop capability to run suite of SCM configurations within E3SM
- Port SCM in E3SM to OLCF's titan, assess performance of ensembles
- Perform sensitivity experiments with SCM ensembles on titan using multiple CPU



## Next steps

- Profile and scope utilizing SCM on multiple accelerator computing systems, target Summit
- Execute multiple SCM on accelerator based computers (Titan, then Summit)
- Optimize SCM ensembles to leverage heterogeneity of Summit



Kate Evans: [evanskj@ornl.gov](mailto:evanskj@ornl.gov)



# 8. Coupling Approaches for Next Generation Architectures (CANGA): Overview

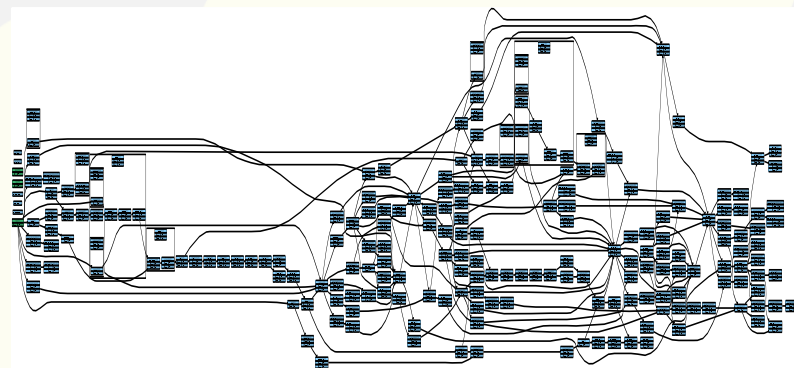
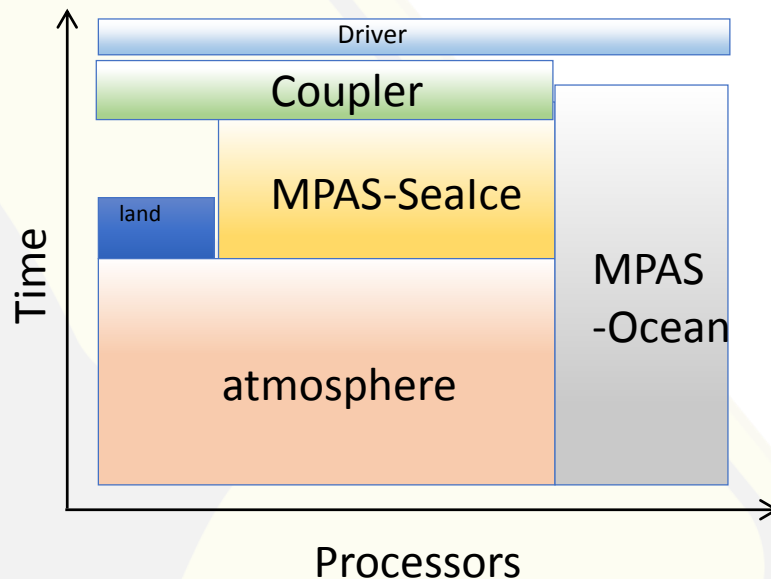
Phil Jones, PI

On behalf of the CANGA project



## 8. CANGA Goals

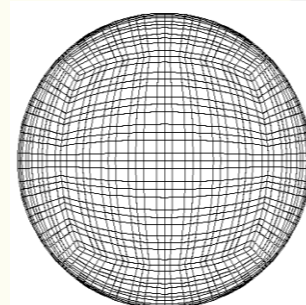
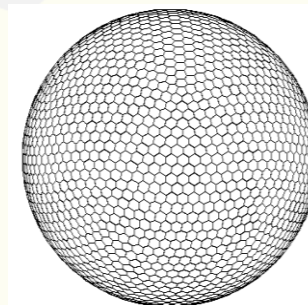
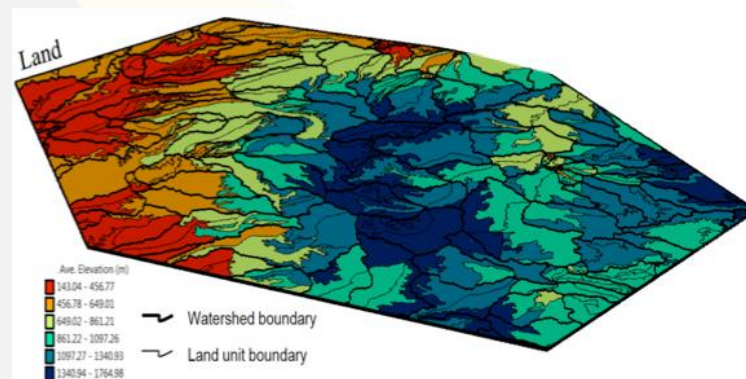
- Highly performant, accurate and robust coupling strategies for a new E3SM
- Prototype Integration of Global models using Legion Execution of Tasks (PIGLET)
  - Replace hub/spoke, monolithic components
  - Asynchronous Many-Task Model
  - Exposes more parallelism
  - Better load balancing
  - Manage both science/software complexity
  - Enable process coupling at proper time, spatial scales
- Legion/Regent implementation
  - Coupler, driver layer
  - Individual components (land, ocean, ice)
  - In situ analysis





## 8. CANGA Goals

- Upgrade coupling algorithms
  - Remapping Online-Offline (ROO)
    - Non-convex cells
    - On-line adaptive remapping
    - Vector and property-preserving
    - Meshfree (agnostic to staggering location)
    - Remap test suite
  - Time InteGration for Greater E3SM Robustness (TIGGER)
    - Replace ad-hoc time-lagging and instability
    - Address multiple space, timescales
  - Integrate into task-based coupler
- Applications, mini-apps
  - Simpler coupled systems to analyze, evaluate





# 8. CANGA organization

ASCR funded

BER funded



## Task-based Models P. Jones (LANL)

Coupler Prototype  
J. Graham, P. Jones (LANL)

Legion Support  
I. Demeshko (LANL)

Land Model  
E. Coon, S. Painter (ORNL)

In Situ analysis  
T. Peterka, H. Guo (ANL)

Ocean, Ice  
I. Demeshko, PD, P. Jones (LANL)

Performant  
accurate, robust  
AMT coupled  
system

## Remapping (ROO) P. Ullrich (UC-Davis)

TempestRemap Extensions  
P. Ullrich (UC-Davis), V Mahadevan (ANL)

Property-preserving and meshless  
P. Bochev, R. Pawlowski, K. Peterson, P. Kuberry (SNL)

Adaptive Remap  
X. Jiao, Stony Brook

## Time Integration and Applications R. Jacob (ANL), P. Bochev (SNL)

Reduced complexity models  
R. Jacob, PD (ANL)

Applications and reduced complexity models  
Z. Liu (Ohio State)

Time integration  
P. Bochev, K. Peterson, D. Ridzal (SNL)

Time Integration  
H. Zhang (ANL)



THE OHIO STATE UNIVERSITY

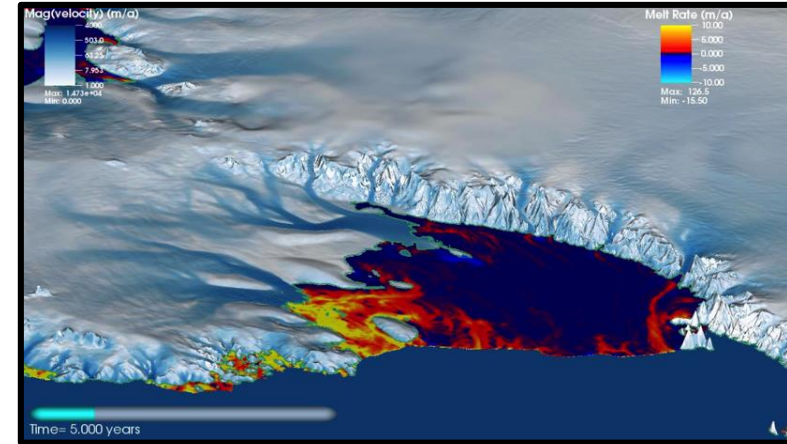


Phil Jones: [pwjones@lanl.gov](mailto:pwjones@lanl.gov); Rob Jacob [Jacob@anl.gov](mailto:Jacob@anl.gov)



# 9. ProSPect: Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models

*ProSPect* will remedy limitations to DOE ice sheet models (ISMs) and Earth System Models (ESMs) that currently prohibit their use in providing accurate sea-level projections. Specific areas to be addressed include:

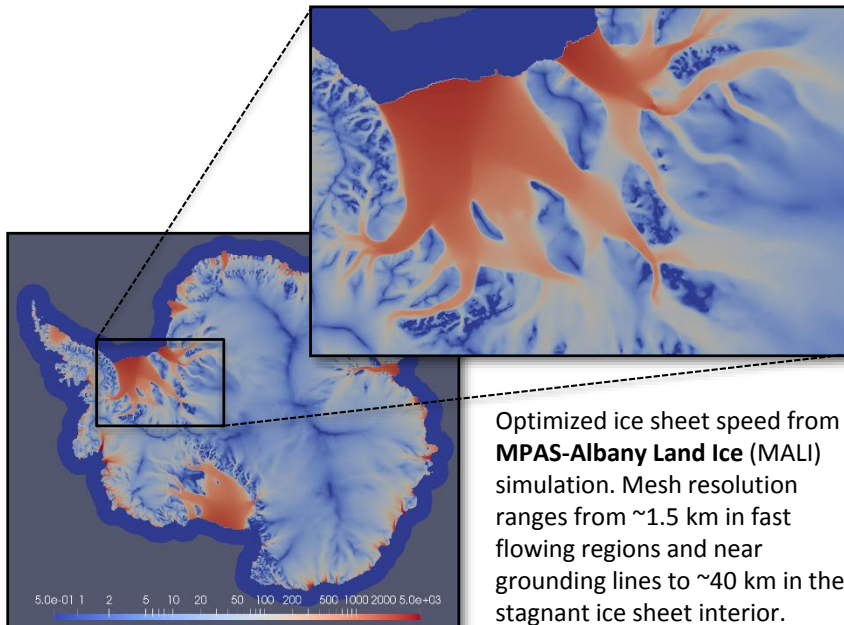


Simulated velocities and submarine melt rates in the Ross Sea Embayment using the **BISICLES AMR ice sheet** model coupled to the POP2x ocean model.

- missing or oversimplified physics
- inadequate initialization methods
- coupling between ISMs & ESMs
- ISM uncertainty quantification

## Institutions:

LANL, LBNL, SNL, ORNL, NYU, U. Mich.

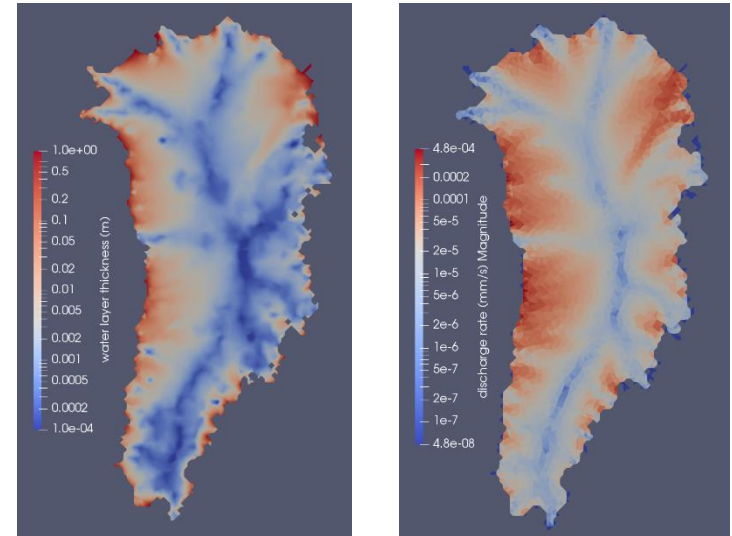


Optimized ice sheet speed from **MPAS-Albany Land Ice (MALI)** simulation. Mesh resolution ranges from  $\sim 1.5$  km in fast flowing regions and near grounding lines to  $\sim 40$  km in the stagnant ice sheet interior.

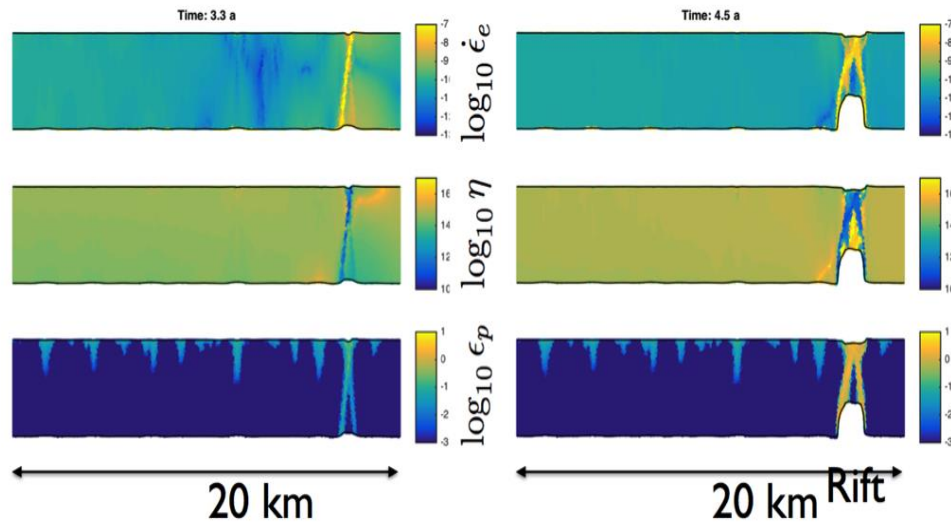
# 9. Coupling of new physics to ice sheet models

## Subglacial Hydrology

- primary control on sliding & hence ice flux to oceans; critical for evolving rather than static basal boundary
- coupled to climate via surface melt & liquid freshwater input to ocean at depth
- challenge: disparate time & spatial scales relative to ISMs; sheet vs. channel flow (mode switches)
- approach: unstruct. FEM or AMR to resolve channels; coupled ice & hydro. solve; dim. reduction via global optimization of hydro. model params.



Subglacial water layer thickness (left) and flux (right) beneath Greenland from a model in development under ProSPect (Figure and results courtesy of L. Burtagna, SNL).



Prototype model of ice shelf "rift" (large cracks) formation based on a damage mechanics approach. Model development and preliminary results under ProSPect courtesy of J. Bassis (Univ. of Michigan).

## Damage, Fracture, Calving

- primary control on ice shelf strength & ability of shelves to limit ice flux to ocean
- coupled to climate via surface melt (hydro-fracture) & solid freshwater flux to ocean
- challenge: accurate grid-scale (km) representation of fracture initiation (micro-scale) & evolution
- approach: damage-mechanics and locally refined meshes with AMR

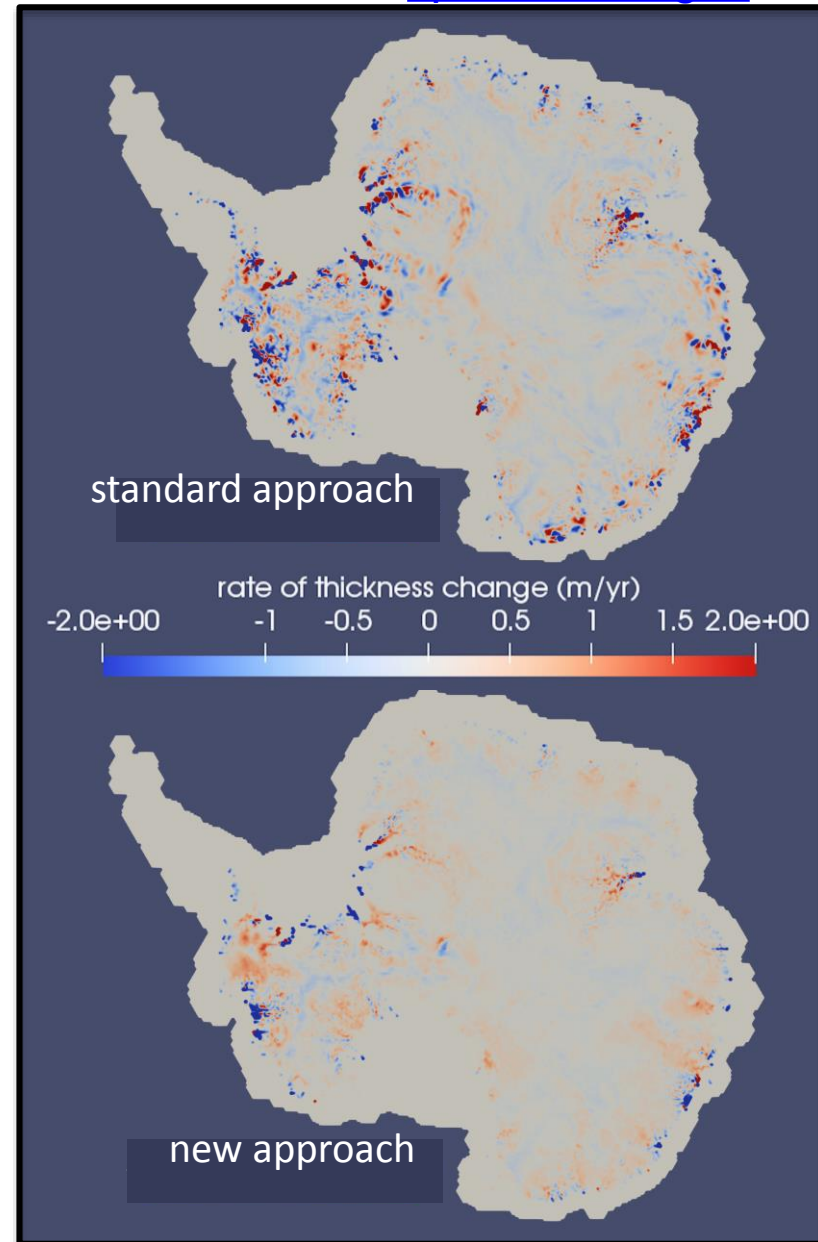
# 9. Coupling to ESMs: Optimization & Initialization

Steve Price: [sprice@lanl.gov](mailto:sprice@lanl.gov)

## Optimization and Initialization

- ISMs & ESMs operate on disparate equilibrium timescales ( $\sim 10^3$ - $10^5$  years for ISMs, )
- standard coupled model “spin-up” methods are not practical for coupling ISMs & ESMs
- one alternative is offline initialization of ISMs but standard optimization leads to large, non-physical ISM transients when coupling to ESMs
- new approaches, specifically aimed at minimizing these transients are being developed & applied under *ProSPect*
- challenges / approach: added constraints & DOFs are numerically & computationally challenging; requires improved solution methods (compute of approx. Hessian; reduced /full-space Newton/Krylov solvers & precondition.)

Rate of initial ice sheet thickness change (i.e., “transient”) for two different optimized initial conditions. Top panel shows a case where the model has only been optimized to match observed ice sheet velocities (standard). The bottom panel, with a greatly reduced transient, also accounts for climate forcing terms – surface and basal mass balance – and allows ice thickness to vary within observational uncertainties (Figures courtesy of M. Perego, SNL).



# 10. Discrete Element Model for Sea Ice (DEMSI)

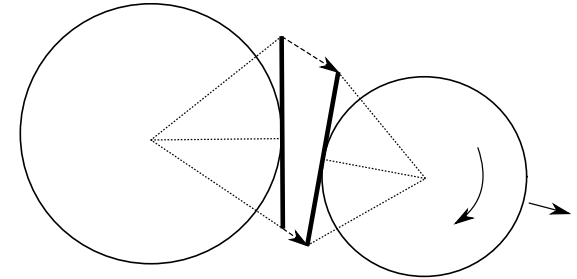
Adrian Turner (LANL), Kara Peterson (SNL), Andrew Roberts (NPS)

## The Challenge

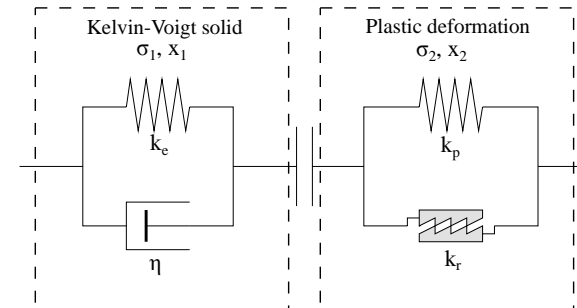
- Develop a Discrete Element Method (DEM) sea ice model suitable for climate applications - improved representation of sea ice dynamics at high resolution.

## Approach

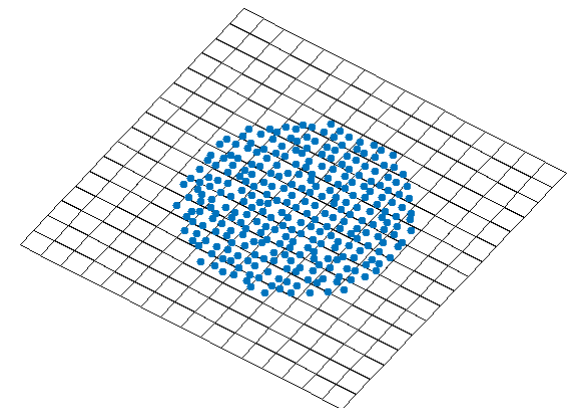
- Combine LAMMPS (dynamics) and Icepack (thermodynamics) codes.
- Develop element contact suitable for sea ice – history dependence, fracture, anisotropy.
- Moving-Least-Squares technique for mapping from particles to coupler
- Kokkos in the dynamics solver.



Bond between two particles undergoing relative motion



Contact model for unbonded elements

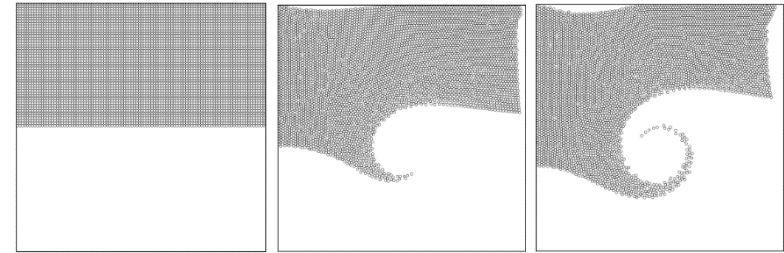


Adrian Turner: [akt@lanl.gov](mailto:akt@lanl.gov)

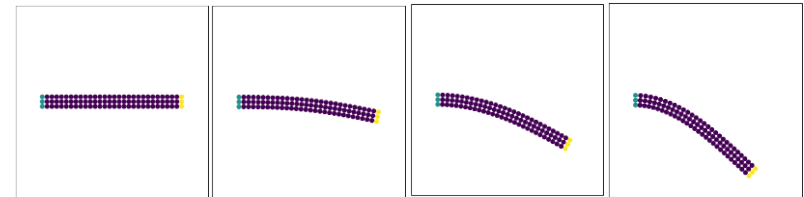
# 10. Discrete Element Model for Sea Ice (DEMSI)

## Results

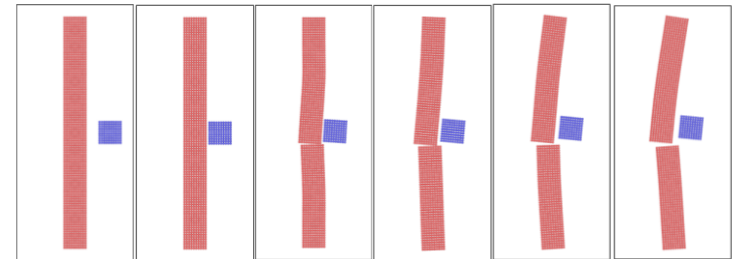
- Element contact model of Hopkins is being validated
- Icepack vertical physics library has been integrated
- Coupling methodology developed
- Framework for performing global climate simulations mostly complete



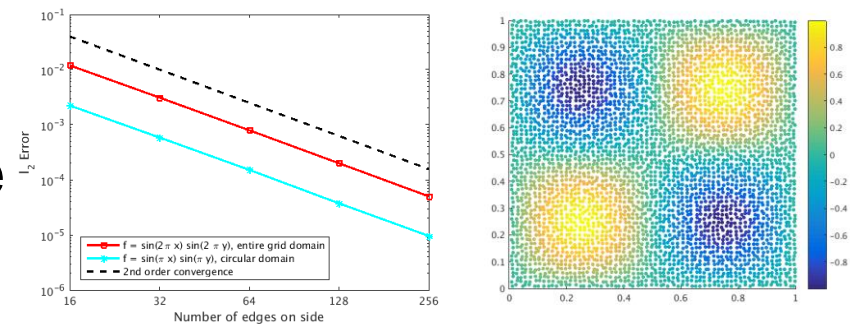
Vortex wind forcing test case



Cantilever testcase without fracture



Impact testcase with fracture



Convergence of coupling interpolation test case

## Next steps

- Improved contact model from ridge and floe resolving sims.
- Regional and global simulations
- Develop methodology to manage element distortion during ice deformation

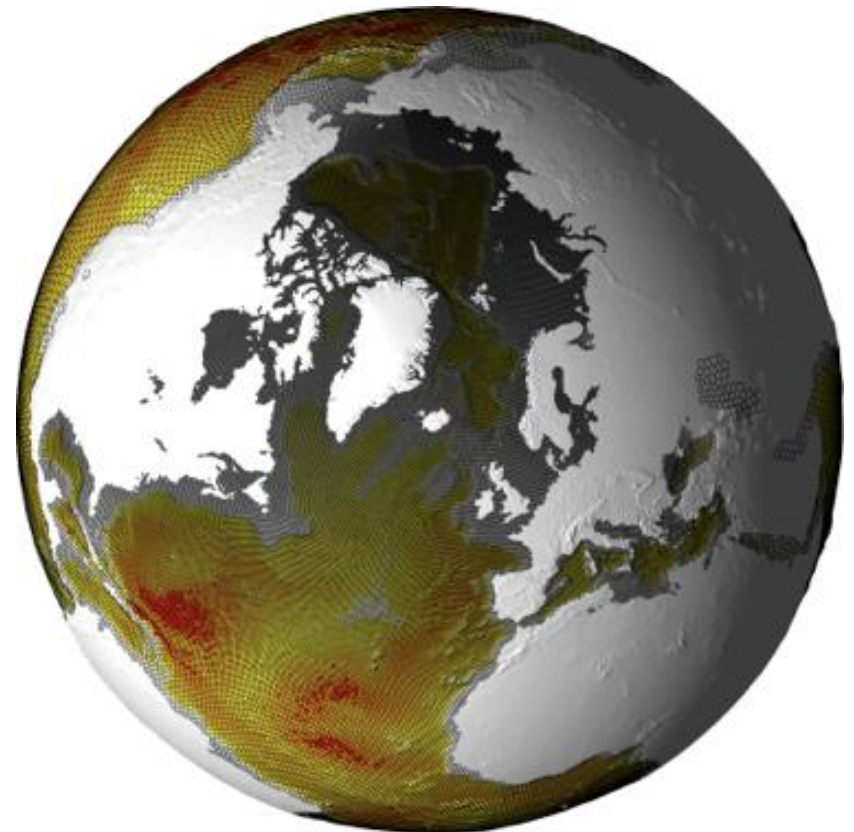
# 11. Multi-resolution Ocean Simulation

## The Challenge

- The ocean component of E3SM supports variable resolutions meshes, with eddy-rich, eddy-permitting, and eddy-parameterized regions within a single simulation. **To exploit the multi-resolution simulation capability, we require a scale-aware parameterization of mesoscale eddies.**

## Approach

- Recast eddy-parameterization in an energetically consistent form (thickness-weighted average equations from Young (2013)).
- Add prognostic equation to track vertically averaged, sub-grid, mesoscale eddy energy.
- Define closure to related sub-grid, mesoscale eddy energy to vertical transport of mean momentum.



# 11. Multi-resolution Ocean Simulation

$$\frac{\partial \langle \mathcal{E}' \rangle_z}{\partial \tilde{t}} = \langle \hat{u} (\nabla \cdot \mathbf{E}) \cdot \mathbf{i} \rangle_z + \langle \hat{v} (\nabla \cdot \mathbf{E}) \cdot \mathbf{j} \rangle_z + \langle \mathcal{D}_e \rangle_z$$

sub-grid  
eddy energy

flow of energy to/from sub-grid  
due to eddy-mean flow interaction

dissipation

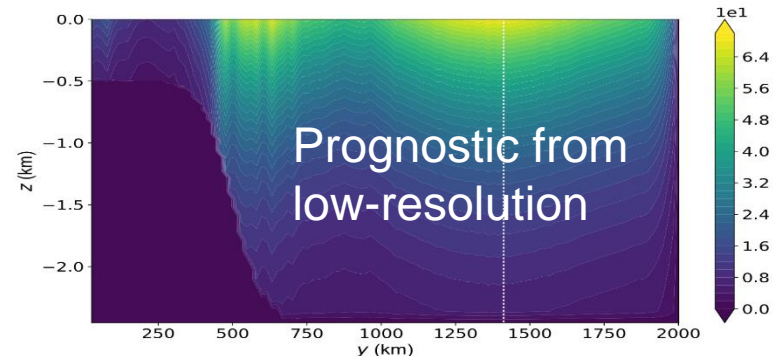
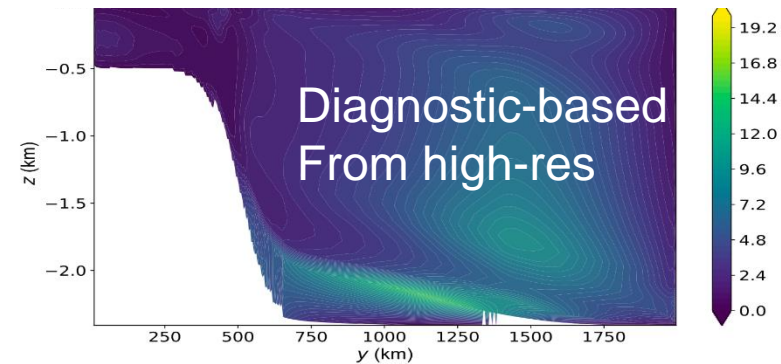
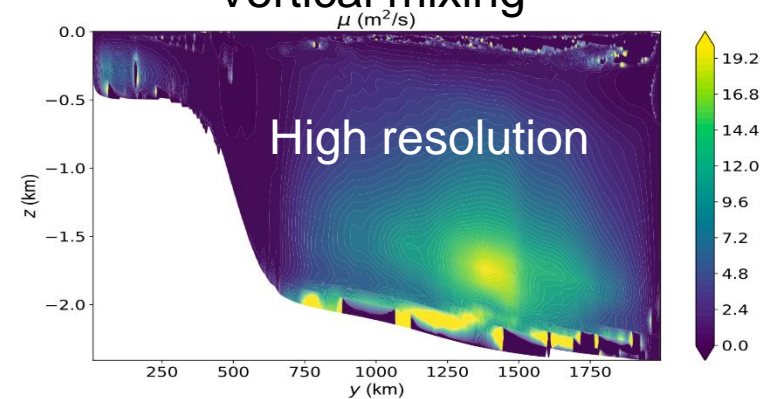
$$\mu_e = \frac{f^2}{N^2} \sqrt{\mathcal{E}'} \ell_m$$

Prandtl mixing-length closure

## Results

- Configure idealized, zonally symmetric annulus as analog to Southern Ocean.
- Conduct eddy-rich, reference solution and eddy-parameterized experiment.
- Compute vertical mixing directly from high-res control (top), diagnostically based on high-res data (middle), and prognostically from low-resolution parameterization (bottom).
- The parameterization deposits too much of the momentum in the thermocline.

## Vertical mixing



# 11. Multi-resolution Ocean Simulation

Saenz, J. and T. Ringler, 2018. A Prognostic, One-Equation Model of Mesoscale Eddy Momentum Fluxes, Ocean Modeling, in preparation.

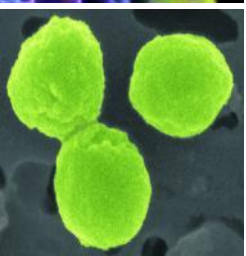
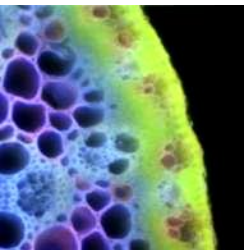
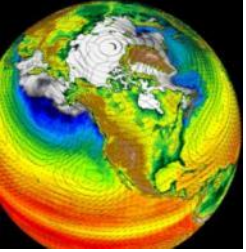
Ringler, T., Saenz, J.A., Wolfram, P.J. and Van Roekel, L., 2017. A thickness-weighted average perspective of force balance in an idealized circumpolar current. *Journal of Physical Oceanography*, 47(2), pp.285-302.

Wolfram, P.J. and Ringler, T.D., 2017. Quantifying residual, eddy, and mean flow effects on mixing in an idealized circumpolar current. *Journal of Physical Oceanography*, 47(8), pp.1897-1920.

Saenz, J.A., Chen, Q. and Ringler, T., 2015. Prognostic residual mean flow in an ocean general circulation model and its relation to prognostic Eulerian mean flow. *Journal of Physical Oceanography*, 45(9), pp.2247-2260.

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# Thank you!

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