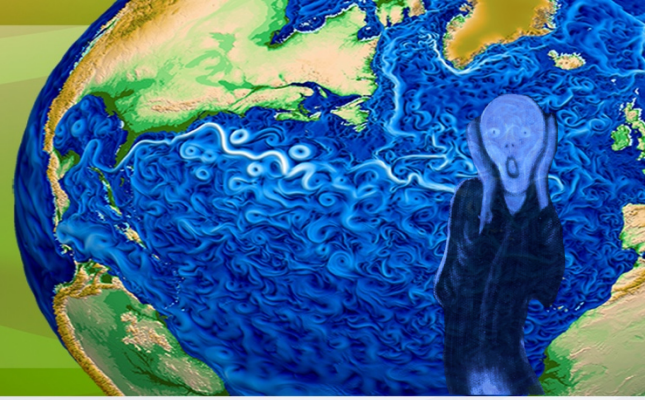
E3SM
Energy Exascale Earth System Model



Next-Generation Developments in Software and Algorithms

Oct 26, 2020

Andy Salinger (Sub-Project Lead)

Hyun Kang Andrew Bradley, Andrew Steyer, Cassidy Krause

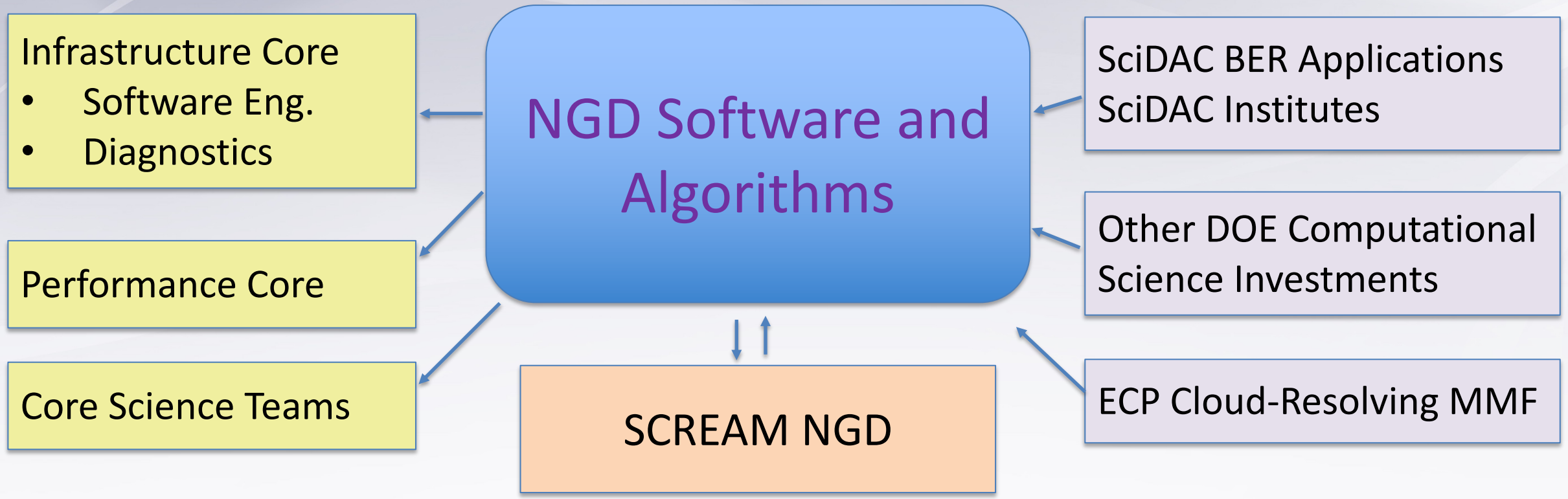
Karen Devine, Iulian Grindeanu, Vijay Mahadevan

Salil Mahajan, Michael Kelleher, Rong-You Chien, Josh Fu

Benj Wagman, Kenny Chowdhury

U.S. DEPARTMENT OF ENERGY

How the NGD Software and Algorithms sub-project Fits in the Larger E3SM Ecosystem



Incorporation into E3SM:
Short Term

Medium Term

Long Term

Software and Algorithms NGD

Major Themes: Make targeted investments to:

1. Improve model throughput on exascale machines
   a. Algorithms, Performance
2. Improve developer productivity
3. Create a culture of Verification
4. Leverage DOE Computational Science investments
5. Entrain talented computational scientists into E3SM

NGD S&A Highlights
October 2020

Key Team Member

For more details, look for the presentation or poster from these authors.

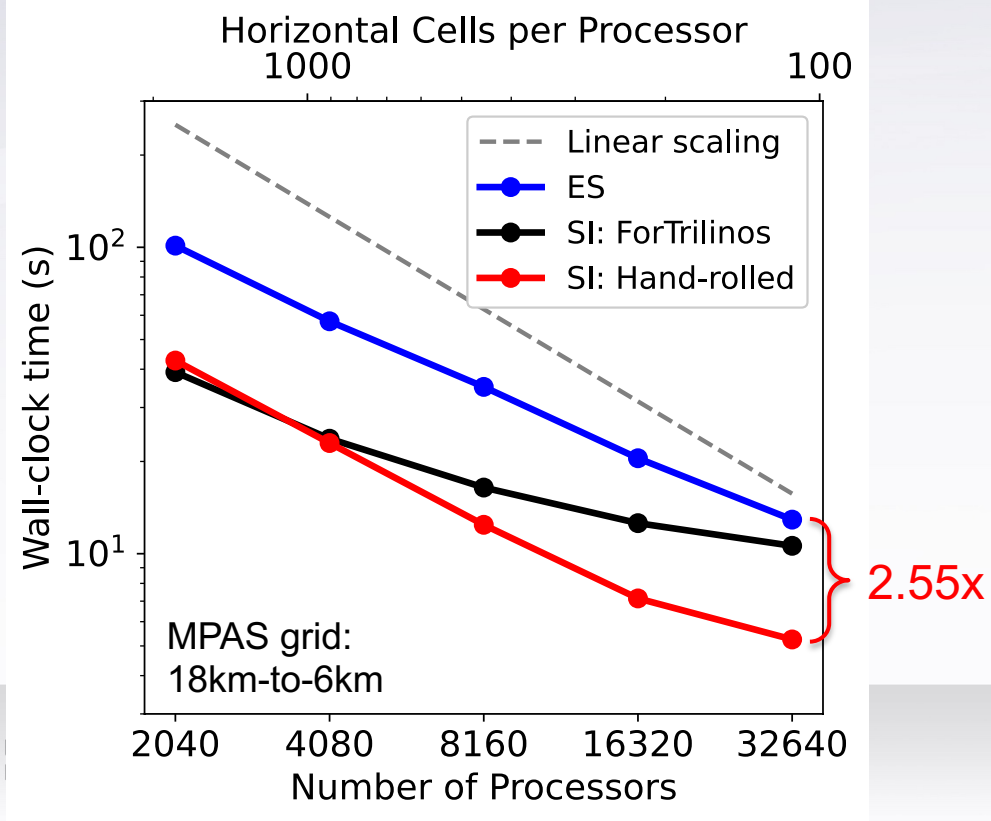
MPAS Barotropic Mode Solver

Hyun Kang

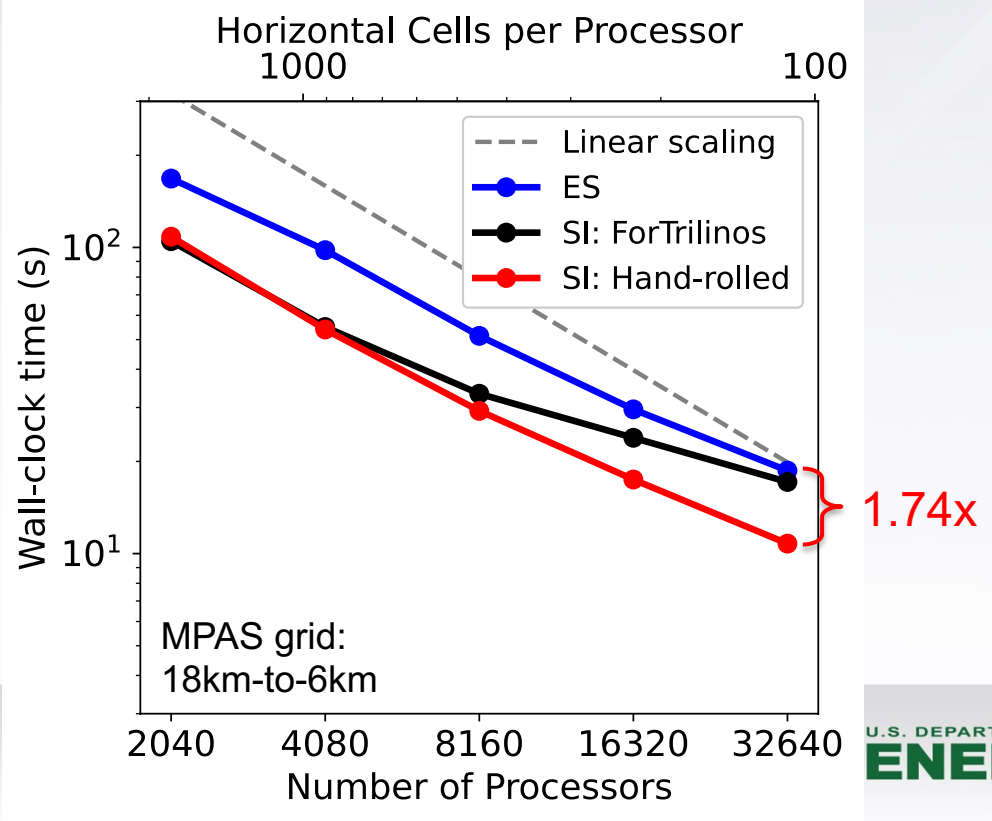
- Ocean barotropic mode
  a. Further improvements in the semi-implicit (SI) barotropic mode solver
     a. 2.55x speedup for barotropic mode solve over explicit subcycling (ES)
     b. 1.74x speedup of MPAS-O at scale
  b. A new semi-implicit solver using ForTrilinos (Fortran interface to Trilinos): AMG preconditioner and CG solver

※ The explicit-subcycling scheme is also improved significantly in MPAS-O v7.0 compared to v6.0.

Barotropic mode solver only



Total runtime



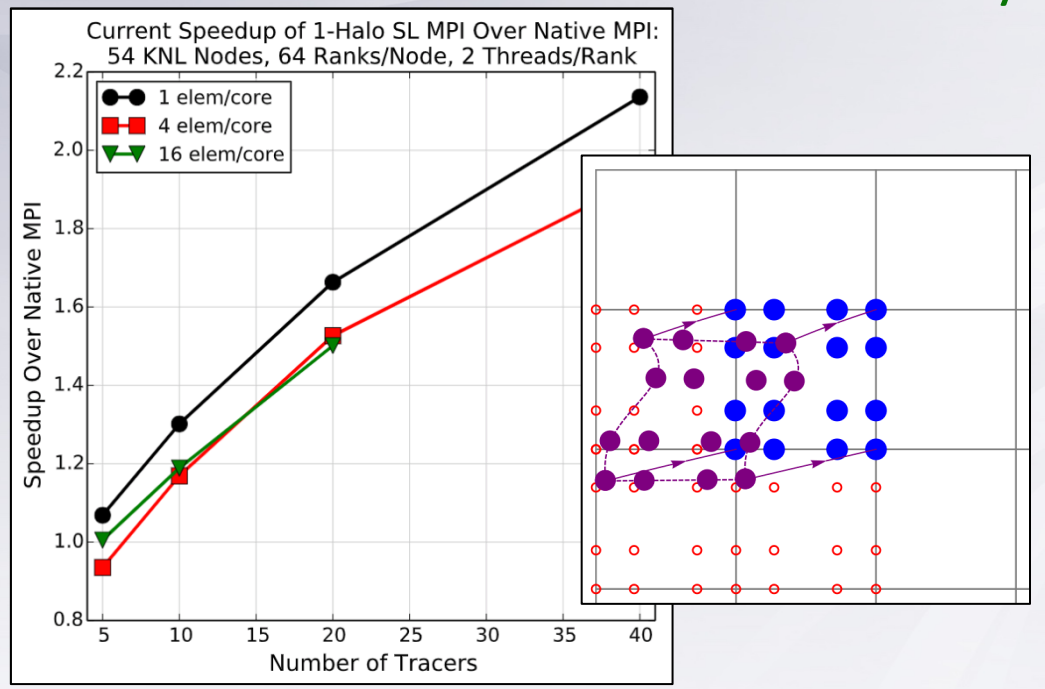
SL Tracer Transport Upwind MPI

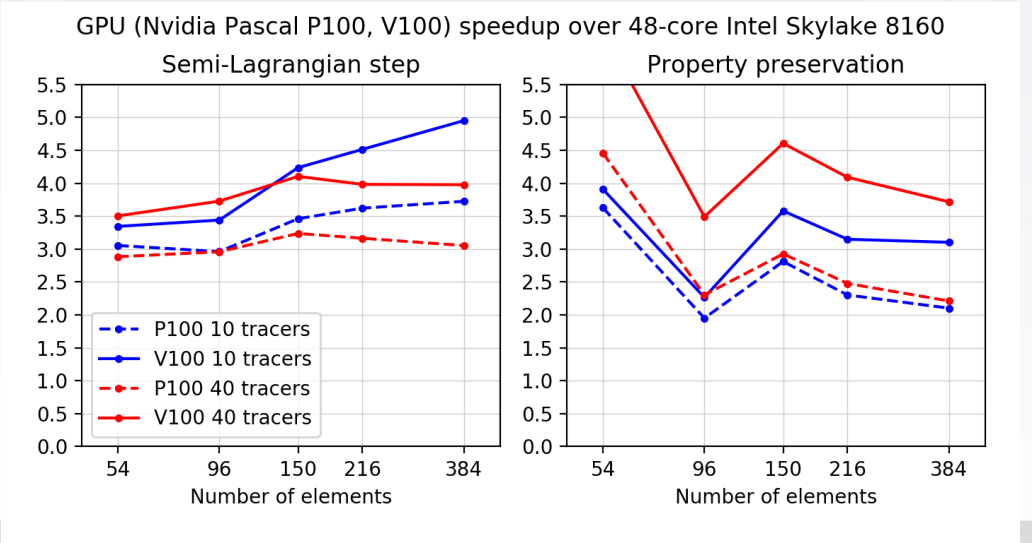
Andrew Bradley

1. Semi-Lagrangian tracer transport speeds up v2 atmosphere dycore by 2-3x.
2. Crucial speedup: communicate only what is needed.
   a. Request red-owning processes to evaluate the purple points. These then update the blue points.
   b. 2x speedup over full halo for 40 tracers.
   c. Enables 2-halo reach with nearly 0 extra cost.
   d. Very unstructured => nontrivial GPU implementation.

✓ **Side Project**: Developed new physics column neighborhood capability

- Supports NGD Atm Physics scale-aware deep convection parameterization work of Guang Zhang.





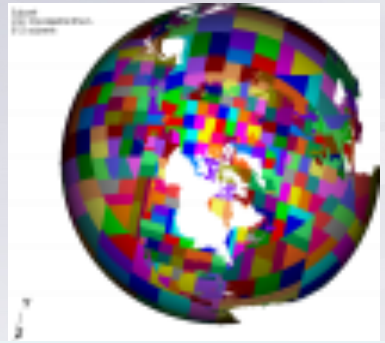
New “coupled” partitioning strategy decreases time for parallel mesh intersection workflow

Karen Devine,
Iulain Grindeanu,
Vijay Mahadevan

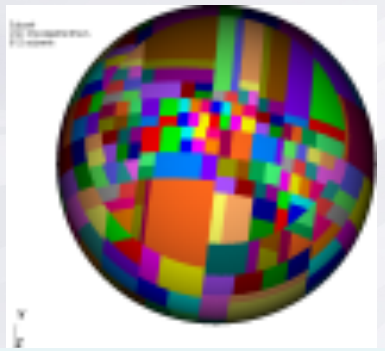
Fast computation of component-mesh intersections and projection weights for solution transfer for high-fidelity cases

- *mbtempest = MOAB + TempestRemap*

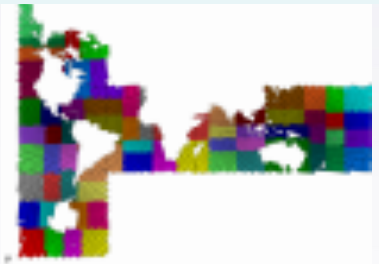
Extensions to on-line intersection / projection underway

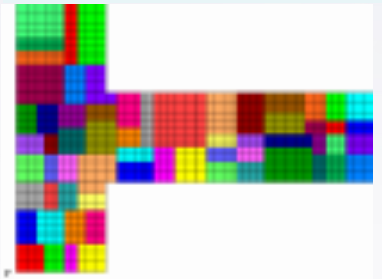


Ocean partitioned via Zoltan’s RCB (recursive coordinate bisection)



Atmosphere partition inferred from ocean’s RCB partitioning tree





2D Gnomonic projection prevents artifacts from partitioning 3D spherical shell

NE256-PG2: OCN (3.7M) -> ATM (1.57M); 1024 cores (bebop KNL)		
Strategy	Coverage time (s)	Intersection time (s)
RCB OCN + RCB ATM	1.81	20.49
RCB OCN + Inferred ATM	0.66	7.72
Gnomonic RCB OCN + Inferred ATM	**0.43**	**3.08**

POCs: I. Grindeanu, V. Mahadevan, ANL;
K. Devine, SNL, SciDAC FASTMath Institute

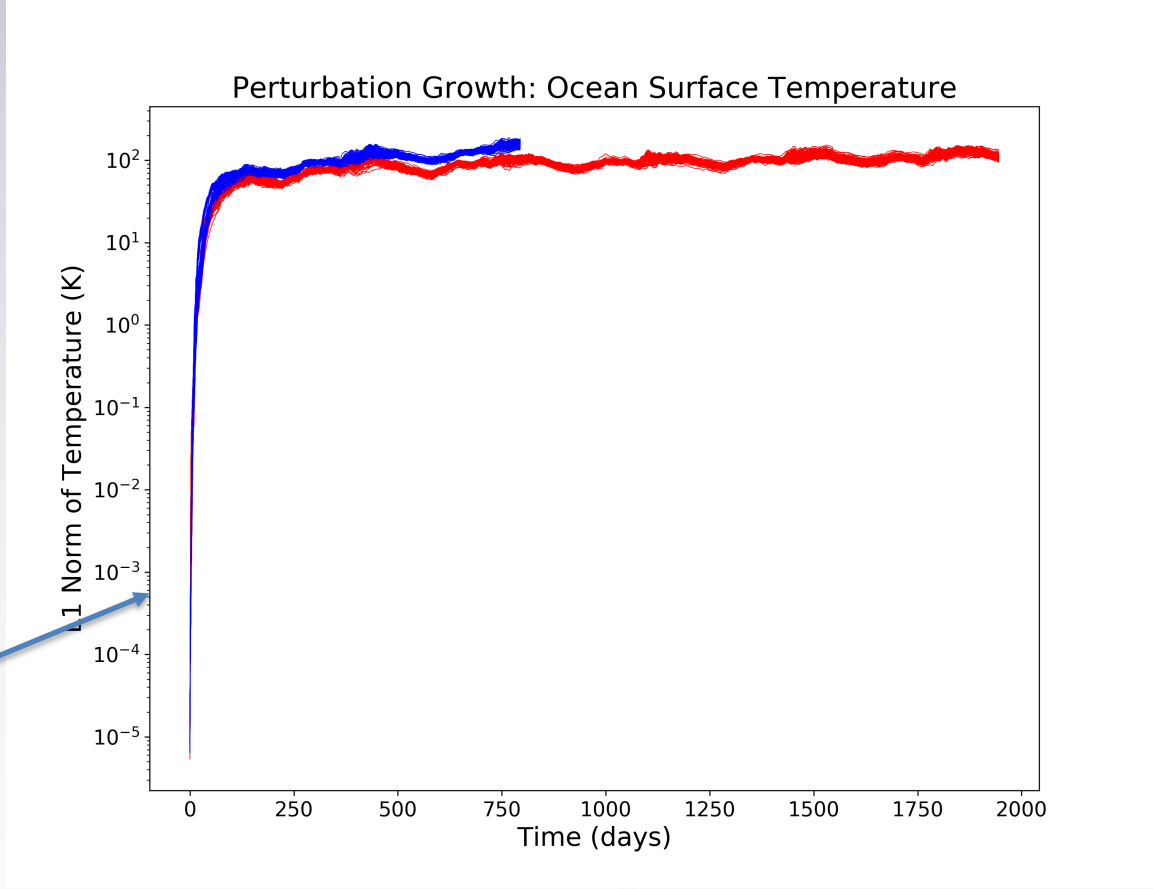
Multivariate Tests for Climate Reproducibility

Salil Mahajan,
Michael Kelleher

1. Developed a ML based multivariate testing framework for climate reproducibility for MPAS-O using short ensembles:
   a. To be ported to EVV – the reproducibility testing framework for EAM.

SST Difference for GM Kappa changing from 1800 to 600, shown:

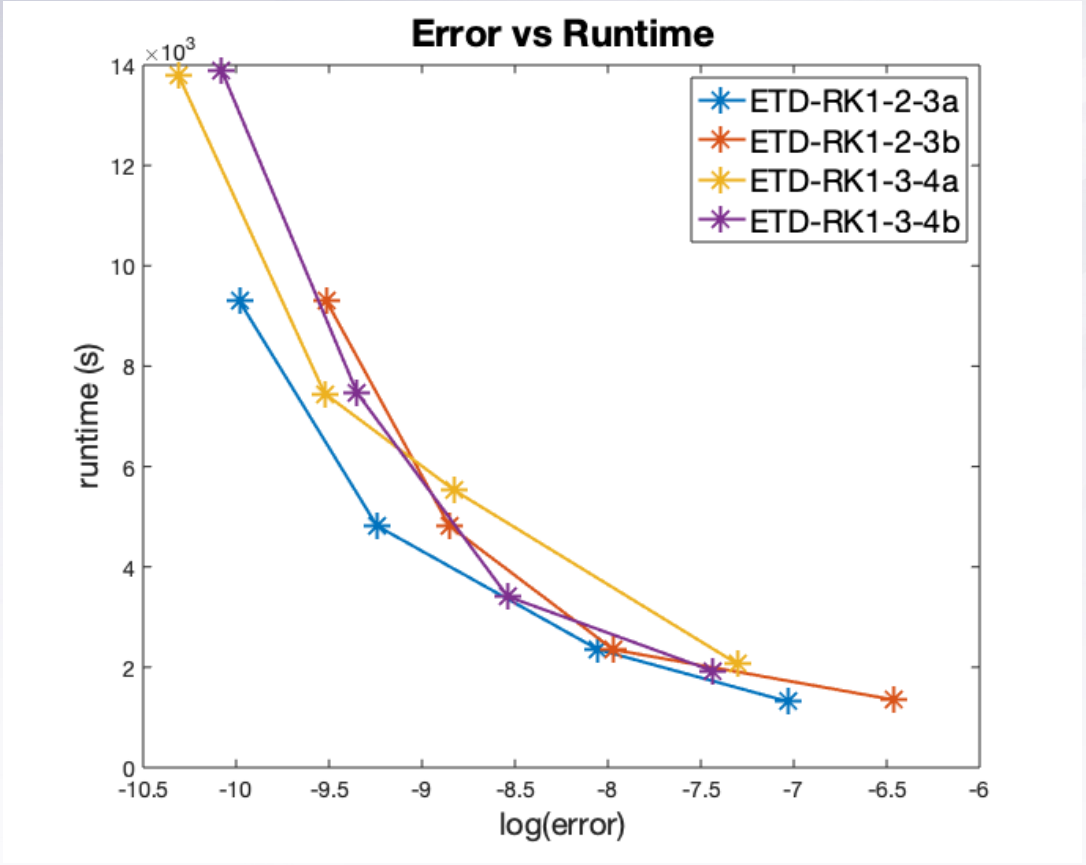
Ensemble testing framework can detect change from 1800 to 1799.



Exponential Time-Differencing Runge-Kutta Methods for Nonhydrostatic Atmosphere

Cassidy Krause,
Andrew Steyer

- Developed new framework for deriving ETD-RK methods for nonhydrostatic models.
- Newly derived ETD-RK methods can take large and accurate time-steps.
- Utilizes time-convergence testing capability in HOMME-NH to evaluate quality of new methods.
- Current aim: Push the ETD-RK methods to be more efficient than current state-of-the-art IMEX-RK methods, by minimizing number of required solves and linear algebra operations
  - ➢ To decrease time-stepping cost of the E3SM atmosphere model.



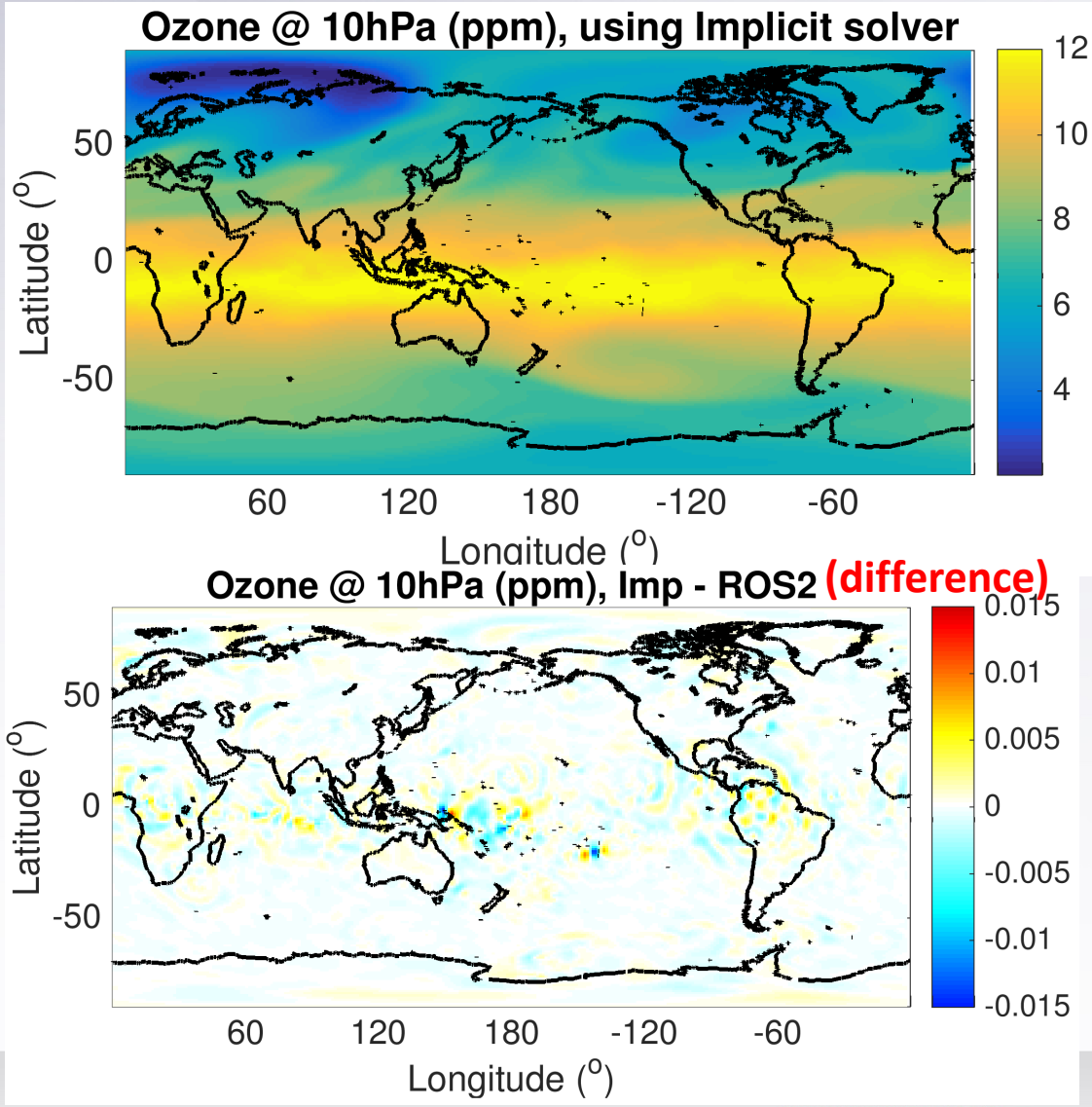
Efficiency of several new custom ETD-RK methods implemented in HOMME-NH.

Krause, C. and Steyer, A. Exponential Rosenbrock integrators for nonhydrostatic atmosphere models. In preparation (2020)

Atmospheric Chemistry Solver

Ron-You Chien,
Josh Fu

1. Using linearization of the second order Rosenbrock (ROS2) to replace the iterative implicit solver in current E3SM
2. 33% of improvement to the UCI_chemistry in the Box model using ROS2 on Single CPU
3. 20% of improvement using E3SM_v1 in Cori 21 nodes
   a. 0.2 SYPD → 0.25 SYPD using ROS2 solver
   b. Difference between two solvers are reasonable. Ozone figures (right panels) show the fidelity of the Model outputs
   c. The ROS2 in E3SM_v2 is under construction, with a longer time period experiment (waiting for Cori)



New “Optimization/UQ-based Calibration” Epic

1. Idea was discussed at Nov 2019 at All-Hands Meeting
2. Staffed for FY21!
   - Benj Wagman (Ran E3SM for postdoc application)
   - Kenny Chowdhury (Opt/UQ/ML expert)
3. Will be soliciting expert involvement with Deep Dives