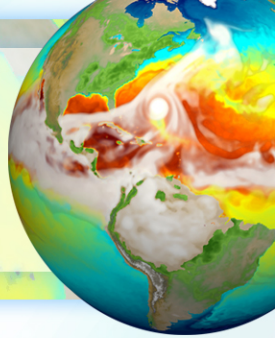
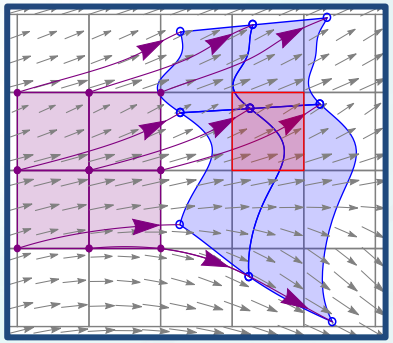
Compact, performance-portable semi-Lagrangian methods for E3SM



Algorithms, software, and science



Sandia National Laboratories

Pete Bosler, Andrew Bradley, Oksana Guba, Mark Taylor

Sandia National Laboratories CCR Center for Computing Research

Los Alamos National Laboratory

Balu Nadiga, Xiaoming Sun, Mat Maltrud

Los Alamos NATIONAL LABORATORY

SciDAC Scientific Discovery through Advanced Computing

E3SM Energy Exascale Earth System Model

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Biological and Environmental Research Program

U.S. DEPARTMENT OF ENERGY

E3SM v2 Impacts for E3SM-Atm. (EAM)

- **Semi-Lagrangian (SL) transport**
  - With new upwind MPI communication pattern [NGD-funded]
  - New Communication Efficient Density Reconstruction (CEDR) algorithms
  - Cell-integrated SL: ~2.5x speedup over v1 Eulerian transport scheme (cpu)
  - Interpolation SL: **~6x speedup over v1,** with 3D trajectories, improved accuracy
  - **PhysGrid** [ECP-funded] algorithms are based on the same principles we used for CISL
  - Verified with standard tests cases
  - Validated with help from the Water Cycle team
- **Dynamics time step stability analysis and improvements**
- Improved energy conservation

Legend:
This SciDAC — Other projects — Technical talk/poster at ESMD — **Good stuff**

Current work

- SL for EAM end-to-end on GPU
- Investigate and quantify non-hydrostatic effects
  - **Baroclinic instability: Effects of vertical resolution**
  - **RCEMIP: Convective self-aggregation**
- Energy conservation in EAM
- *p*-refined tracers for EAM; increased resolution with no time step penalty
- SL Transport for Ocean BGC
  - CISL: Standalone implementation developed
  - **Testing found & fixed bug in v2 FCT**
  - ISL: Ongoing

Legend:
This SciDAC — Other projects — Technical talk/poster at ESMD — **Good stuff**

At this meeting

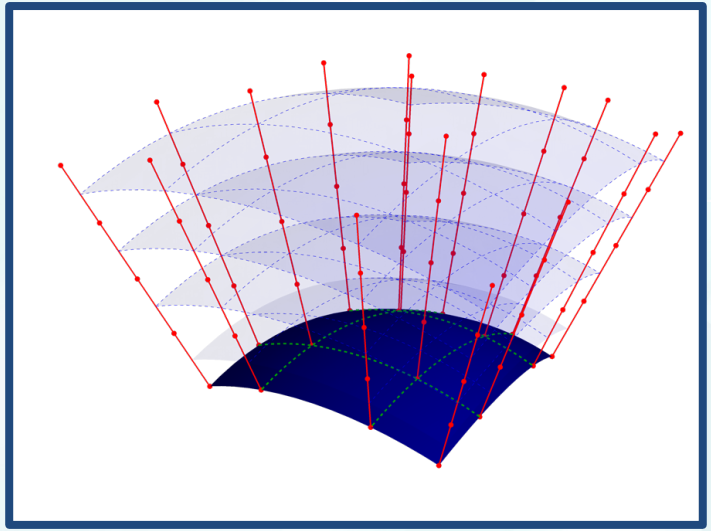
Presenter	Title	Session
Andrew Bradley	High-order, property-preserving, semi-Lagrangian tracer transport in E3SM	Computational Science Breakout Today, 3:15 PM (1:15 Mtn)
Oksana Guba	A framework to evaluate IMEX schemes for atmospheric models	Poster Session 2 Today, 4:30 PM (2:30 Mtn)
Xiaoming Sun	Hydrostatic and Non-hydrostatic Convective Self-aggregation in E3SM	Poster Session 2 Today, 4:30 PM (2:30 Mtn)
Balu Nadiga	Quantification of non-hydrostatic effects and the role of vertical resolution in HOMME	Poster Session 2 Today, 4:30 PM (2:30 Mtn)
Andrew Bradley	High-order, property-preserving physics-dynamics-grid remap in E3SM	Water Cycle Breakout Tomorrow 11:05 am (9:05 Mtn)

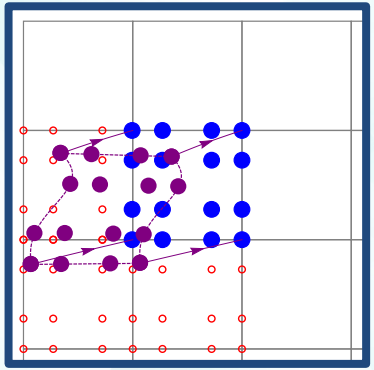
Outline

- ☑ E3SM v2 Impacts
- ☑ Current work
- ☑ Also at this meeting
- ❑ Our approach:
  - Match algorithms to both science applications and HPC architectures
  - Rigorous verification
  - Validate with expert help
  - Use high-resolution tests to identify future challenges
  - Stay connected and keep pace with the rest of E3SM
  - In-scope: Our main objectives ***and*** anything that presents an obstacle to them
  - Follow-through: Deliver to E3SM

Match algorithms to application & architecture

- Application:
  - Non-hydrostatic atmosphere model
  - Horizontal: spectral elements
  - Vertical: Lorenz staggering, HEVI splitting
  - High throughput requirements
- Architectures:
  - Reward high workloads with minimal data movement
  - Punish large communication volumes



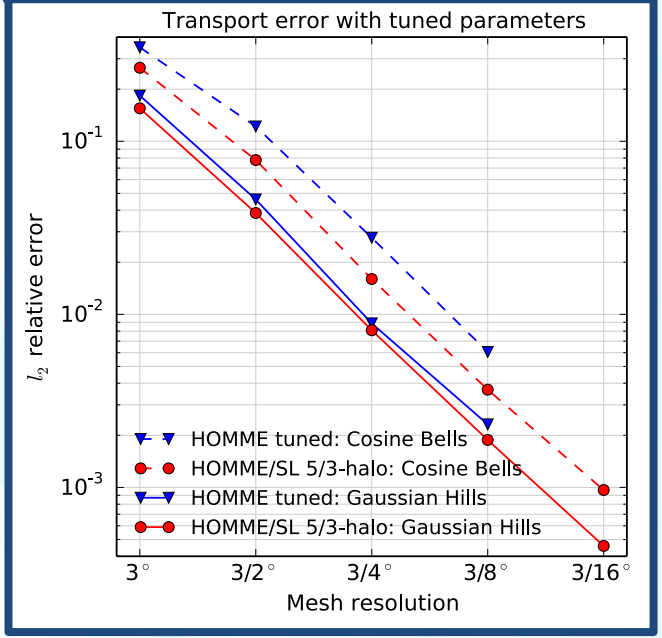


- Algorithms:
  - Communication Efficient Density Reconstruction (CEDR): Conservative shape preservation in **exactly 1 all-reduce**
  - SL Transport exploits **compact, high-order data** stencils

Andrew Bradley: CS and WC breakouts
Today 3:15 pm, Tomorrow 11:05 am

Rigorous verification

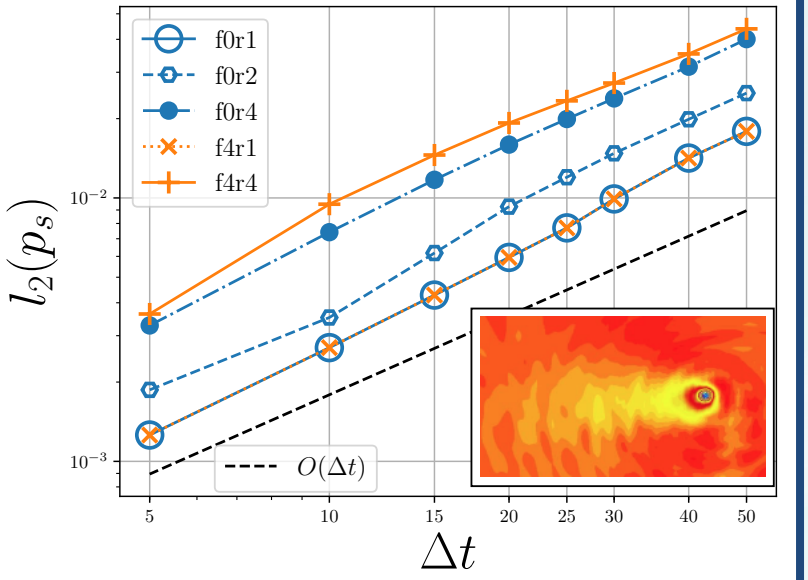
Mesh refinement convergence



Rigorous verification

Mesh refinement convergence

Time step convergence

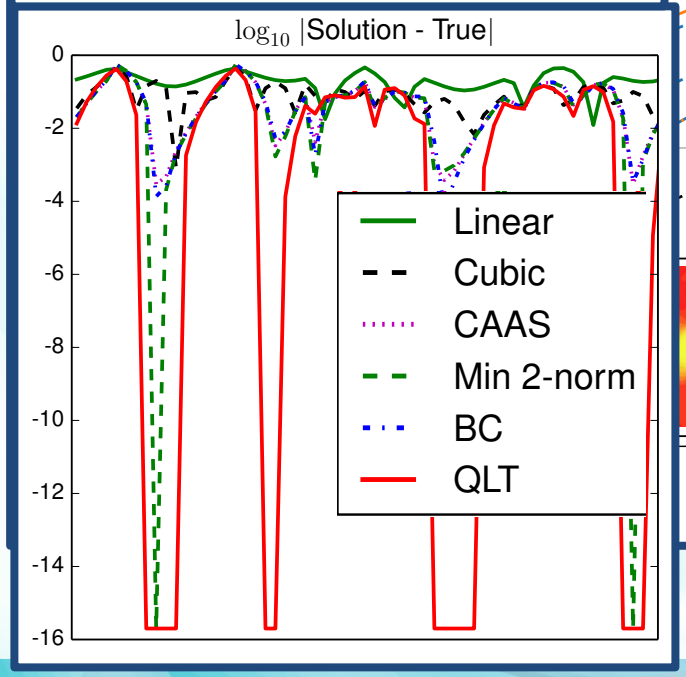


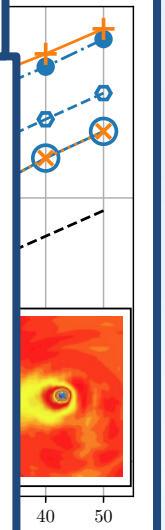
Rigorous verification

Mesh refinement convergence

Time step convergence

CEDR: With conservative trans.



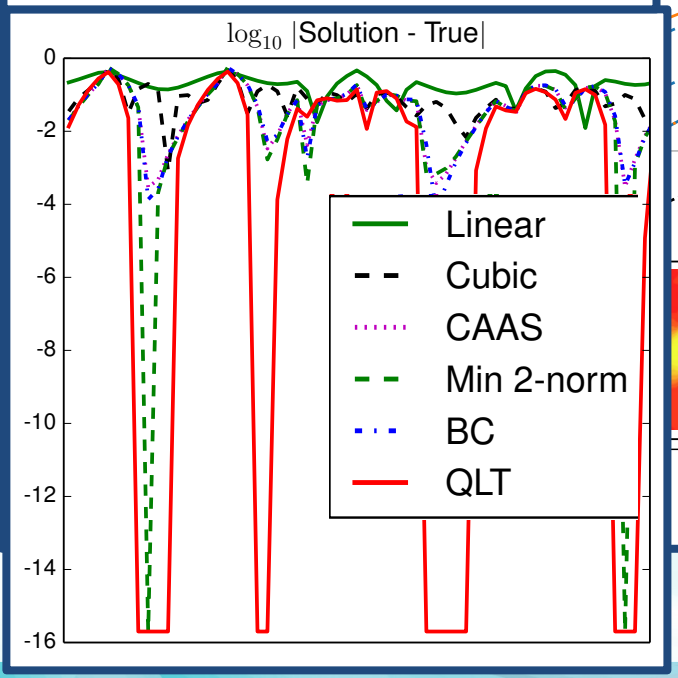


Rigorous verification

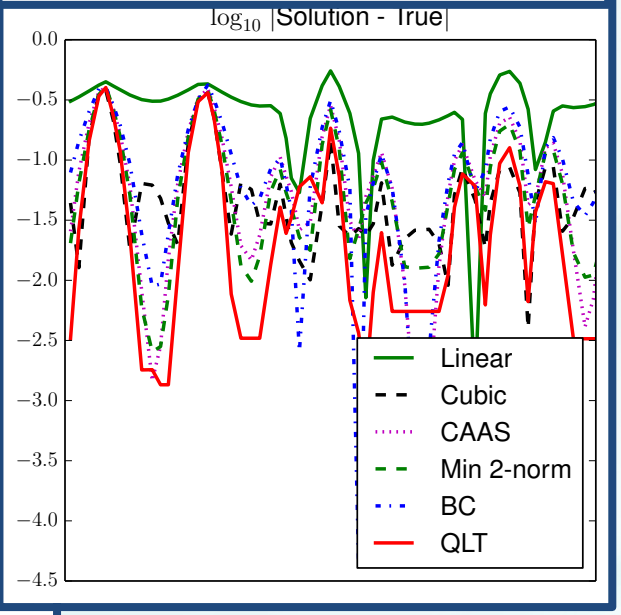
Mesh refinement convergence

Time step convergence

CEDR: With conservative trans.



CEDR: non-cons. transport

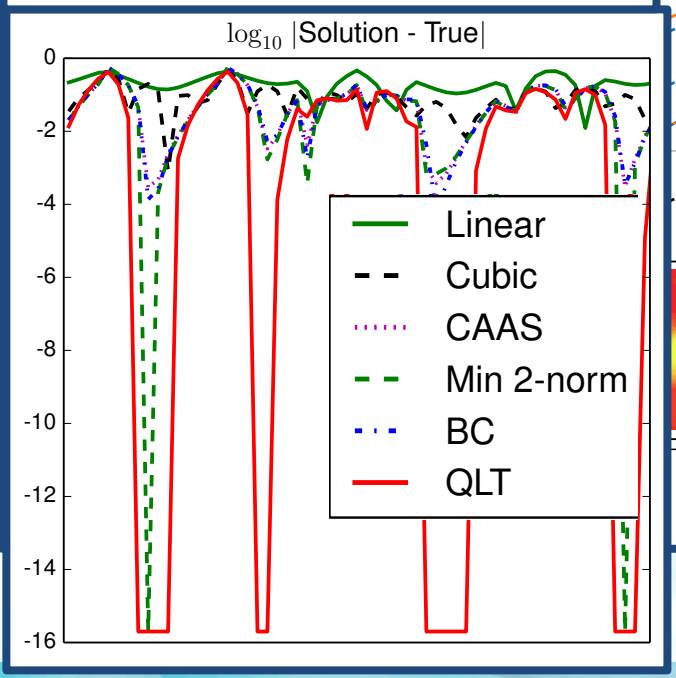


Rigorous verification

Mesh refinement convergence

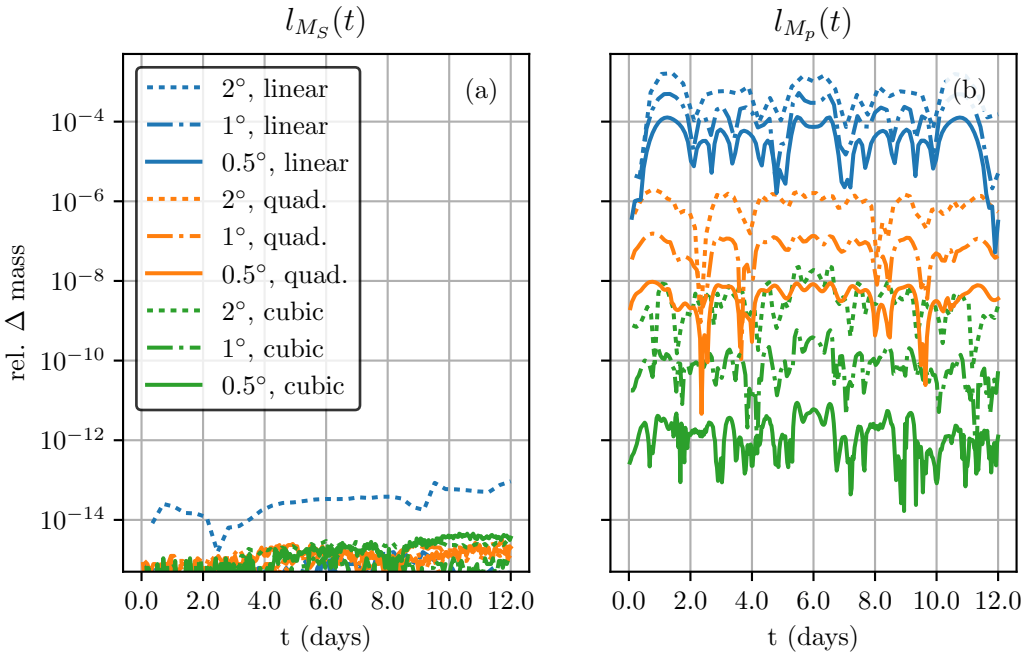
Time step convergence

CEDR: With conservative trans.



CEDR: non-cons. transport

Standalone tests

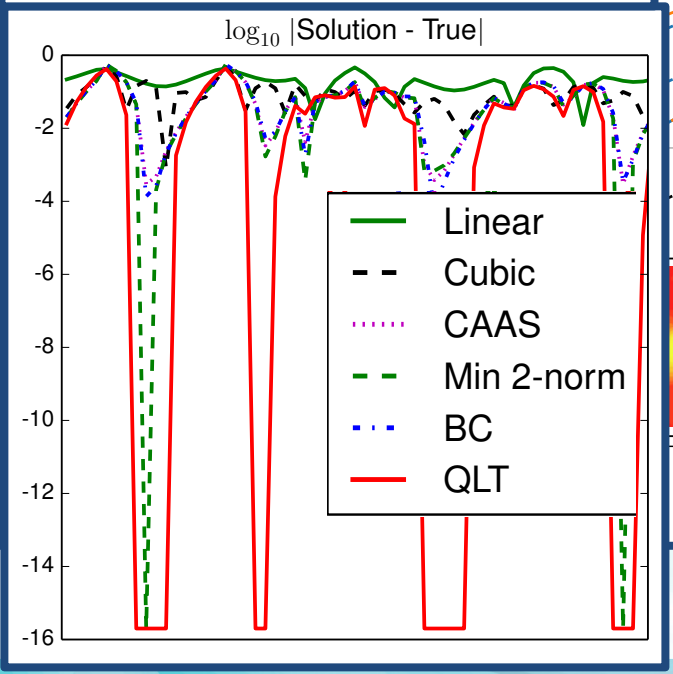


Rigorous verification

Mesh refinement convergence

Time step convergence

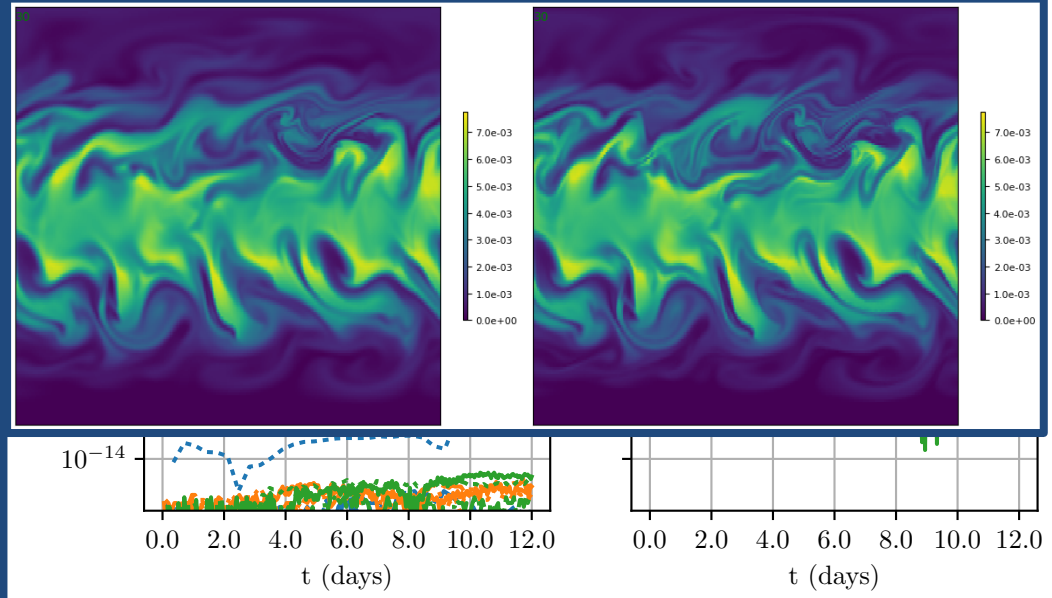
CEDR: With conservative trans.



CEDR: non-cons. transport

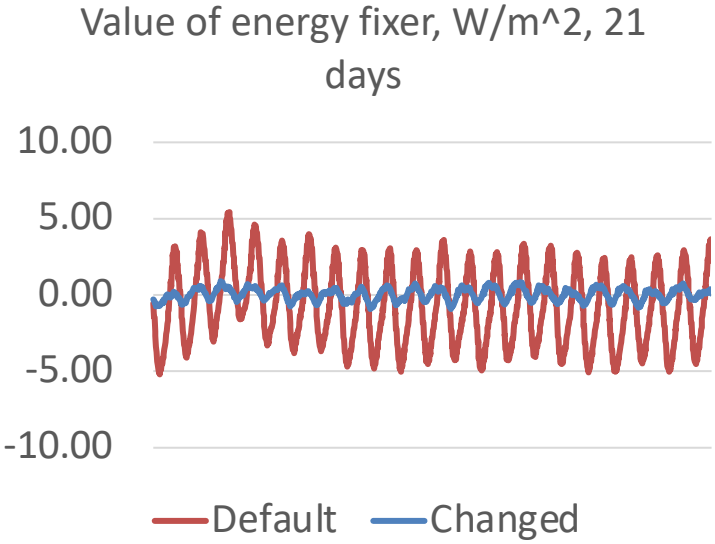
Standalone tests

Coupled tests, with & without RRM

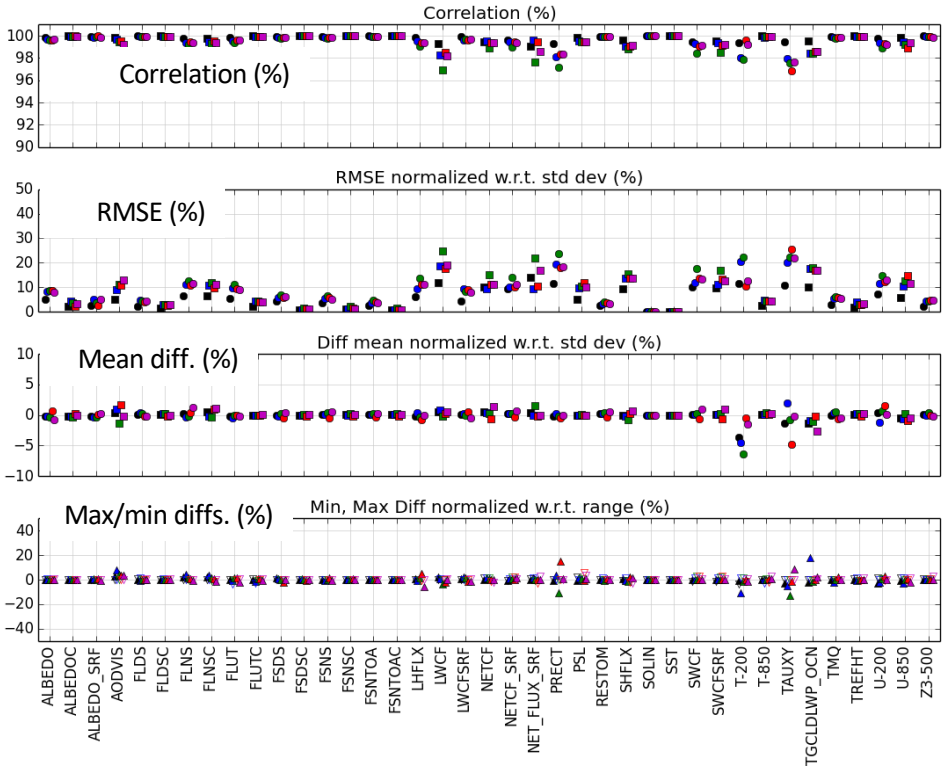


Validation, with help from science experts

- Example: Energy fixer update
- "*Energy considerations in the Community Atmosphere Model (CAM)*", 2015, by D. Williamson, J. Olson, C. Hannay, T. Toniazzo, M. Taylor, V. Yudin

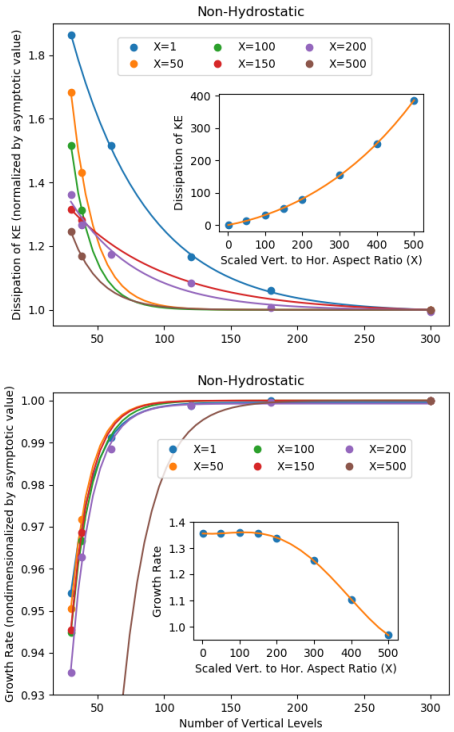


Climatology comparison vs. default setup

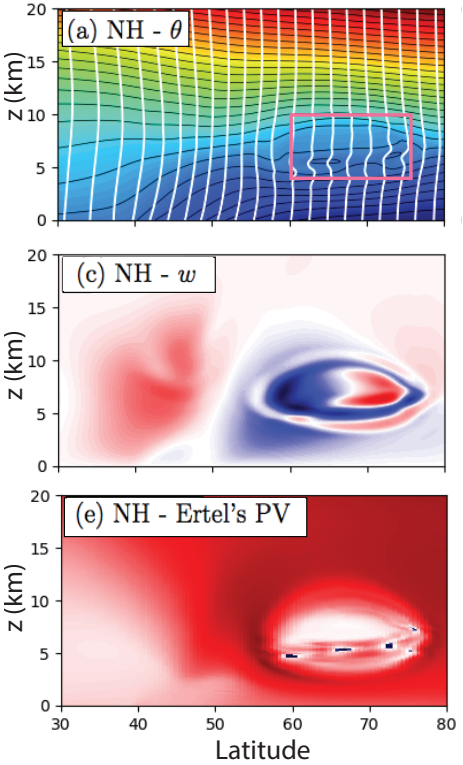


High resolution tests: Identify future challenges

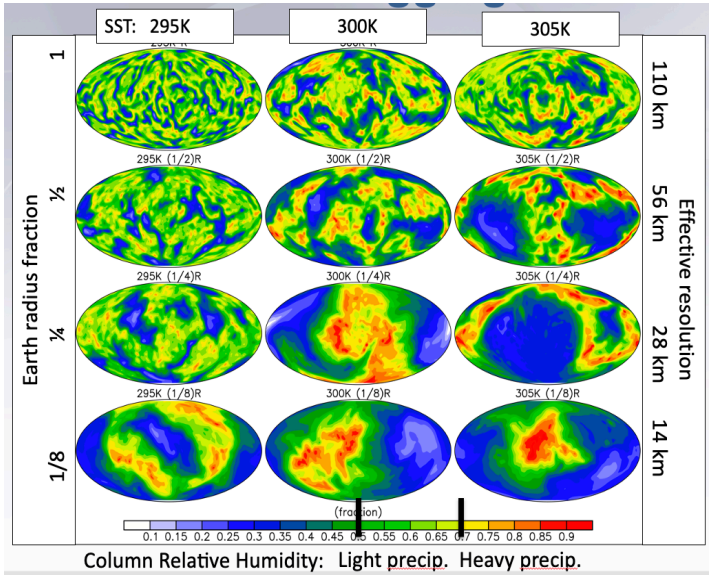
NH Effects: Dependence on vertical resolution



Mesoscale instability: Real vs. Numeric



RCEMIP: Convective self-aggregation



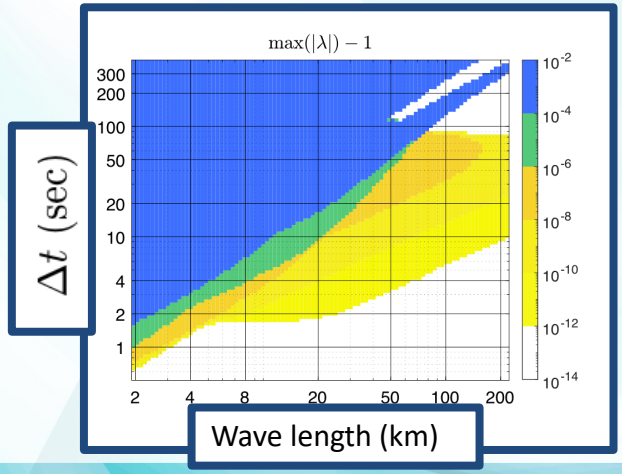
Balu Nadiga (Today): Poster Session 2

Xiaoming Sun (Today): Poster Session 2

Challenges and Opportunities

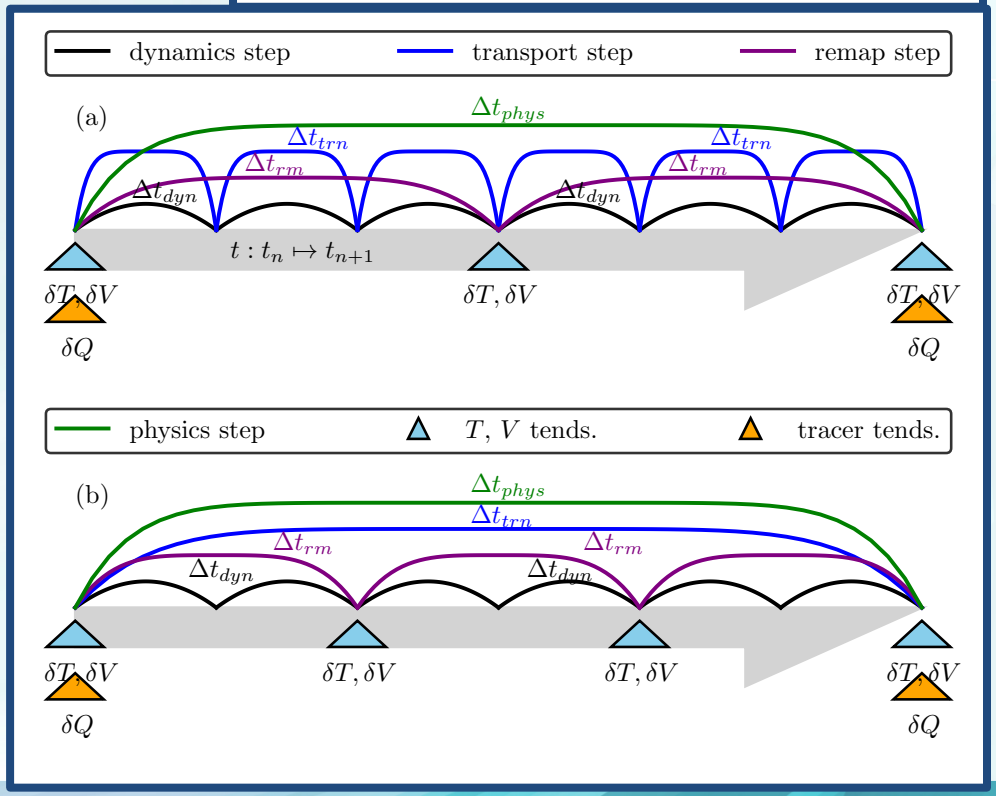
- Time step coupling (right) & vertical remap with new BC
- Stabilized basis polynomials for SL on GLL grids
- IMEX stability analysis (below)

Oksana Guba: Today, Poster Session 2



(a) Project start. Short transport time steps (CFL) and coupled software implementation.

(b) EAM v2. Long tracer time steps, decoupled from physics and remap. Better control of vertical dynamics for nonhydrostatic model.



Publications

- Accepted/Published:
  - Bradley, Bosler, Guba, Taylor, Barnett, 2019; Communication-efficient property preservation in tracer transport, ***SIAM J. Sci. Comput.,*** 41(3): C161—C193.
  - Bosler, Bradley, Taylor, 2019; Conservative multimoment transport along characteristics for discontinuous Galerkin methods, ***SIAM J. Sci. Comput.,*** 41(4): B870—B902.
  - Nadiga, Verma, Weijer, Urban, 2019; Enhancing skill of initialized decadal predictions using a dynamic model of drift, ***Geophys. Res. Ltr.,*** 46: 9991—9999.
- In review:
  - Guba, Taylor, Bradley, Bosler, Steyer, 2020; A framework to evaluate IMEX schemes for atmospheric models, ***Geosci. Model Dev.***
- In preparation:
  - Bradley, Guba, Bosler, Taylor: Islet: Algorithms and software for stabilized high-order interpolation semi-Lagrangian transport on spectral elements