High-order, property-preserving, semi-Lagrangian tracer transport in E3SM

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Funding: LEAP-T (BER), SciDAC (ASCR and BER), NGD Software and Algorithms
Thanks also to MMF, Water Cycle, NGD NH Atm., and Performance Groups

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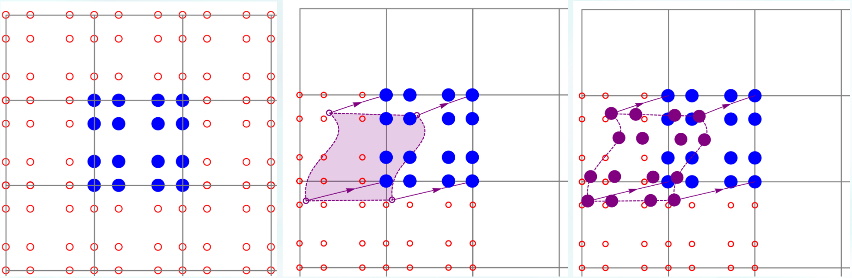
SAND2020-11715 C

Overview

- *Computational efficiency*: Solution accuracy for given computational resources.
- Two new methods increase E3SM Atmosphere Model (EAM) computational efficiency:
  - *Semi-Lagrangian tracer transport* (this talk).
  - Separate physics parameterizations grid with physics-dynamics-grid remap.
- Property preserving, to mimic continuum equations:
  - Conserve mass.
  - Limit extrema.
  - Tracer consistent.
- High order: Order of accuracy (OOA) is at least 2.
  - In general, strict property preservation limits formal OOA to 2-3.
- Together, speed up EAM by roughly $2\times$ roughly independent of architecture and problem configuration.
- Work seamlessly in the Regionally Refined Mesh (RRM) configuration.

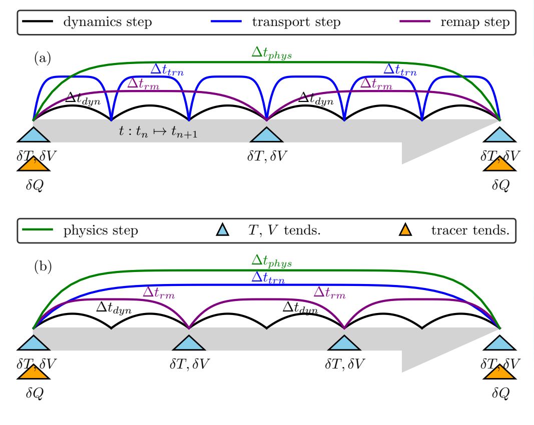
Motivation

- In EAMv1, Eulerian flux-form tracer transport is the dominant dynamical core cost.
- In EAMv2, switch to a semi-Lagrangian method to take very long time steps per communication round.



Time stepping

- Hardest part of integrating an algorithm into a dycore.
- To exceed the dynamics vertical remap time step, created a fully 3D SL method.
  - Reconstruct Lagrangian levels with 2nd-order accuracy.
  - 2D advection within levels.
  - Vertically remap to reference levels.



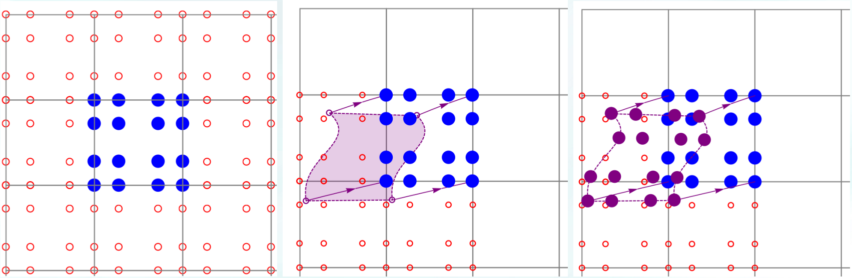
Algorithms

- Semi-Lagrangian ⇒ very long time steps.
- Remap form ⇒ communication volume is roughly independent of time step.
- Interpolation ⇒ extremely efficient, both in computations and data volume of discrete domain of dependence.
- Use a *communication-efficient density reconstructor*[1] (CEDR) for mass conservation, limiting extrema, and tracer consistency.
  - Exactly one all-reduce(-like) communication round.
  - Clear and practical necessary and sufficient conditions for feasibility.
  - Clear and practical bounds on mass modifications.
- Implemented using an *upwind communication pattern* to communicate no more than what is needed.

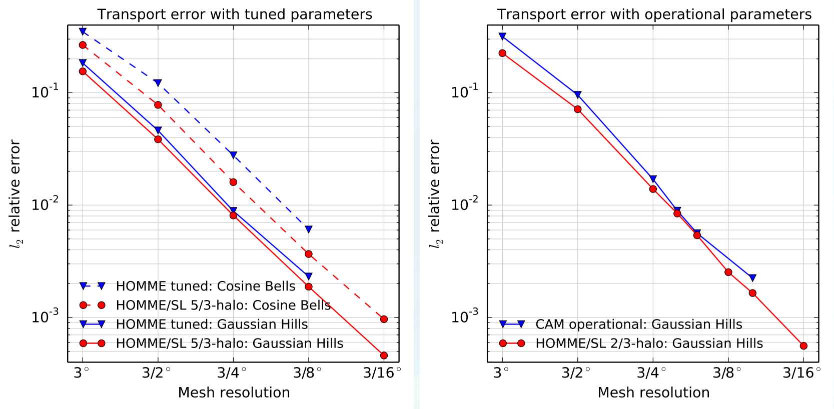
[1] A. M. Bradley, P. A. Bosler, O. Guba, M. A. Taylor, G. A. Barnett, *Communication-efficient property preservation in tracer transport*, SIAM J. Sci. Comput., 41(3), 2019, doi:10.1137/18M1165414.
Software: `github.com/E3SM-Project/COMPOSE`.

Upwind MPI

- Communicate only what is needed.
- Send and receive evaluation requests (location data).
- Interpolate to these locations.
- Send and receive fulfilled requests.
- Unstructured communication pattern: in general, different at every level and time step.



2D accuracy[2]

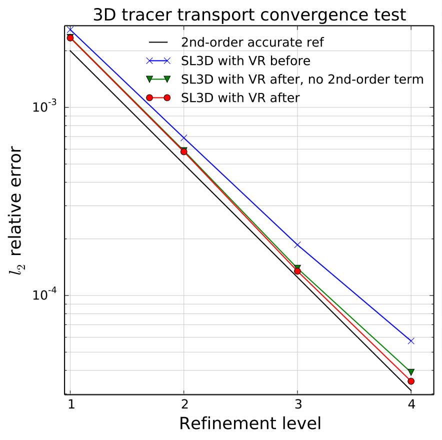


- Nondivergent flow test case.
- Compare (left) tuned parameters and (right) operational parameters.
- SL transport is uniformly more accurate.

[2] "HOMME tuned" data are from O. Guba, et al, *Optimization-based limiters for the spectral element method*, JCP 2014. "CAM operational" data are from P. H. Lauritzen, et al. "Geoscientific Model Development A standard test case suite for two-dimensional linear transport on the sphere: results from a collection of state-of-the-art schemes." GMD 7(1) 2013.

3D accuracy

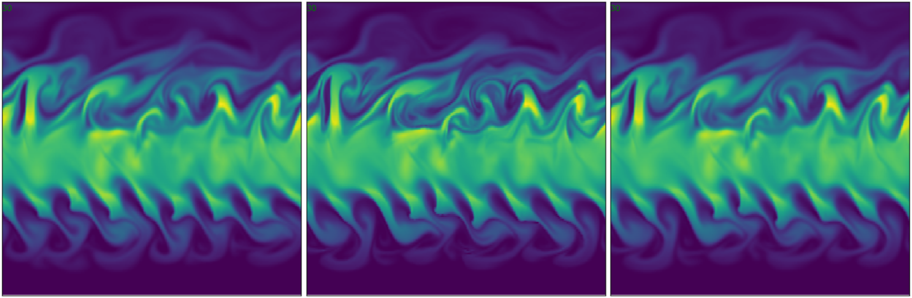
- Modification of DCMIP 2012 test 1-1: smooth ICs and vertical flow to permit empirical OOA test.
- Nondivergent flow test case with a vertical velocity component and a divergence-compensating horizontal component.



Dissipation

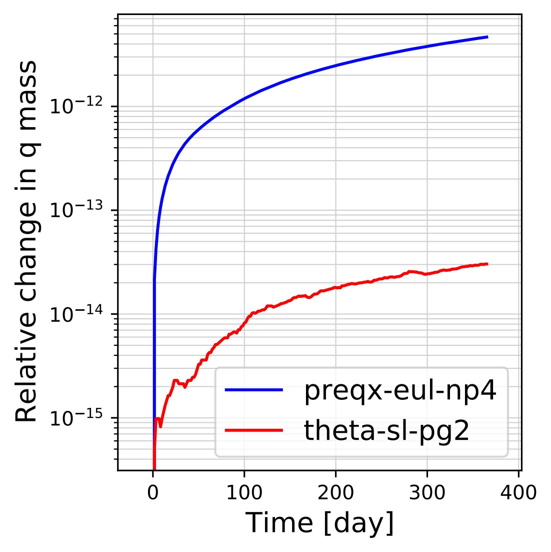
- Eulerian flux-form method requires hyperviscosity for stability.
- SL transport does not.
- But optionally can apply hyperviscosity.
- Example: Specific humidity at approximately 500 hPa, on day 30 in DCMIP 2016 moist baroclinic instability test.

Eulerian flux-form | SL, no hyperviscosity | SL with hyperviscosity



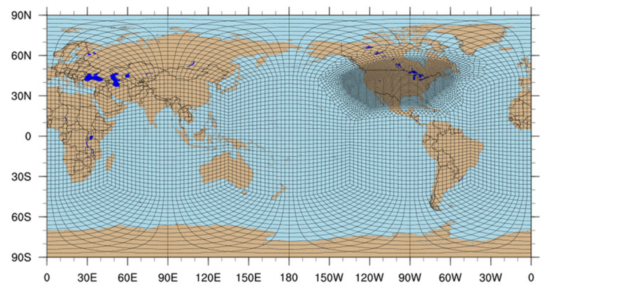
Mass conservation

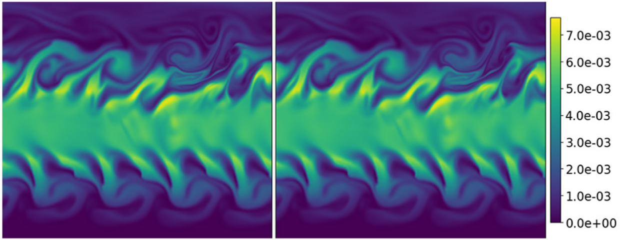
- Mass conservation of a source/sink-less tracer in one year of simulation of an `ne30` F-case.
- Two orders of magnitude better than EAMv1.



RRM

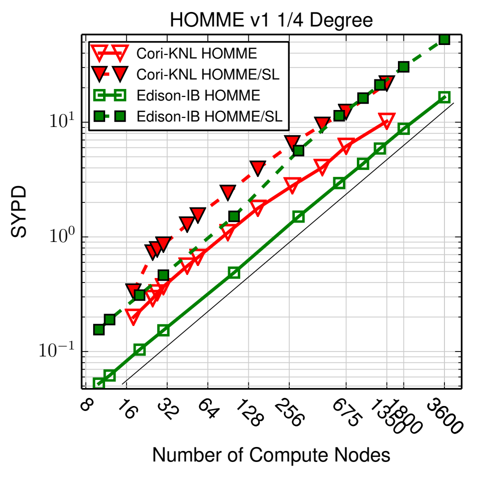
- Specific humidity at approximately 600 hPa on day 25 from DCMIP 2016 Test 1: Moist Baroclinic Instability on the CONUS 1/4-degree RRM grid.
- Left image shows Eulerian flux-form transport with physics on the dynamics grid.
- Right image shows SL transport with the pg2 grid configuration.

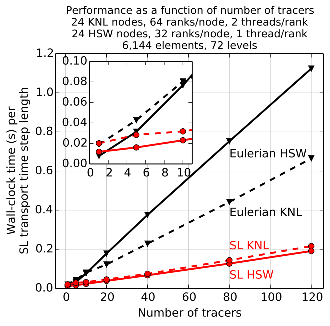


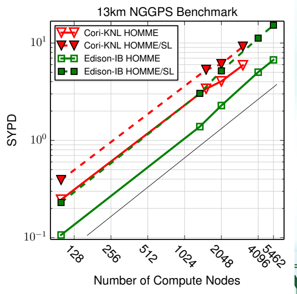


Dycore-only performance

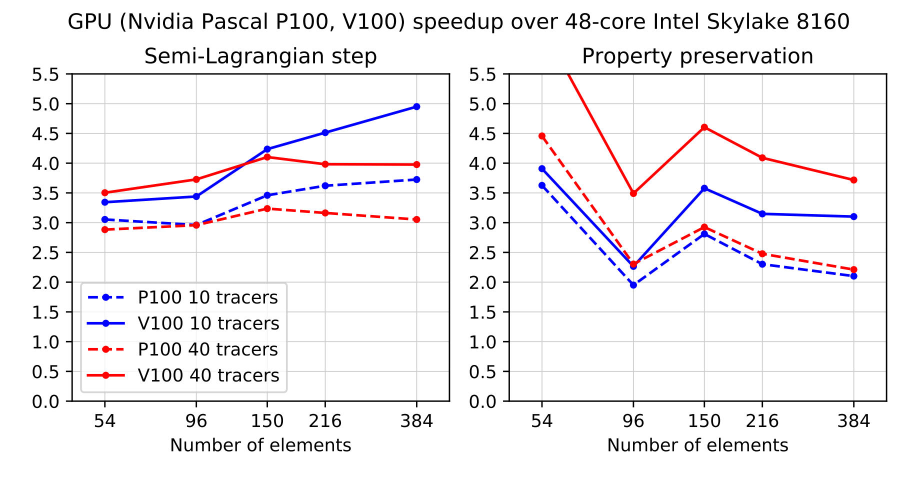
- preqx dycore is $>$**2.1**$\times$ faster on KNL at 1350 nodes (strong-scaling limit) with SL transport.
- preqx dycore is $>$**3.2**$\times$ faster on Edison at 3600 nodes (strong-scaling limit) with SL transport.







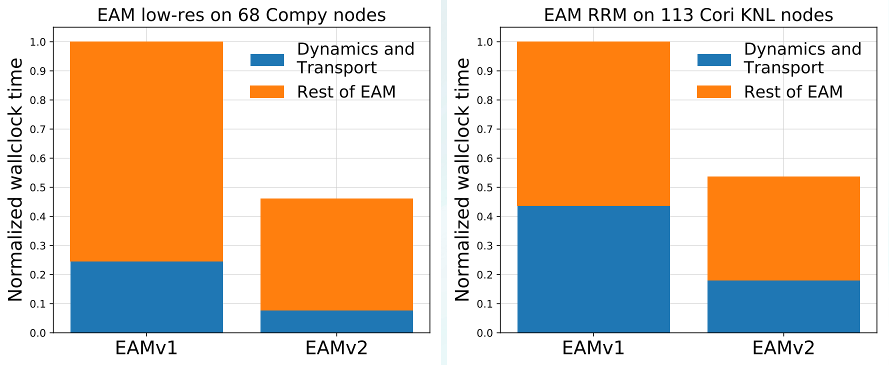
GPU performance



EAMv2 performance

Max timers for

- `CPL:RUN_LOOP` (total time-stepping time) and
- `CAM_run3` (total dycore time-stepping time).



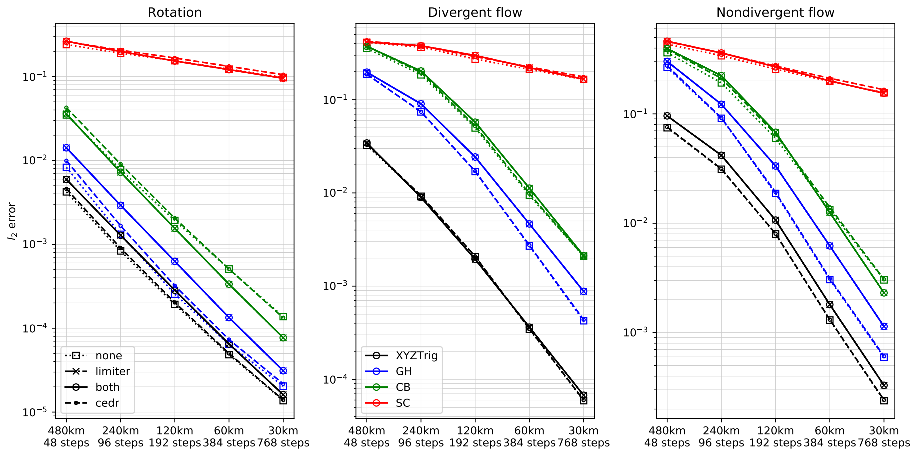
Ocean passive tracers for BGC

- Remap-form, property-preserving, cell-integrated, semi-Lagrangian passive tracer transport method[3] for MPAS-Ocean.
- CISL rather than ISL
  - MPAS-O's finite volume discretization makes CISL substantially faster than CISL for HOMME's SE discretization
    - ★ 3 quadrature points instead of 32 per triangle facet.
    - ★ No nonlinear iteration to solve for reference coordinates at quadrature points.
  - Immediate stability from L2 projection.
    - ★ Helpful because ocean boundaries could make ISL stability hard to achieve.
  - 1-halo is enough to obtain a 3rd-order reconstruction; 2 neighbor cells are enough to obtain a 2nd-order reconstruction.
- 2nd-order accurate trajectories using edge normal velocities.
- CEDR for tracer consistency.
  - As long as we're using a CEDR, use it for shape preservation, too.

[3] P. A. Bosler, A. M. Bradley, M. A. Taylor, *Conservative multimoment transport along characteristics for discontinuous Galerkin methods*, SIAM J. Sci. Comput., 41(4), 2019, doi:10.1137/18M1165943.

Ocean passive tracers for BGC

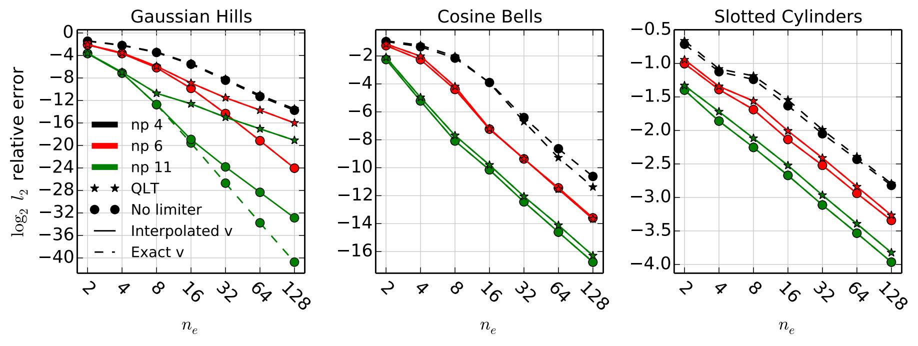
2D correctness and convergence tests on a global MPAS grid sequence[4]



[4]Lauritzen, P. H., Skamarock, W. C., Prather, M. J., and Taylor, M. A. (2012). A standard test case suite for two-dimensional linear transport on the sphere. Geoscientific Model Development, 5(3), 887-901.

Current and future work: Ultra-accurate atm. tracers

- *Islet* subpackage of COMPOSE will extend current interpolation formula up to 9th-order accuracy.
- Interpolate velocity data from dycore.
- Remap tendencies between grids.
- Increase accuracy by up to >100×.



Summary

- EAMv2 is roughly 2$\times$ faster than EAMv1 roughly independent of architecture and problem configuration.
- NGD NH Atm. (aka SCREAM) and E3SM-MMF are also using these methods.
- We have developed and are developing a set of high-order, property-preserving remap tools for
  - tracer transport in the atmosphere (v2)
  - physics-dynamics-grid remap in the atmosphere (v2)
  - passive tracer transport in the ocean for BGC (target: v3)
- Library: `github.com/E3SM-Project/COMPOSE`