High-order, property-preserving *semi-Lagrangian tracer transport* and *physics-dynamics-grid remap* in EAMv2

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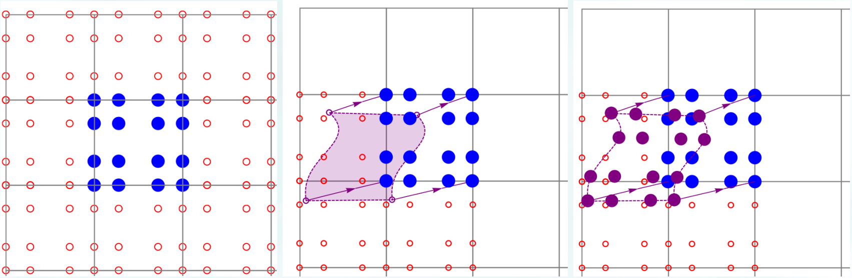
Overview

- *Computational efficiency*: Solution accuracy for given computational resources.
- Two new methods increase E3SM Atmosphere Model (EAM) computational efficiency:
  - *Semi-Lagrangian tracer transport*.
  - Separate physics parameterizations grid with *physics-dynamics-grid remap*.
- Property preserving, to mimic continuum equations:
  - Conserve mass.
  - Limit extrema: no new nodal value, element-neighborhood-local global extrema.
  - Tracer consistent: A constant mixing ratio remains constant.
- High order: Order of accuracy (OOA) is at least two.
  - In general, strict property preservation limits formal OOA to two.
- Speed up EAM by roughly $2\times$ roughly independent of architecture and problem configuration.
- Work seamlessly in the Regionally Refined Mesh (RRM) configuration.

SL Transport: Overview

- 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.

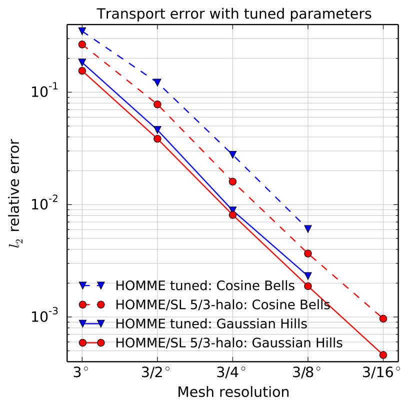


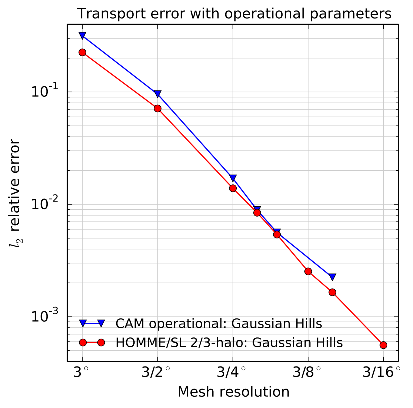
SL Transport: Algorithms

- 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.
- End-to-end on GPU; currently integrating into HOMMEXX-NH.

[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`.

SL Transport: Accuracy[2]





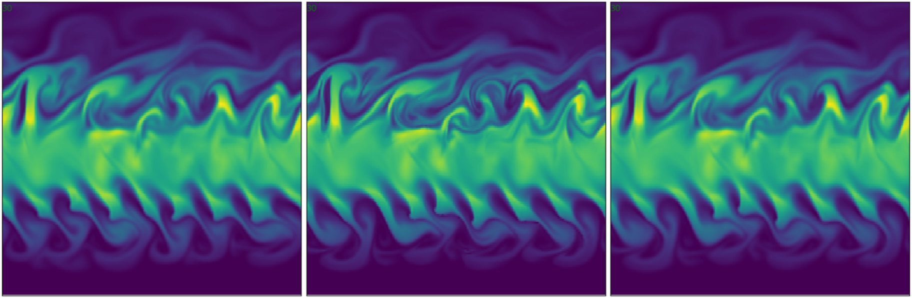
- Nondivergent flow test case.
- Compare (left) tuned parameters and (right) operational parameters.
- SL transport is uniformly more accurate.

[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.

SL Transport: Dissipation

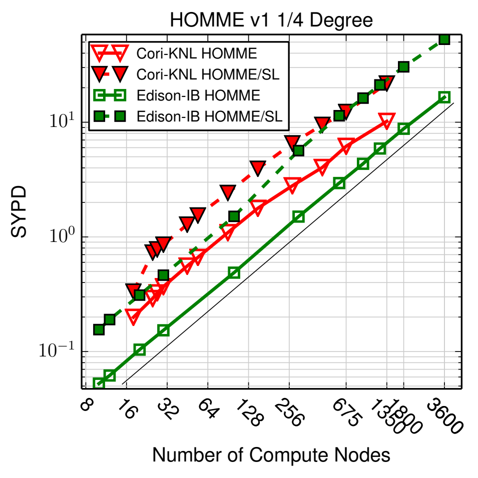
- Eulerian flux-form method requires hyperviscosity for stability.
- SL transport does not.
- But optionally can apply hyperviscosity.
- Example: Specific humidity at approximately 500 hPa, on day 30 in DCMIP 2016 moist baroclinic instability test.

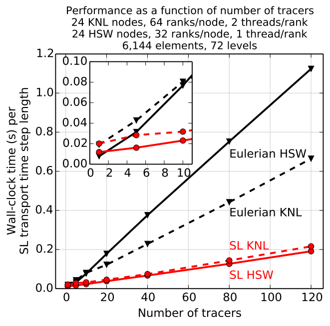
Eulerian flux-form | SL, no hyperviscosity | SL with hyperviscosity

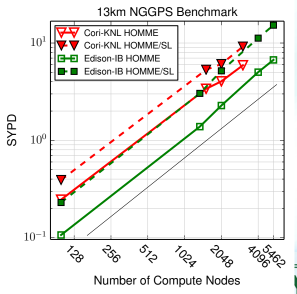


SL Transport: Dycore-only performance

- `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.

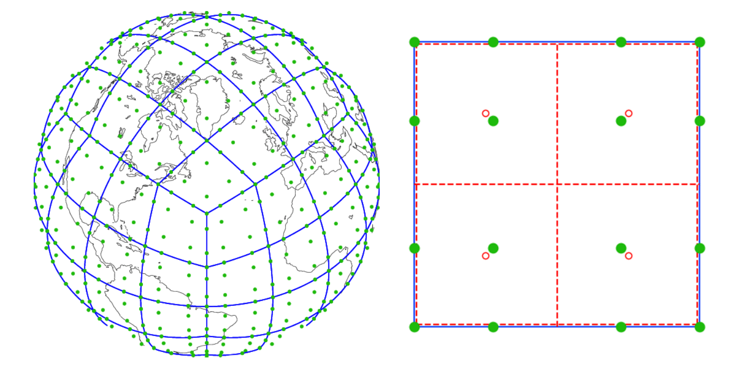






Physgrid Remap: Overview

- Previously: Physics column at each dynamics grid GLL point.
- Many ways to define dycore's effective resolution. All imply assigning a physics column to every GLL point is inefficient.
- New: Physics column at each subcell of a spectral element.
- "pg2" has 4/9 as many columns as in EAMv1, better matching the effective resolution.
  - $>2\times$ greater computational efficiency: approximately the same answer for half the cost.



Physgrid Remap: Algorithms

Linear operator requirements:

1. Mass conserving.
2. Remap is local to the element.
3. If $\boldsymbol{d} = A^{p \to d} \boldsymbol{p}$, then $A^{d \to p} \boldsymbol{d} = \boldsymbol{p}$.
4. If $\boldsymbol{p} = A^{d \to p} \boldsymbol{d}$, and $\boldsymbol{d} = \mathcal{I}^{d' \to d} \boldsymbol{d}'$ with $n_{d'} = n_p$, then $A^{p \to d} \boldsymbol{p} = \boldsymbol{d}$.

Rationale:

- Requirement 2 means there is no communication round beyond what is strictly necessary.
- Requirements 3 and 4 specify limited forms of idempotence; these help to minimize dissipation from remap.
- Requirement 4 assures the remap operator has order of accuracy $n_{d'} = n_p$ because an $n_{d'}$-basis-representable field is recovered exactly.

Dynamics $\to$ physics:

- Simply average the GLL density over the physics subcell.
- Call this $A^{d \to p}$.
- Satisfies requirements 1, 2.

Physics $\to$ dynamics:

- $A^{d \to p}$ and requirements 2 and 4 uniquely specify $A^{p \to d}$.
- Satisfies requirement 3.

Nonlinear operator:

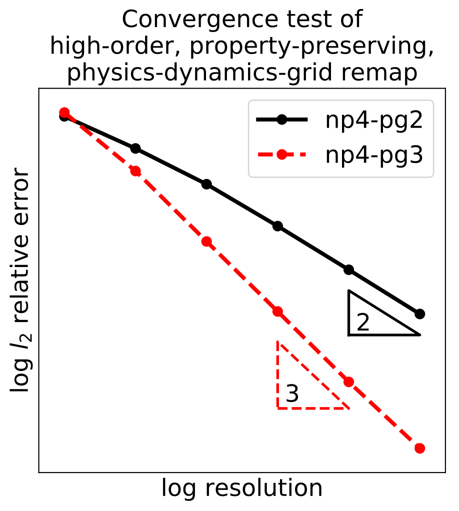
- Mass-conserving local limiter.

Communication:

- None in dynamics $\to$ physics remap.
- Physics $\to$ dynamics requires:
  - Limiter: min/max communication round from HOMME.
  - Final DSS to restore continuity.

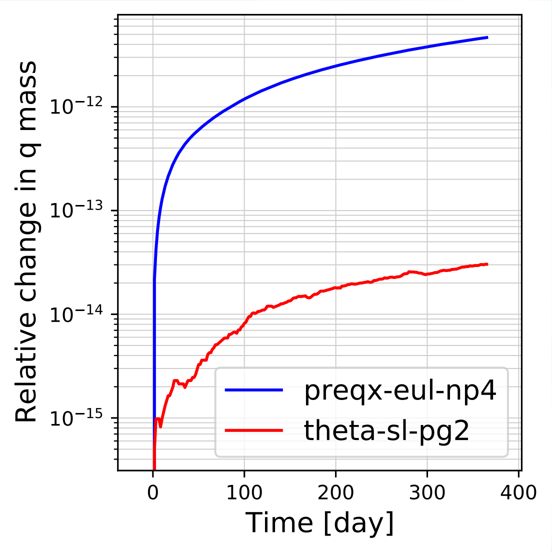
Physgrid Remap: Accuracy

- Remap a test function from dynamics grid to physics grid and then back.
- Compare error under grid refinement.



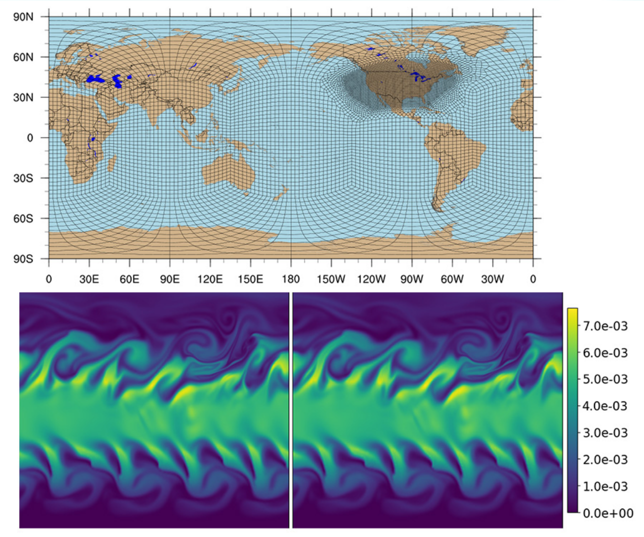
Together: Accuracy

- 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.



Together: Accuracy

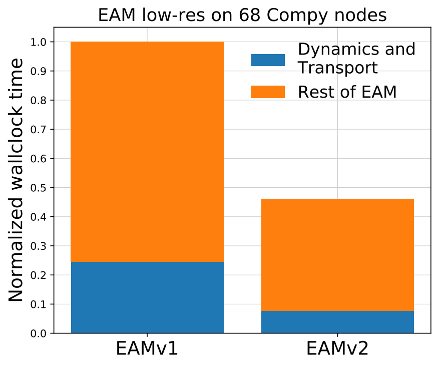
- Specific humidity at approximately 600 hPa on day 25 from DCMIP 2016 Test 1: Moist Baroclinic Instability on the CONUS 1/4-degree RRM grid.
- Left image shows Eulerian flux-form transport with physics on the dynamics grid.
- Right image shows SL transport with the pg2 grid configuration.

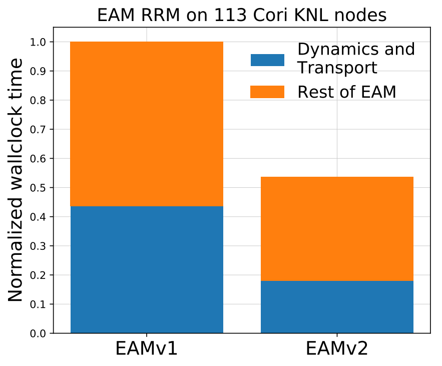


Together: Performance

Max timers for

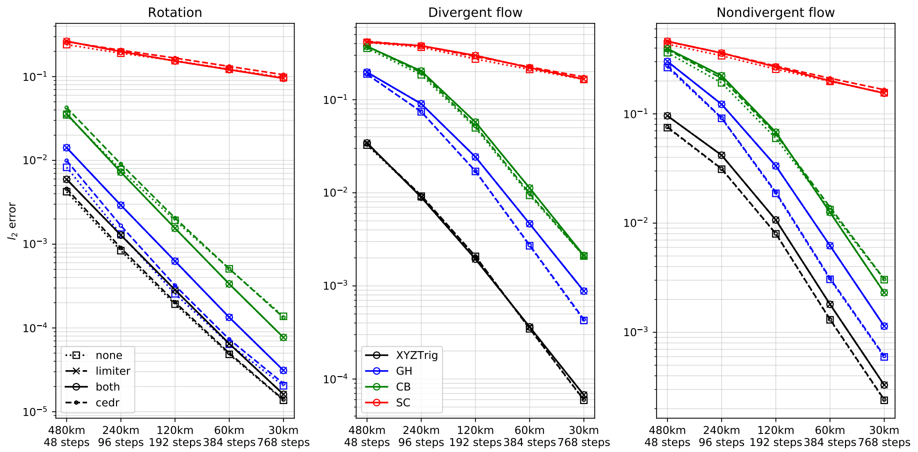
- `CPL:RUN_LOOP` (total time-stepping time) and
- `CAM_run3` (total dycore time-stepping time).





Current and future work: Ocean passive tracers for BGC

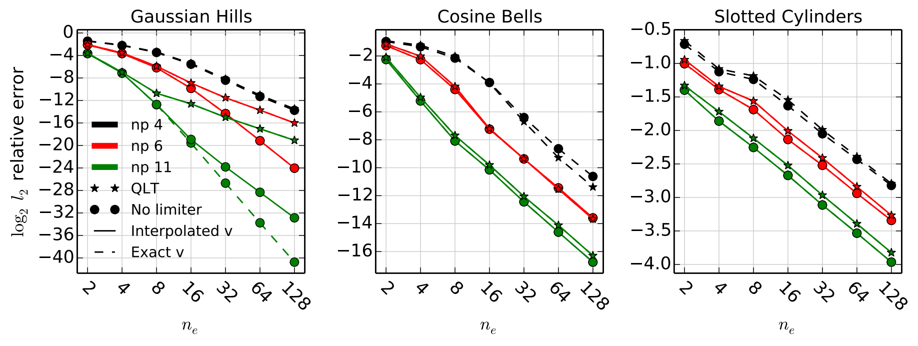
- Remap-form, property-preserving, cell-integrated, semi-Lagrangian passive tracer transport method[3] for MPAS-Ocean.
- 2D correctness and convergence tests on a global MPAS grid sequence:



[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.

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× 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`