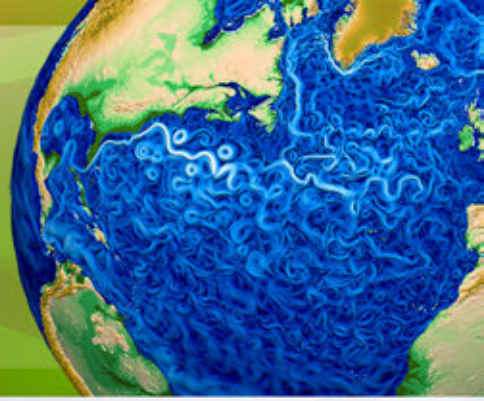
E3SM
Energy Exascale Earth System Model



LEAP-T: Multi-Moment Semi-Lagrangian Tracer Transport

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**As part of COMPOSE*

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Outline

- Introduction
- Challenges and Opportunities
- Methods and results
- Conclusions and future work

LEAP-T

Launching an Exascale ~~ACME~~ E3SM Prototype (Transport)

- Research and develop:
  - Performance portable implementations of existing tracer transport algorithms;
  - New NGP-friendly tracer transport algorithms (today's talk).
- 2 years: Oct 2015 to Sep 2017.
- Main themes:
  - Legion for MPAS (not today)
  - Characteristic Discontinuous Galerkin (CDG) in flux form (ocean)
  - CDG, Incremental Remap in remap form (atmosphere)
  - Portable intersection library
  - Multi-moment shape preservation and tracer consistency library

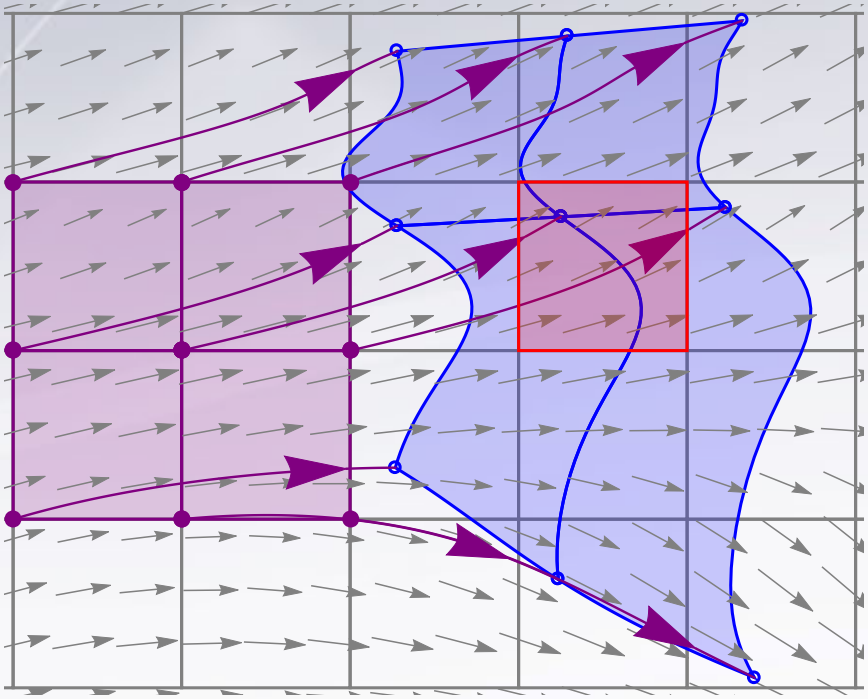
Challenges and Opportunities

- Tracer transport is computationally demanding
  - 10s of tracers vs <10 dynamical variables
  - Property preservation
    - Property: A quantity that must be computed to machine precision despite an overall solution that is (of necessity) approximate.
    - Mass conservation, shape preservation, tracer consistency
- Advection only: thus, semi-Lagrangian methods
  - Different spatial discretization
  - Different (larger) time step
    - No Courant number limit
    - Substantially lower Comm/UST
      - Comm: Communication volume, communication rounds
      - UST: Unit of simulated time
    - Property preservation is harder

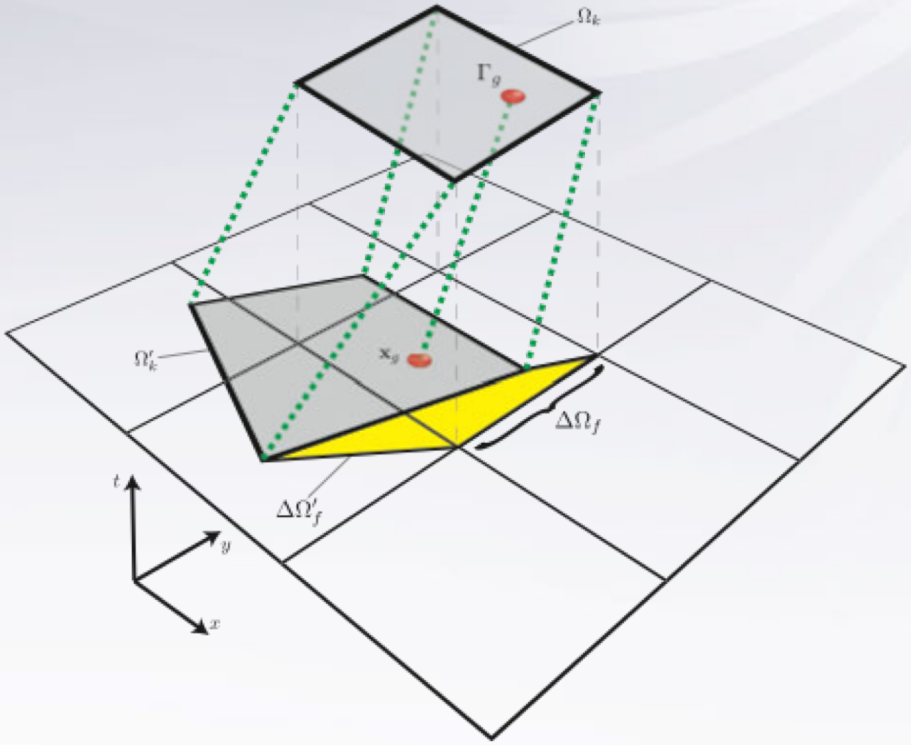
Design Space and Decisions

- Atmosphere
  - Spectral Element spatial discretization
    - Discontinuous Galerkin followed by discrete stiffness summation (DSS) to continuous Galerkin
  - Thus, multi-moment DG with same basis
  - Remap form (definitely harder but potentially faster)
  - Cell integrated for local mass conservation
  - CDG and Incremental Remap (IR)
- Ocean
  - Flux form, multi-moment DG, cell integrated

Methods: Conceptual



Remap form



Flux form

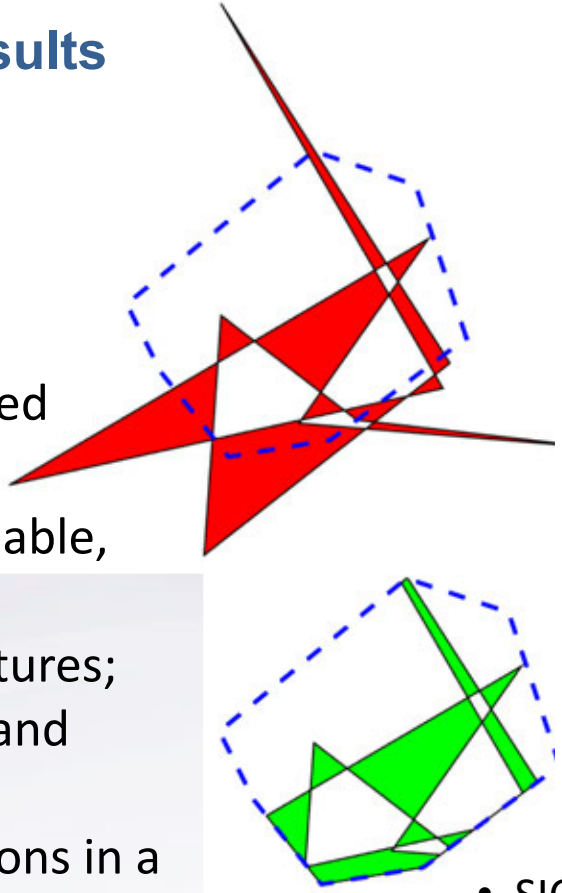
Methods: Overview of Components

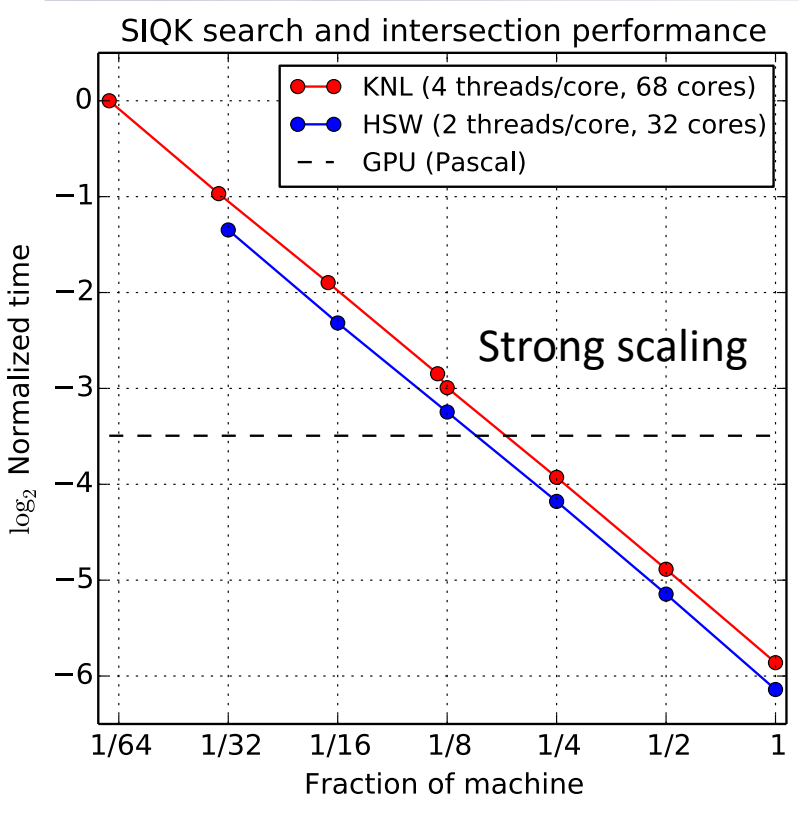
- SIQK: Spherical polygon intersection and quadrature with Kokkos
  - Used by both ocean and atmosphere
- CEDR/QLT: Communication-Efficient Density Reconstruction for property preservation
  - Assured shape preservation *and* tracer consistency
  - Efficient Quasi-Local Tree algorithm
- MPAS/CDG: Ocean Semi-Lagrangian Characteristic Discontinuous Galerkin (CDG)
- SLMM: Atmosphere Semi-Lagrangian CDG/Incremental Remap

Methods and Results

SIQK

- Portable spherical polygon intersection code for cell-integrated transport methods.
- Uses only thread-scalable, robust operations.
- (No global data structures; do not mix topology and geometry.)
- Expose these operations in a standalone Kokkos-based library.
- Kokkos: C++ framework to enable performance portability





- SIQK is used in HOMME and MPAS prototype CDG implementations.
- Aggressive usage in standalone SLMMIR test program shows SIQK is very robust.
- Standalone library can be used in other applications.

Reference: ***Bosler, Bradley, Taylor, "Conservative multi-moment transport along characteristics for discontinuous Galerkin methods", in preparation.***

Methods and Results

CEDR/QLT

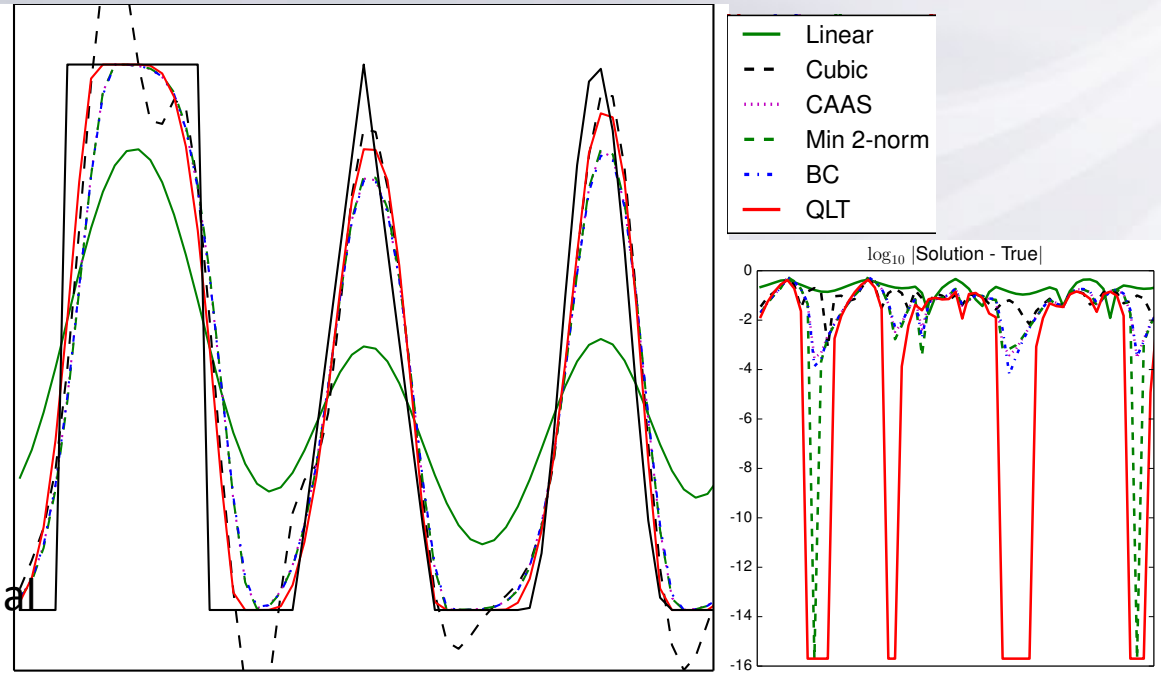
QLT algorithm: Preserve properties
- assuredly,
- in exactly one reduction equivalent,
- quasi-locally.

- Enables remap form.
- Only extremely loosely dependent on details of discretizations.

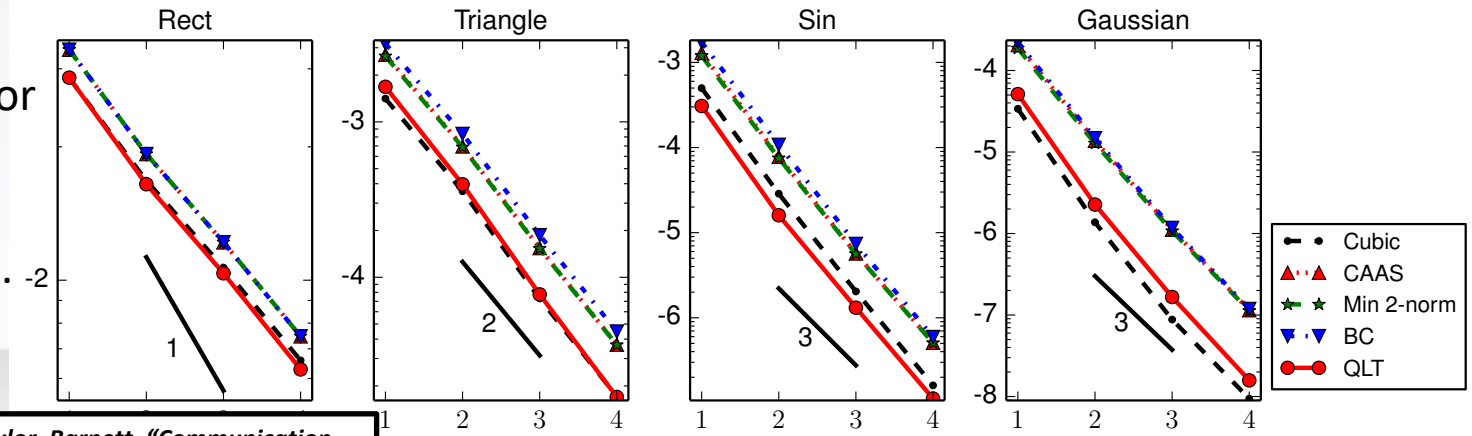
Mass conservation

Shape preservation
- Mimic advection equation
- Mixing ratio value at time step n+1 bounded by extrema in domain of dependence at time step n

Tracer consistency
- *Tracer transport method* and continuity equation from *dynamics* agree exactly …
- … despite completely different spatial and temporal discretizations.



- Previous methods for remap form are *iterative* or *cannot assure preservation*.

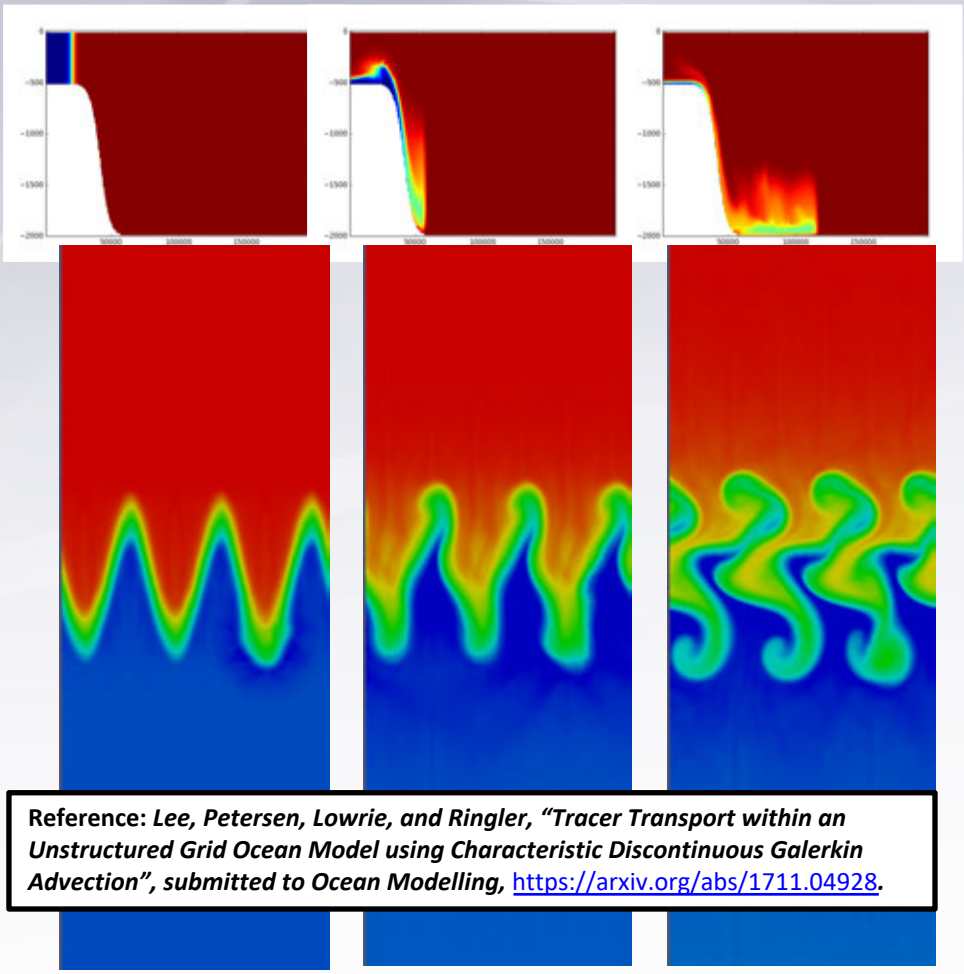


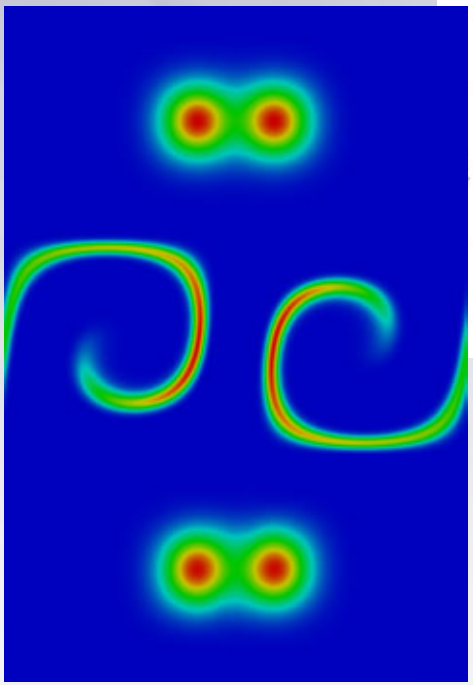
$\log_{10}$ Relative Error *vs.* Mesh Refinement Level

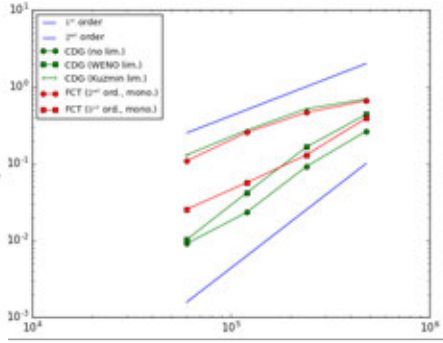
Reference: ***Bradley, Bosler, Guba, Taylor, Barnett, "Communication-efficient property preservation in tracer transport", in preparation.***

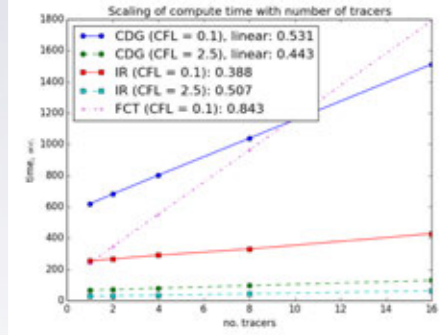
Methods and Results

MPAS/CDG









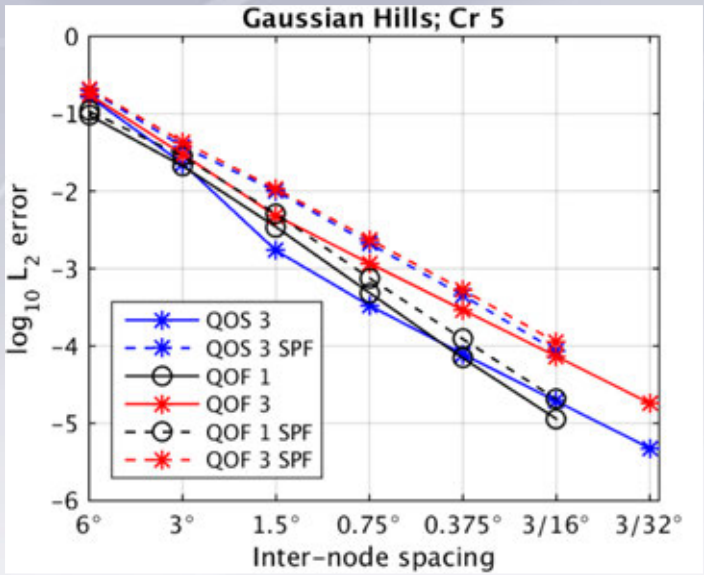
- More computationally efficient than existing FCT scheme for O(10) tracers.
- Superior error convergence to FCT in both unlimited and WENO limited form.
- Conservative and supported on both planar and spherical unstructured grids.

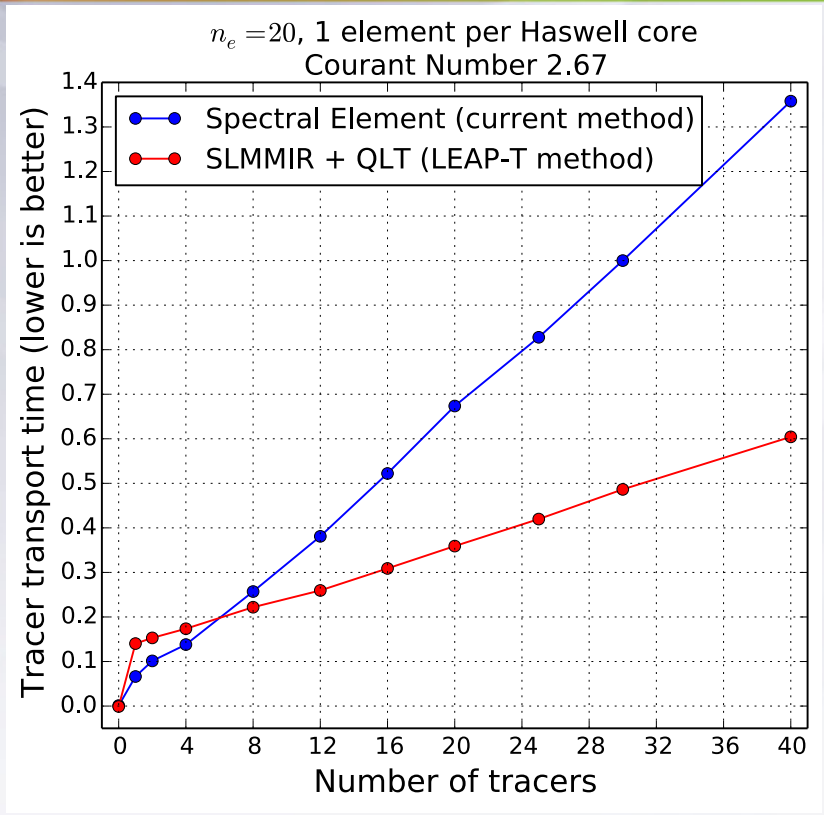
Reference: ***Lee, Petersen, Lowrie, and Ringler, "Tracer Transport within an Unstructured Grid Ocean Model using Characteristic Discontinuous Galerkin Advection", submitted to Ocean Modelling,*** https://arxiv.org/abs/1711.04928.

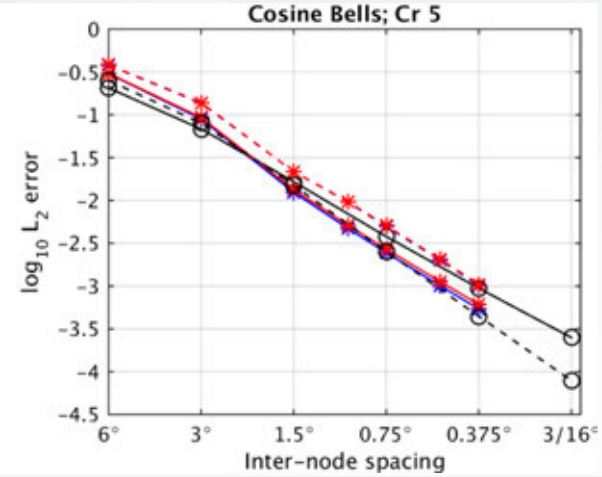
Reference: ***Lee, Lowrie, Petersen, Ringler and Hecht, "A High Order Characteristic Discontinuous Galerkin Scheme for Advection on Unstructured Meshes", Journal of Computational Physics 324, 289-302.***

Methods and Results

SLMM







- Full atmosphere test case in HOMME
- At strong-scaling limit (1 element per core)
- SLMMIR faster than current transport for number of tracers > 7
- Transport speedup at 30 tracers: > 2x
- (Much) more communication-reduction speedup to go:
  - Match MPI communication pattern to remap-form SL
  - Localize QLT reduction adaptively
- SLMM+QLT: Suite of methods enabling a large design space

E3SM Energy Exascale Earth System Model

Reference: ***Bosler, Bradley, Taylor, "Conservative multi-moment transport along characteristics for discontinuous Galerkin methods", in preparation.***

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Conclusions and Future Work

- Demonstrated semi-Lagrangian methods for tracer transport in E3SM
  - Speedup based on *substantially lower communication*
- Prototyped multiple general-use components
  - Portable spherical polygon intersection
  - Communication-efficient property preservation
  - C++ with Kokkos
- CANGA: Coupling Approaches for Next-Generation Architectures
  - DOE (BER and ASCR) SciDAC
- COMPOSE: Compact Multi-Moment Performance-Portable Semi-Lagrangian Methods
  - DOE (BER and ASCR) SciDAC