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

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*As part of COMPOSE
**High school summer intern
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.

Methods and Results

CEDR/QLT

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.

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

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

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.


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

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