E3SM All Hands: NGD: Efficient Communication Pattern for Interpolation Semi-Lagrangian Tracer Transport

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Outline

1. Motivation

2. SL MPI

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COMPOSE: Semi-Lagrangian Tracer Transport for E3SM

- Problem: Tracer transport is expensive.
- Solution: Semi-Lagrangian (SL) transport. Long time steps; less communication.

- Problem: Transport requires property preservation, and SL makes that harder.
  - (mass conservation, shape preservation, tracer consistency, linear correlation preservation)
- Solution: CEDR: Property preservation in exactly 1 all-to-all reduction equivalent.[1]

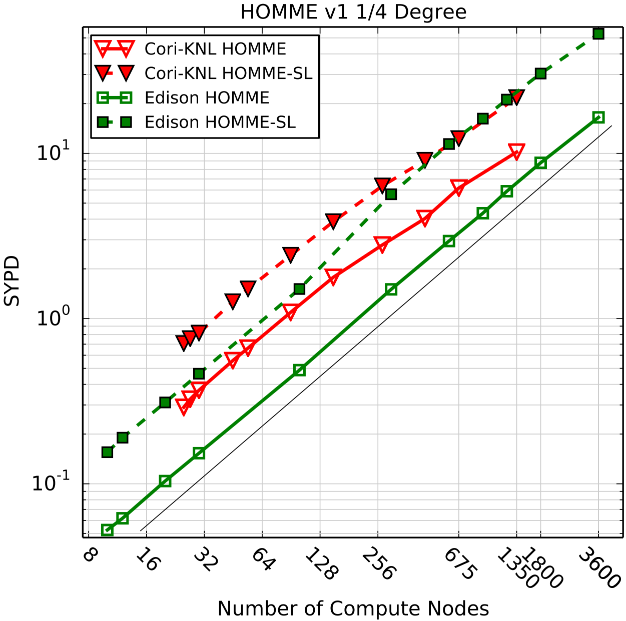
- Opportunity: CEDR enables using the fastest, lowest-communication SL method there is: Interpolation SL (ISL) with compact stencil.

- Problem: ISL based on high-order compact stencil (GLL element, $n_p \geq 4$) is unstable.
- Solution: Stabilized ISL.

- Problem: HOMME's deterministic halo exchange is suboptimal for SL.
- Solution: ISL-specific optimal communication pattern.
  - This project.

[1] A. M. Bradley, P. A. Bosler, O. Guba, M. A. Taylor, G. A. Barnett, *Communication-efficient property preservation in tracer transport*, to appear in SIAM J. Sci. Comp.
Software: `github.com/E3SM-Project/COMPOSE`

Strong scaling HOMME: Status for 40 tracers



- `preqx` dycore is >**2.1**× faster on KNL at 1350 nodes (strong-scaling limit).
- `preqx` dycore is >**3.2**× faster on Edison at 3600 nodes (strong-scaling limit).

Outline

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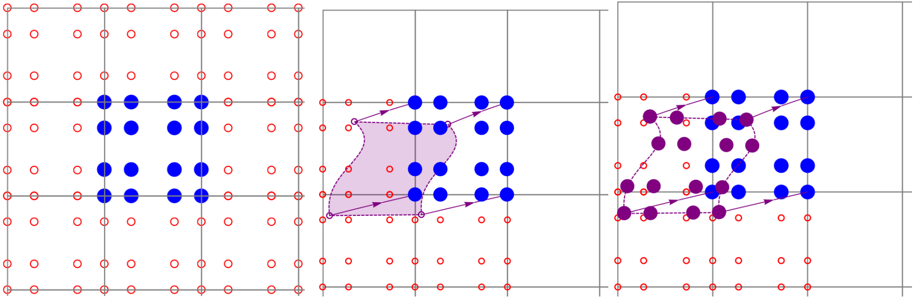
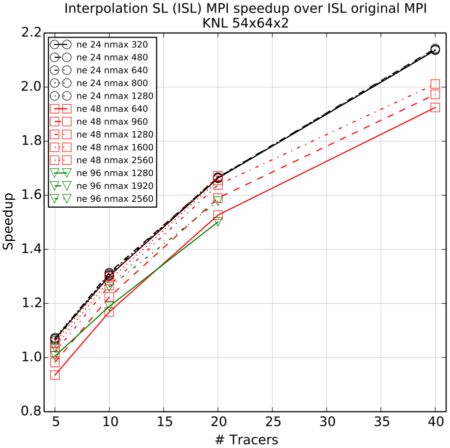
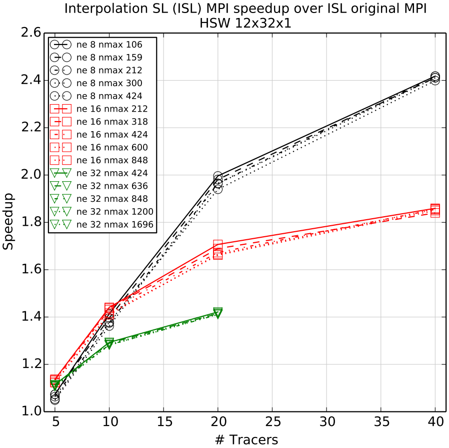
- Communicate only with ranks holding relevant data.
- For Interpolation SL (ISL), send requests for interpolation.
  - Send/receive departure point data to make requests for interpolation.
  - Send/receive interpolation and bounds data, fulfilling these requests.
  - In both rounds, overlap communication and computation.



SL MPI speedup

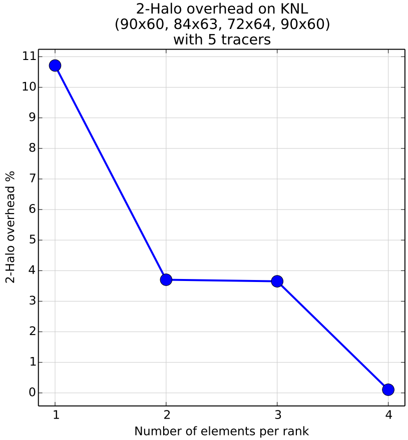
- Prescribed velocity field driver on Mutrino KNL, HSW; time step requires only 1-halo.
- Vary number of elements per rank, number of tracers.
- Measure end-to-end time using original MPI and new SL MPI communication patterns and report speedup.

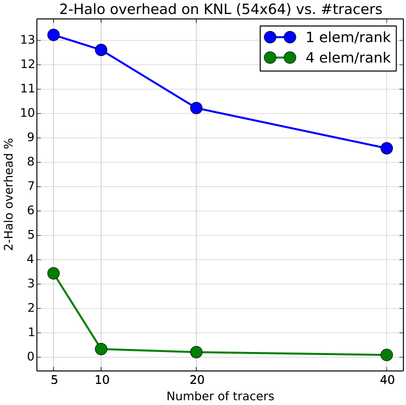




2-halo overhead

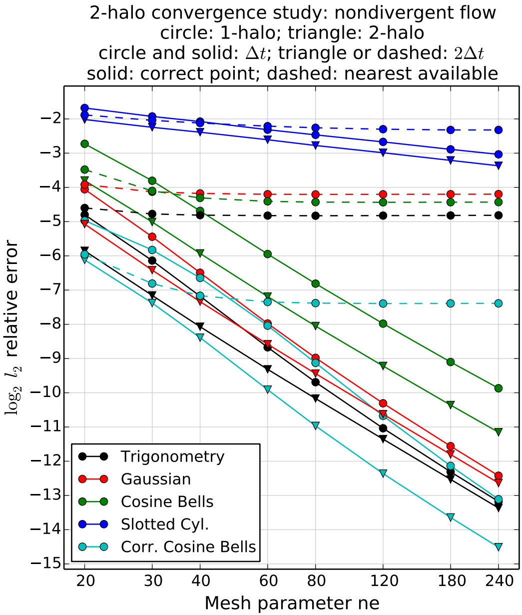
- Prescribed velocity field driver on Mutrino KNL; time step requires only 1-halo.
- Vary number of elements per rank, number of tracers.
- Measure extra time taken when 2-halo is active and report percent overhead.
- *Except for this overhead*[2]*, speedup of 2-halo is exactly the factor time step increase.*



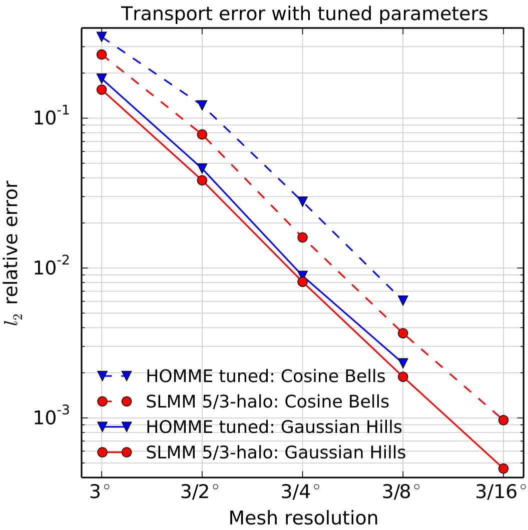


[2] still possibly to do: more accurate velocity, which will also have overhead

2-halo convergence (correctness)



Fidelity study



- Nondivergent flow test case
- "HOMME tuned" data are from Guba et al, *Optimization-based limiters for the spectral element method*, JCP 2014.
- SL MPI is used with 2-halo capability.

To do

- Algorithm: Communicate and compute once per node (currently redundant for edge nodes).
- Algorithm: Expose all available parallelism for GPU implementation; rework metadata and metadata setup as necessary.
- Software: Rewrite several target-cell, local-mesh data structures so bulk data are shared.
  - Bulk data memory footprint independent of halo size.

Thanks!

Semi-structured messages

- Set of departure points in remote elements is nondeterministic.
- $\Rightarrow$ unstructured messages.
- Requirements:
  - No memory allocation except in initialization.
  - But don't use more memory than deterministic 1-halo method does.
  - Message size roughly proportional to number of departure points (up to a little metadata).
- Preferences during time stepping (not initialization):
  - Two passes to set up message structure rather than one pass plus a sort.
  - $O(1)$ accesses with *no* hash table, just linear arrays.
  - No holes in arrays, i.e., unused index space.
- Strategy:
  - At initialization, do everything necessary to make the above feasible during time stepping.
  - Assemble and parse messages using these initialization-phase metadata.

```
xs: (#x-tgt-rank   integer           < send/recv departure points
     pad           i
     (lid-src-rank i      packed only when #x in lid > 0
      #x-in-lid    i      > 0
       (lev        i      packed only when #x in (lid,lev) > 0
        #x         i      > 0
        x        3 real
         *#x) *#lev) *#lid) *#rank
qs: (q-extrema    2 qsize r    (min, max) packed together
     q              qsize r
      *#x) *#lev *#lid *#rank     < send/recv q data
```

Top-level algorithm at each time step

```
/* xs: (#x-tgt-rank   int
       pad            i
       (lid-src-rank i      only packed if #x in lid > 0
        #x-in-lid     i      > 0
        (lev          i      only packed if #x in (lid,lev) > 0
         #x           i      > 0
         x          3 real
          *#x) *#lev) *#lid) *#rank                          */

setup_irecv(cm); // Set up to receive departure point requests.

// Determine where my departure points are. Set up requests to
// remotes as well as to myself to fulfill these. Fill metadata.
//   In parallel over my elements, determine element containing
// departure point. Count:
//     # points in an element,
//     # points in an (element, level).
analyze_dep_points(cm, nets, nete, dep_points);
//   In parallel over remote ranks, calculate offsets and fill in
// xs metadata.
pack_dep_points_sendbuf_pass1(cm);
//   In parallel over elements having remotes in halo, fill x
// bulk data and record some offsets.
pack_dep_points_sendbuf_pass2(cm, dep_points);

isend(cm); // Send requests.
```

Top-level algorithm at each time step

```
// While waiting, compute q extrema in each of my elements.
calc_q_extrema<np>(cm, nets, nete);

// Wait for the departure point requests.
recv_and_wait_on_send(cm);
```

Top-level algorithm at each time step

```
// Compute the requested q for departure points from remotes.
calc_rmt_q<np>(cm);

// Send q data, skipping messages to ranks who made 0 requests.
isend(cm, false /* want_req */, true /* skip_if_empty */);
```

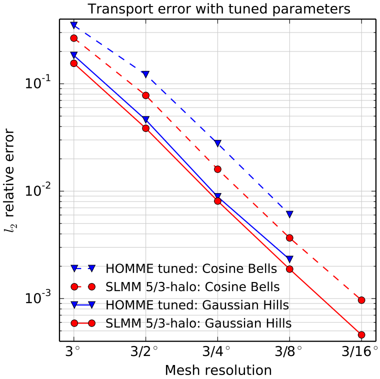
Top-level algorithm at each time step

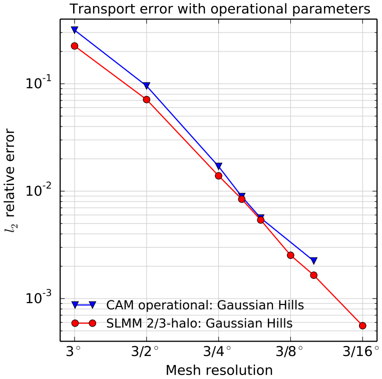
```
// Set up to receive q for each of my departure point requests
// sent to remotes.
setup_irecv(cm, true /* skip_if_empty */);

// While waiting to get my data from remotes, compute q for
// departure points that have remained in my elements.
calc_own_q<np>(cm, nets, nete, dep_points, q_min, q_max);

// Receive remote q data.
recv(cm, true /* skip_if_empty */);
// Copy these data into my data structures.
copy_q(cm, nets, q_min, q_max);
```

Fidelity study[4]





- Nondivergent flow test case.
- Compare (1) tuned parameters and (2) operational parameters, as in previous slide.
- SL transport is uniformly more accurate.
- For climate results, see Nov 2018 DOE Modeling PI Meeting poster[3].

[3] https://acme-climate.atlassian.net/wiki/spaces/CNCL/pages/840073634/E8.1+Semi-Lagrangian+tracer+transport+in+the+E3SM+atmospheric+dycore

[4] "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.

Resolution: DCMIP2016 Baroclinic Instability

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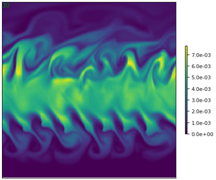
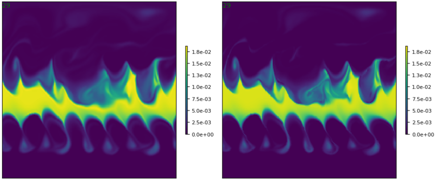
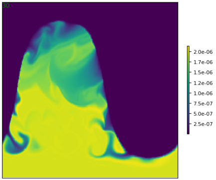
- Configuration: `theta-l`, nonhydrostatic mode, moist, `ne` = 30, `tstep` = 300, `rsplit`×`qsplit` = 6
- Eulerian at left; SL at right



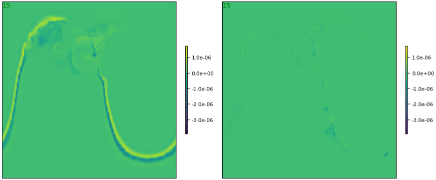
(a) q_v, level 20, day 30



(b) q_v, level 30, day 29



(c) Toy chemistry tracer, level 30, day 30



(d) Toy chemistry diagnostic, level 30, day 15