A performance portable implementation of HOMME via the Kokkos programming model


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1. The E3SM and CMDV projects

2. Kokkos and HOMME

3. From HOMME to HOMMEXX

4. Results
What is E3SM?

- DOE effort for a high resolution earth model.
- Branched from Community Earth System Model (CESM) in 2014.
- Modular library, with several components: atmosphere dynamics/physics, land, land-ice, ocean, sea-ice, biogeochemistry, ...
- All component can run with variable-resolution, unstructured grids.
- Mostly written in Fortran 90.
- Broad variety of time and space scales.
- 2018: E3SM version 1 is released in April.
Project goal is to improve

- trustworthiness of the model for decision support,
- code agility for adapting to exascale architectures,
- productivity through leveraging of cutting-edge computational science.

Coding challenge: have a single code base, performant on a variety of architectures, and capable of rapidly adapting to new ones.

Task: study the feasibility of using Kokkos (a library for on-node parallelism, more on it later) to achieve a single code base which is performant on a variety of architectures (CPU, MIC, GPU).

Path: convert a component of E3SM, namely the atmosphere component HOMME (more on that later), to C++, using Kokkos.

Metrics: correctness (bit-for-bit with original HOMME), and performance (on par with original HOMME on CPU/MIC).
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The Kokkos library

- Developed at Sandia National Labs, written in C++ (with C++11 required).
- Provides templated constructs for on-node parallel execution: execution space (host vs device), execution policy (range vs team), parallel operation (for, scan, reduce).
- Provides template abstraction for a multidimensional array: data type, memory space (host, device, UVM), layout (left, right, ...), memory access/handling (atomic, unmanaged, ...).
- Supports several back-ends: Serial, OpenMP, Pthreads, Cuda, ....
- Available at http://github.com/kokkos/kokkos.
- Component of E3SM (and CESM) for dynamics and transport in the atmosphere.
- Accounts for 20-25% of total run time of typical fully-coupled simulation.
- Highly optimized for MPI and OpenMP parallelism.
- Horizontal (2D) and vertical (1D) differential operators are decoupled.
- Spectral Element Method (SEM) in the horizontal direction.
- Eulerian or Lagrangian schemes for vertical operators.
- Solves for 4 prognostic variables (2 horizontal velocities, temperature, pressure), and the transport of N tracers (usually, N~10-40).
From HOMME to HOMMEXX

- Incremental conversion of original Fortran code to C++.
- Heavily tested (~85% of kernels are individually tested).
- Bit-for-bit agreement with original implementation.
- Minimization of architecture-specific code.
- Primary design goals:
  - expose parallelism,
  - maximize vectorization,
  - minimize memory movement.
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HOMMEXX design: exposing parallelism

- HOMME has 3 layers of nested for loops: element($\times$ \# variables), GLL points, vertical levels.
- Elements and levels independently processed through majority of code.
- 2D differential operators couple GLL points.
- Kokkos supports up to 3 levels of hierarchical parallelism:
  - team level: a parallel region over the number of teams (of threads)
  - thread level: a parallel region over the number of threads in a team
  - vector level: a parallel region over the number of vector lanes of a thread.
- Hierarchical parallelism allows to expose maximum parallelism with minimal index bookkeeping.
A simple nested loop:

```c
for (int i=0; i<dim0; ++i) {
  for (int j=0; j<dim1; ++j) {
    for (int k=0; k<dim2; ++k) {
      // do some work on i, j, k
    }
  }
}
```

Expose parallelism by flattening:

```c
for (int idx=0; idx<dim0*dim1*dim2; ++idx) {
  int i = idx / (dim1*dim2);
  int j = idx / dim2;
  int k = idx % dim2;
  // do some work on i, j, k
}
```

Embarassingly parallel.
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Embarassingly parallel.
A more complex scenario: divergence on the sphere

```c
for (int ie=0; ie<num_elements; ++ie) {
    for (int idx=0; idx<NP*NP; ++idx) {
        int i = idx / NP; int j = idx % NP;
        double v0 = v(ie,0,i,j); double v1 = v(ie,1,i,j);
        buf(0,i,j) = (J(0,0,i,j)*v0 + J(1,0,i,j)*v1)*metdet(i,j);
        buf(1,i,j) = (J(0,1,i,j)*v0 + J(1,1,i,j)*v1)*metdet(i,j);
    }

    for (int idx=0; idx<NP*NP; ++idx) {
        int i = idx / NP; int j = idx % NP;
        double dudx = 0.0, dvdy = 0.0;
        for (int k = 0; k < NP; ++k) {
            dudx += D(j,k) * buf(0,i,k);
            dvdy += D(i,k) * buf(1,k,j);
        }
        div(ie,i,j) = (dudx+dvdy) / (metdet(i,j)*rearth);
    }
    ...
}
```
HOMMEXX design: exposing parallelism

A more complex scenario: divergence on the sphere

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for (int ie=0; ie<num_elements; ++ie) {
    || over # teams
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        buf(1,i,j) = (J(0,1,i,j)*v0 + J(1,1,i,j)*v1)*metdet(i,j);
    }

    team barrier

    for (int idx=0; idx<NP*NP; ++idx) {
        int i = idx / NP; int j = idx % NP;
        double dudx = 0.0, dvdy = 0.0;
        for (int k = 0; k < NP; ++k) {
            dudx += D(j,k) * buf(0,i,k);
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        }
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}
...
HOMMEXX design: exposing vectorization

- Core data type is a packed (Vector) of N doubles.
- On GPUs, N=1 (no SIMD, only SIMT).
- Vectorization via call to compiler intrinsics.

Two natural choices for vectorization: GLL points and vertical levels. But:

- 2D differential operator much more frequent than 1D vertical integrals, and
- matching N with # vertical level feasible, while matching N with # of GLL point could become prohibitive.

⇒ Vectorization over vertical levels (and data laid out accordingly in memory).
Results: tested architectures

(IB) Intel Ivy Bridge: 2 sockets/node, 12 cores/socket, 2 threads/core, DDR3
(HSW) Intel Haswell: 2 sockets/node, 16 cores/socket, 2 threads/core, DDR4
(KNL) Intel Xeon Phi: 68 cores/node, 4 threads/core, HBM+DDR4
(SKX) Intel Skylake: 2 sockets/node, 24 cores/socket, 2 threads/core, DDR4
(P9) IBM Power9: 2 sockets/node, 10 cores/socket, 4 threads/core, DDR4
(P100) NVidia Pascal: 2 sockets/node, 2 GPUs/socket, 1792 DP cores/GPU
(V100) NVidia Volta: 2 sockets/node, 2 GPUs/socket, 2560 DP cores/GPU

Note: IB, HSW and KNL tested at large scale, SKX, P100, V100, P9 only available on testbeds.
Results: strong scaling at large scale

Strong Scaling for 86,400 Elements

- Cori-HSW HOMME
- Cori-HSW HOMMEXX
- Cori-KNL HOMME
- Cori-KNL HOMMEXX
- Edison HOMME
- Edison HOMMEXX

Thousands of Element-Timesteps / Node / Second

Number of Compute Nodes
Results: single node performance (40 tracers)

Power consumption (at high workload):
- IB: 260W
- HSW: 360W
- KNL: 260W
- SKX: 330W
- P9: 360W (?)
- P100: 190W
- V100: 200W
Results: single node performance (no tracers)

Power consumption (at high workload):
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Conclusions

- With Kokkos, HOMMEXX can run on multiple architectures with a (mostly) single implementation.
- HOMMEXX slightly faster than HOMME on CPU/MIC (\(\sim 1.1 \times\) on HSW, and up to \(1.4 \times\) on KNL).
- Reasonable performance on GPUs. Need to test performance with NVLink 2.0.
- Skylake-like architectures could become very interesting for E3SM.
- C++ and Kokkos is a viable path to achieve a performance portable code.