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A performance portable implementation of HOMME via the Kokkos programming model

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Energy **E**xascale **E**arth **S**ystem **M**odel (E^{3}SM)

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What is E3SM?

- DOE effort for a high resolution earth model.
- Branched from **C**ommunity **E**arth **S**ystem **M**odel (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.

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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.

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Coding challenge: have a single code base, performant on a variety of architectures, and cabable 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).

The Kokkos library

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- 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`.

(HOMME)

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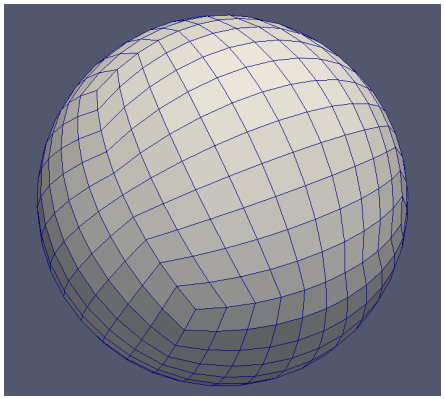
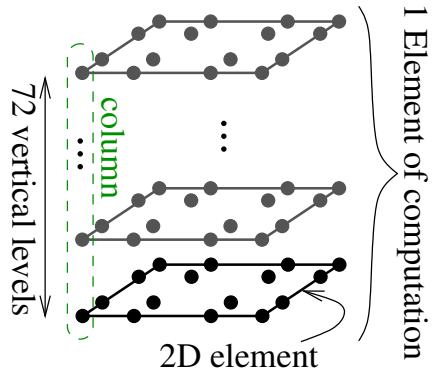
- Component of E3SM (and CESM) for dynamics and transport in the atmosphere.
- Accounts for 20-25% of total run time of typical fully-coupled simulation.
- Highly optimized for MPI and OpenMP parallelism.
- Horizontal (2D) and vertical (1D) differential operators are decoupled.
- Spectral Element Method (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

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- 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

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- 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 bookkeping.

HOMMEXX design: exposing parallelism

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A simple nested loop:

```
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
}}}
```

HOMMEXX design: exposing parallelism

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}}}
```

Expose parallelism by flattening:

```
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
}
```

HOMMEXX design: exposing parallelism

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}
```

Embarassingly parallel.

HOMMEXX design: exposing parallelism

A more complex scenario: divergence on the sphere

```
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

```
for (int ie=0; ie<num_elements; ++ie) {   ← || over # teams
  for (int idx=0; idx<NP*NP; ++idx) {
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    double v0 = v(ie,0,i,j); double v1 = v(ie,1,i,j);
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HOMMEXX design: exposing parallelism

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  }

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    }
    div(ie,i,j) = (dudx+dvdy) / (metdet(i,j)*rearth);
  }
  ...
}
```

← ∥ over # teams

← ∥ over # threads in a team

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HOMMEXX design: exposing parallelism

A more complex scenario: divergence on the sphere

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    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);
  }
  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);
      dvdy += D(i,k) * buf(1,k,j);
    }
    div(ie,i,j) = (dudx+dvdy) / (metdet(i,j)*rearth);
  }
  ...
}
```

← ∥ over # teams

∥ over # threads in a team

∥ over # threads in a team

shared within team

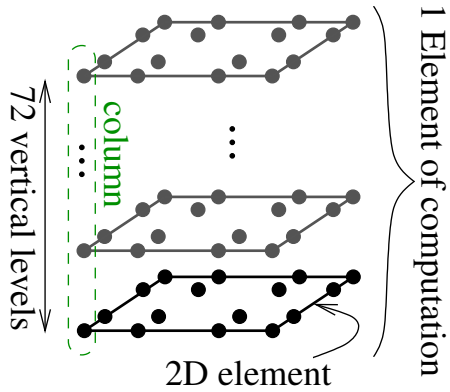
HOMMEXX design: exposing vectorization

- Core data type is a packed (`Vector`) of N doubles.
- On CPU, N varies: KNL/SKX N=8, HSW N=4.
- 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.

$\Rightarrow$ Vectoriation over vertical levels (and data laid out accordingly in memory).



Results: tested architectures

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(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

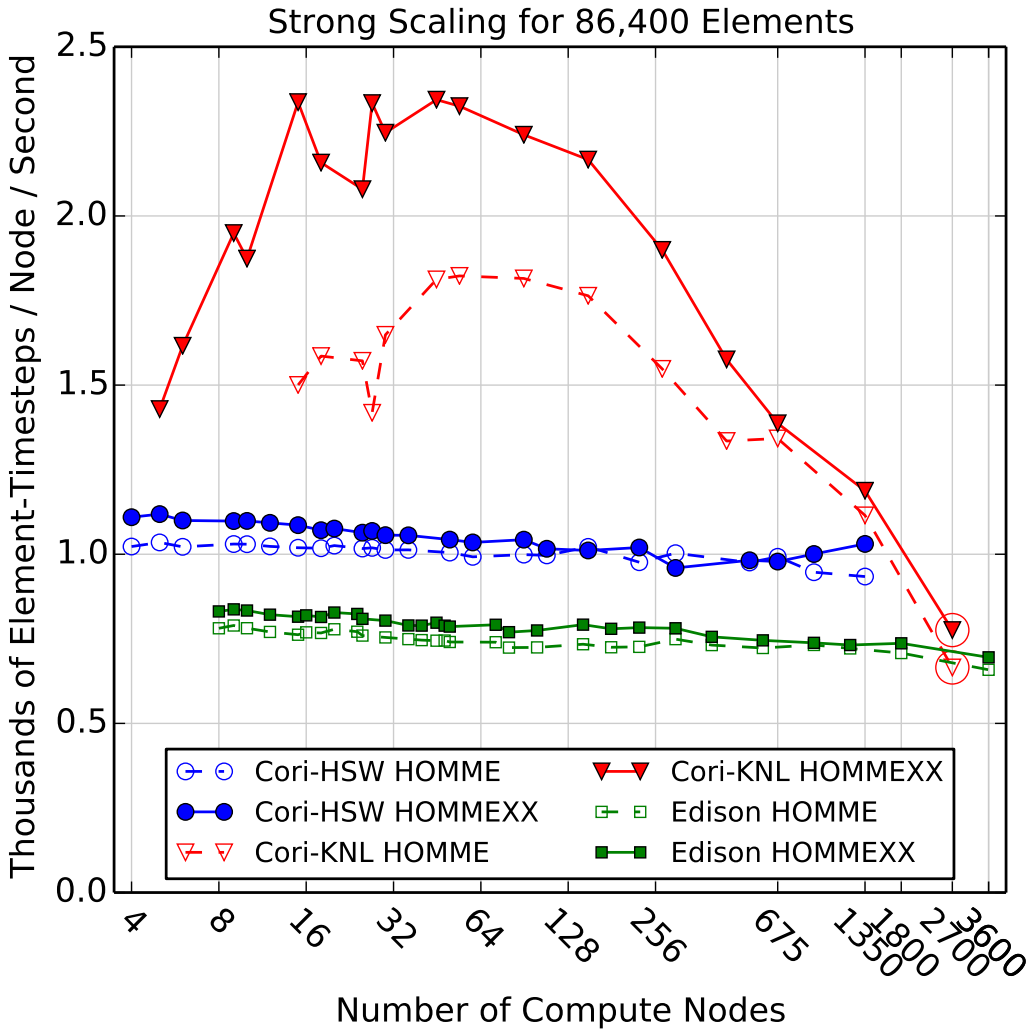
(P9) IBM Power9: 2 sockets/node, 10 cores/socket, 4 threads/core, DDR4

(P100) NVidia Pascal: 2 sockets/node, 2 GPUs/socket, 1792 DP cores/GPU

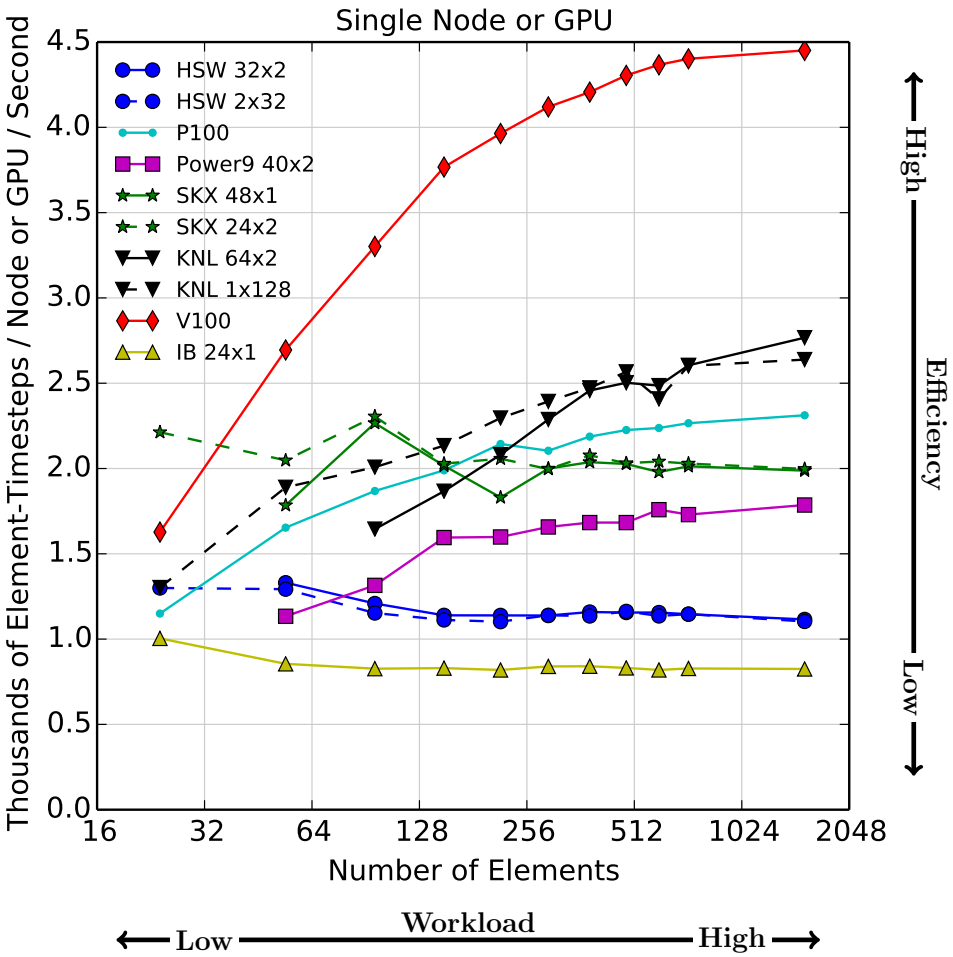
(V100) NVidia Volta: 2 sockets/node, 2 GPUs/socket, 2560 DP cores/GPU

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

Results: strong scaling at large scale



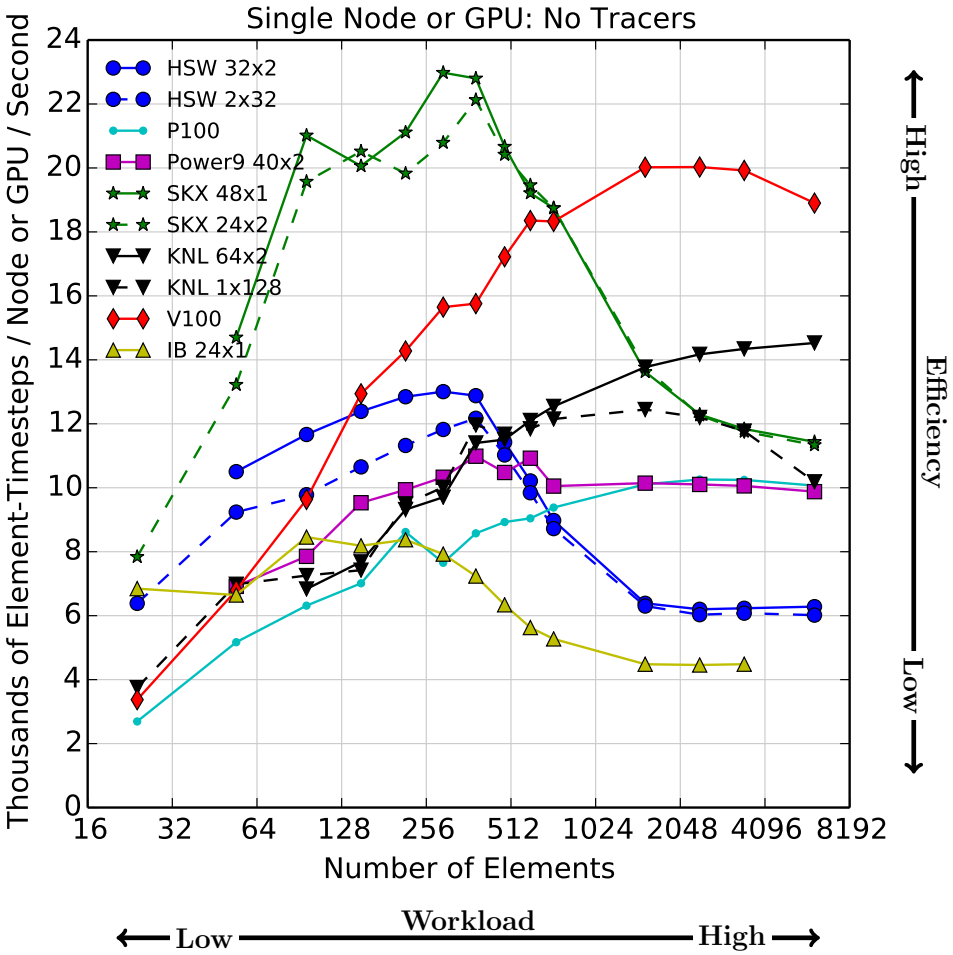
Results: single node performance (40 tracers)



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)



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- P100: 190W
- V100: 200W

Conclusions

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- 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.