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A Performance-Portable C++ Implementation of Atmospheric Dynamics

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Outline

Energy Exascale Earth System Model (E3SM)

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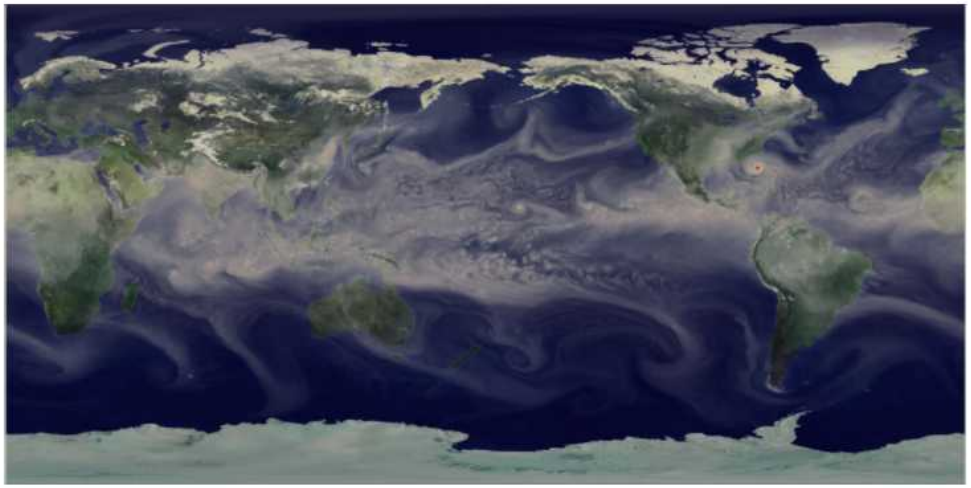
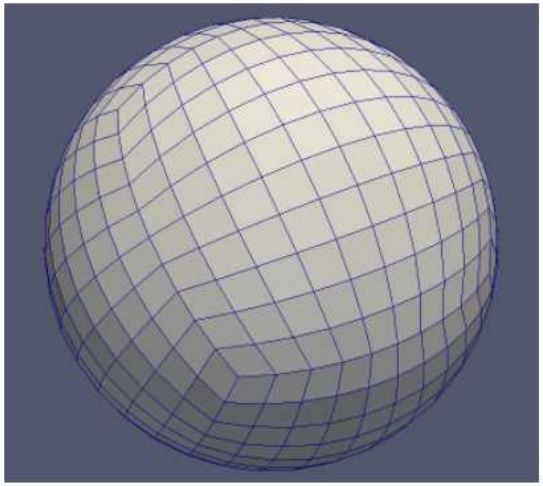
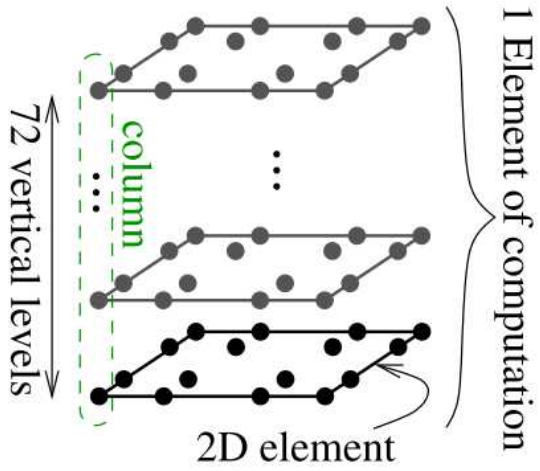


- Open source with open development at `https://github.com/E3SM-Project/E3SM`
- Fork of Community Earth System Model (CESM)[9] from 2014
- Several Components: **Atmosphere Dynamics**, Atmosphere Physics, Ocean, Sea Ice, ...
  - We are only concerned with the Atmosphere Dynamics

HOMME Atmosphere Dynamics

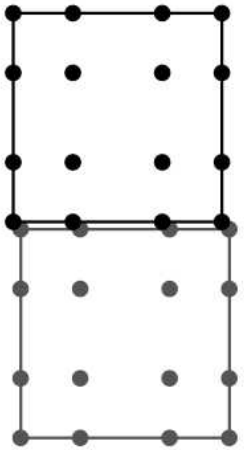
- High-Order Methods Modeling Environment (HOMME)[6]
- Joint project among the DOE, NSF, NCAR, and several laboratories and universities
- Cubed Sphere Mesh with 72 level extruded elements
  - Terrain following vertical coordinate with material surfaces, ie no vertical flux

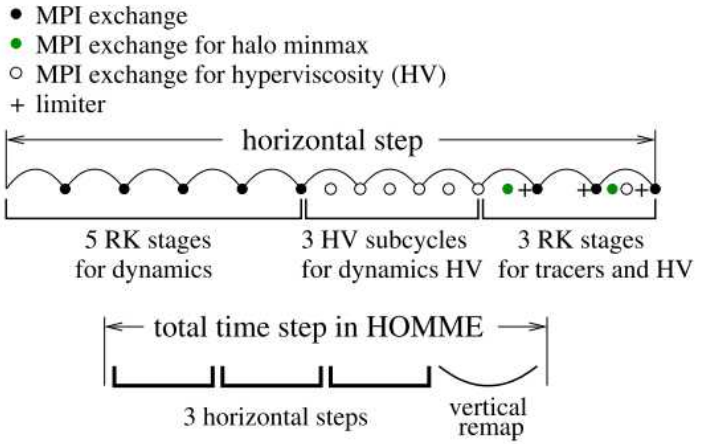




HOMME Atmosphere Dynamics

- Spectral Element Method (SEM) horizontal discretization [4]
  - Continuous Galerkin method with high accuracy and scalability
  - DOFs and quadrature points chosen to coincide
- Solves for 4 prognostic variables: Pressure, Temperature, and 2 Velocity components





Kokkos [5]

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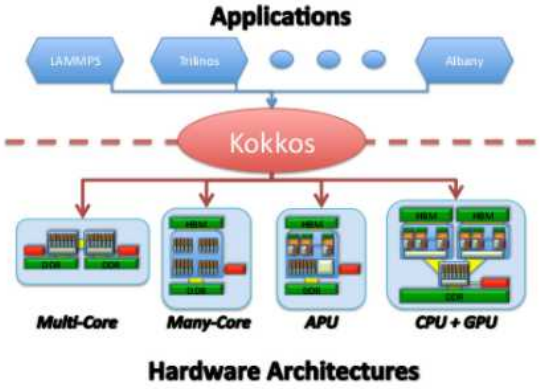
- Open source with open development at `https://github.com/kokkos/kokkos`
- Performance Portability Layer, similar to RAJA [8], HEMI [7], OpenACC [3], and future C++ STL features[1]
- Not pragma based, C++11 compliant, uses template metaprogramming
- Provides memory space abstractions in addition to parallel dispatch abstractions
- Performance overhead of at most 10%



[11]

Kokkos

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Key Definitions:

- **Kernel**: A body of work to be performed
- **Execution Space**: Describes the device kernels should execute on
- **Execution Pattern**: Scan, Reduce, or Map; primitives for parallel algorithms
- **Execution Policy**: How a kernel receives work items.
  - Range: Work is mapped to a range of integers from $[L, U)$
  - Team: Provides a team of warps/threads to each work item. Exposes hierarchical parallelism, avoids duplicating work and extra buffers
- **View**: A multi-dimensional array reference. Abstracts memory (de)allocation and accesses

Kokkos Examples

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```
Kokkos::parallel_for(
  Kokkos::RangePolicy<ExecSpace>(0, elements.num_elems()*NP*NP*NUM_LEV),
  KOKKOS_LAMBDA(const int it) {
     const int ie = it / (NP*NP*NUM_LEV);
     const int igp = (it / (NP*NUM_LEV)) % NP;
     const int jgp = (it / NUM_LEV) % NP;
     const int ilev = it % NUM_LEV;
     t(ie,nm1,igp,jgp,ilev) = (5.0*t(ie,nm1,igp,jgp,ilev)-t(ie,n0,igp,jgp,ilev))/4.0;
     v(ie,nm1,0,igp,jgp,ilev) = (5.0*v(ie,nm1,0,igp,jgp,ilev)-v(ie,n0,0,igp,jgp,ilev))/4.0;
     v(ie,nm1,1,igp,jgp,ilev) = (5.0*v(ie,nm1,1,igp,jgp,ilev)-v(ie,n0,1,igp,jgp,ilev))/4.0;
     dp3d(ie,nm1,igp,jgp,ilev) = (5.0*dp3d(ie,nm1,igp,jgp,ilev)-dp3d(ie,n0,igp,jgp,ilev))/4.0;
});
```

Figure : Example of range parallelism in HOMMEXX

Kokkos Examples

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```
Kokkos::parallel_for(
  Homme::get_default_team_policy<ExecSpace>(m_elements.num_elems()),
  KOKKOS_LAMBDA (const TeamMember& team) {
    KernelVariables kv(team);
    Kokkos::parallel_for (
      Kokkos::TeamThreadRange(kv.team, NP*NP),
      [&] (const int loop_idx) {
        const int i = loop_idx / NP;
        const int j = loop_idx % NP;
        Kokkos::parallel_for(
          Kokkos::ThreadVectorRange(kv.team, NUM_LEV),
          [&] (const int& k) {
            buf(kv.ie,i,j,k) =
              dp(kv.ie,i,j,k) - rhsmdt * divdp_proj(kv.ie,i,j,k);
          });
      });
  });
```

Figure : Example of hierarchical parallelism in HOMMEXX

HOMMEXX Design Overview

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- Incremental conversion of algorithms from FORTRAN to C++
- Maintained bit-for-bit compatibility (even on GPU!)
- Heavily unit tested, $\sim 85\%$ of kernels individually verified
- Abstracted most architecture dependent code
- First converted RK stages and spherical operators; used to evaluate design choices such as data structures
- Primary performance goals: Expose Parallelism, Minimize Memory Movement, Expose Vectorization
- In addition, minimize code specific to different architectures, and use C++11 in the design

HOMMEXX Design - Expose Parallelism

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4 levels of parallelism in HOMME: Elements, Variables/Tracers, Vertical Levels, GLL Points.
Expose parallelism by mapping these to hierarchical parallelism

- Kokkos' hierarchical parallelism only supports 3 levels... Solve by treating elements and variables as one level
- Naturally maps to spherical operators and other interior parallel regions

HOMMEXX Design - Vectorization

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Explicit Vectorization used on CPU

- Abstracted data type `double` as a packed `vector` type
- GPUs use SIMT rather than SIMD, so packs are size 1
- CPU vector size varies, KNL, Skylake size 8, Haswell size 4
- Alternative: pack data and surround loops with `#pragma simd`
  - C++ compilers don't generally vectorize well [10]
  - Explicit vectorization provides a $\sim 15\%$ boost over this method
  - C++ has a proposal for explicit vectorization support [2]

HOMMEXX Design - Data Layout

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Three priorities

- Enable vectorization
- Reduce required buffers
- Match fast indices with loop order

Two simple non-tiling solutions: make GLL point indices fast, or vertical level indices fast. Each choice has trade-offs:

- Vectorization in (common) spherical operators vs Vectorization in vertical integrals (rare)
- Kokkos' hierarchical parallelism has a parallel scan implementation for fast indices, not for slower ones
- Matching the number of vertical levels with vector sizes is feasible, matching the number of points is more difficult

HOMMEXX Design - Modern C++11

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- Template metaprogramming enabled static polymorphism.
  Can reduce low level `if` statements
  Can reduce register pressure on GPUs, improving functionality without performance costs
- Pointer to Implementation to reduce compilation times, esp for static polymorphism.
- Memory ownership semantics prevent memory leaks.

Architectures

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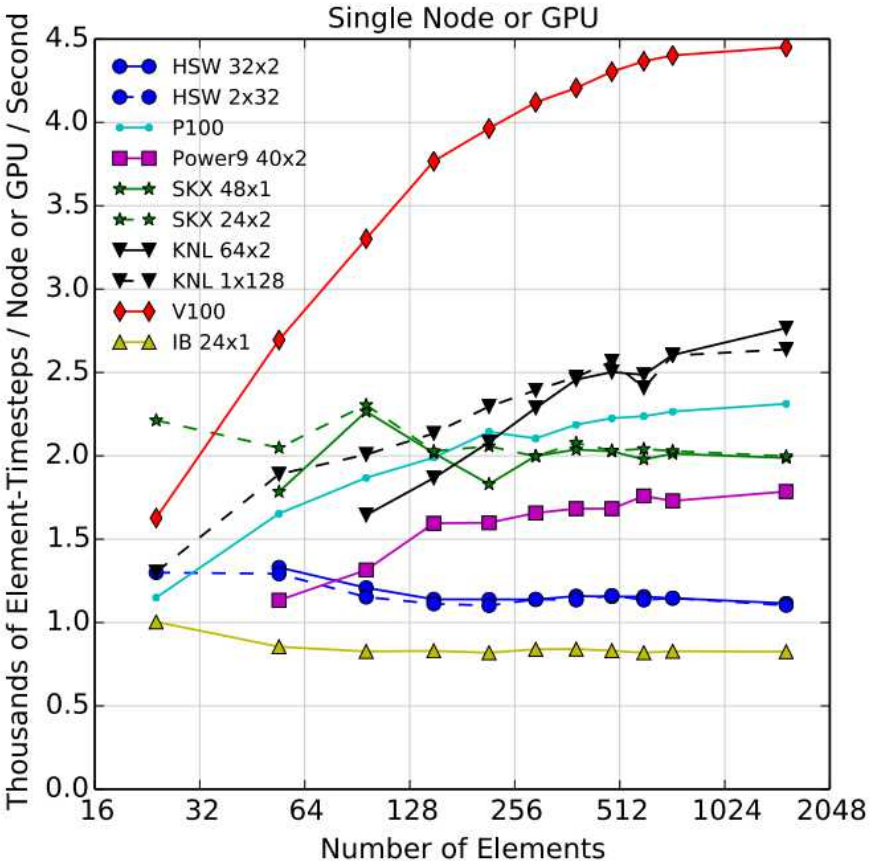
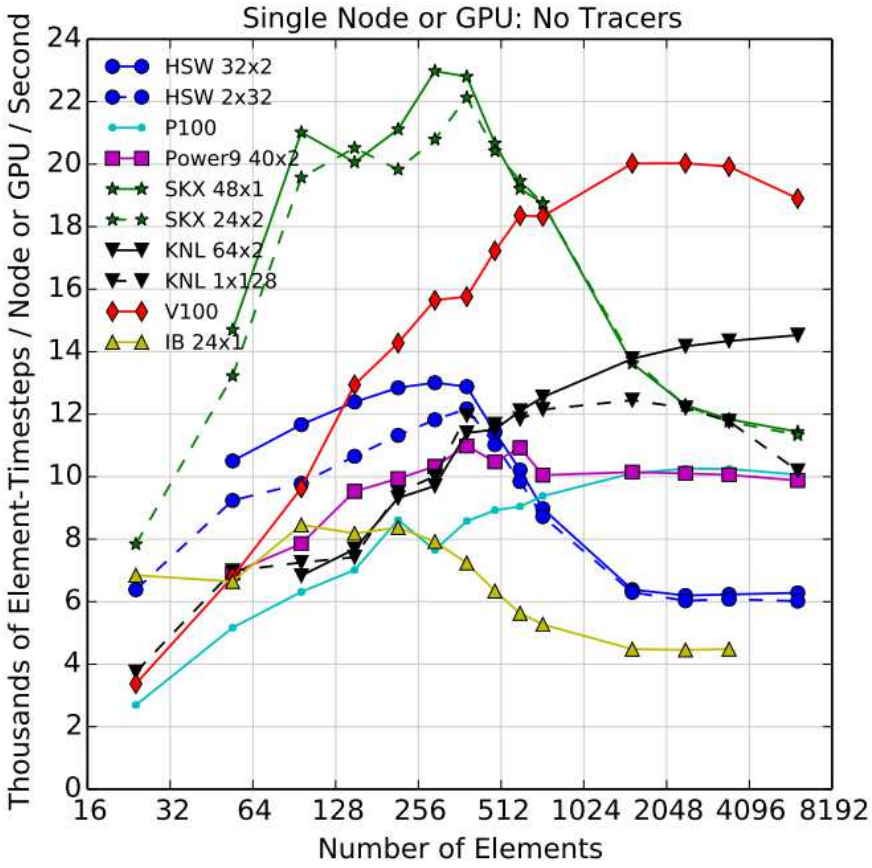
Compared performance of CPU to HOMME on several machines, and examined GPU performance.
Architectures tested:

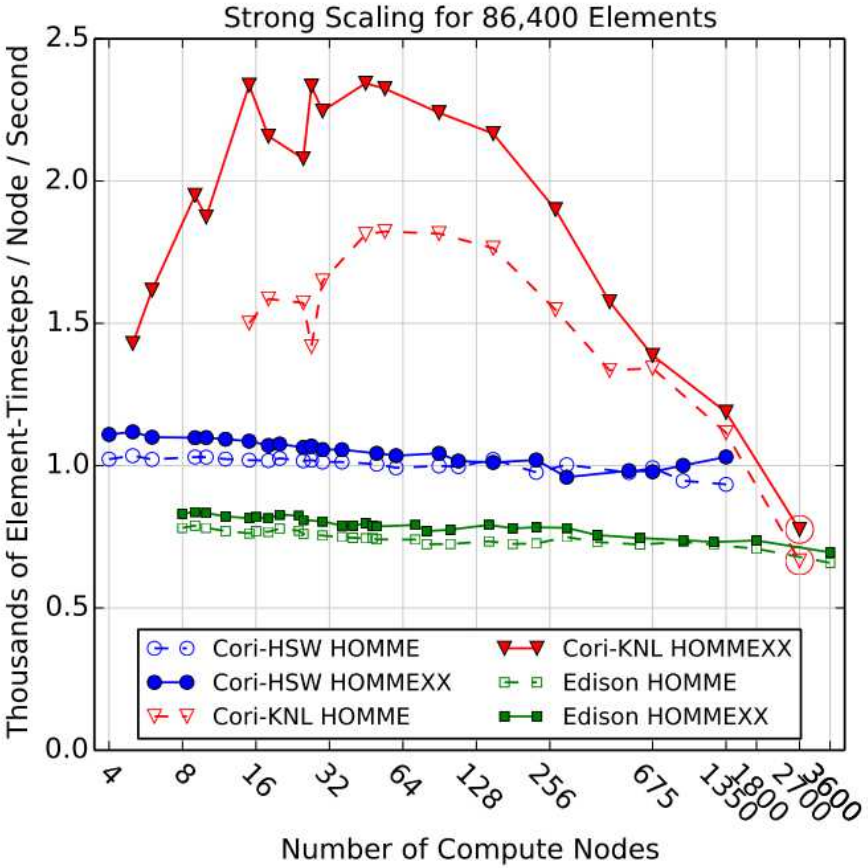
- Edison (IB): 2 sockets, 12 cores, 2 threads, Ivy Bridge, DDR3
- Cori Haswell (HSW): 2 sockets, 16 cores, 32 threads, Haswell, DDR4
- Cori KNL (KNL): 68 cores, 272 threads, Xeon Phi Knights Landing, MCDRAM
- Skylake (SKX): 2 sockets, 24 cores, 2 threads, DDR4
- GPU Testbed (V100, Power 9): 2 POWER9 CPUs, 10 cores, 2 threads, 4 Nvidia V100 GPUs

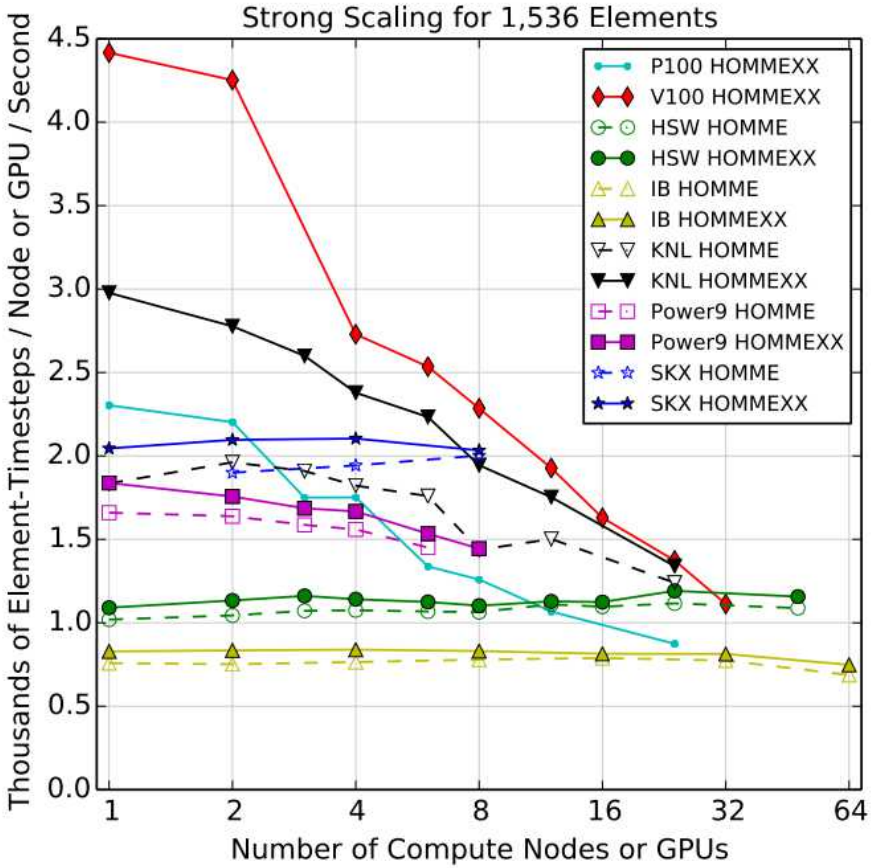
HOMMEXX Performance





HOMMEXX Performance





Conclusions

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- HOMMEXX is performant across multiple architectures
- C++ and Kokkos are a viable combination to achieve performance portability
- Modern C++ designs with template metaprogramming can be performance portable

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