E3SM All Hands: NGD Nonhydrostatic Atmosphere: Performance-Portable Physics Parameterizations

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Outline

1. Machines

2. Methods

3. Mini-app

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Summit

- Summit
  - 4608 IBM Power9 nodes
  - 27,648 16GB Nvidia V100 GPUs
  - 2560 double precision cores/GPU (80 SM $\times$ 32 cores/SM)
  - 32 threads/core
- Nonhydrostatic 3km atmosphere
  - $n_e = 1024$
    - 6,291,456 horizontal elements
    - 56,623,106 columns
  - 128 levels
- Implied minimum parallelism in each column
  - $\sim$2048 columns/GPU
  - Must use $\geq$ 40 threads/column
  - In practice, 2–4 cores controlled by a thread block (Cuda) = team (Kokkos)
  - Must parallelize in each column.
- 1/4-degree model ($n_e = 120$, 72 levels) with 2 (3) cores/column can occupy $\sim$608 ($\sim$973, accounting for unused 2 cores/SM when team size is 3) GPUs.

Outline

Methods: Expose all Parallelism

- C++/Kokkos
- Hierarchical parallelism
- Team per column
- Parallel map (for), reduction, scan within team
- Kokkos tutorial and documentation:
  - `github.com/kokkos/kokkos/tree/master/doc`
  - `github.com/kokkos/kokkos-tutorials`
  - `github.com/kokkos/kokkos/tree/master/example/tutorial`
  - `github.com/kokkos/kokkos-tutorials/tree/master/Intro-Full/Slides`

Methods: Vectorize

Sandia National Laboratories

- Vector processing units (VPU) are important on current CPU/KNL.
- Adding VPUs to an architecture is an efficient means to increase FLOPS and optimize use of available memory bandwidth.
- Thus, I predict VPUs will never go away.
- V100 already supports limited vector intrinsics.

Implementation:

- Fortran auto-vectorizes well if code is written carefully.
- C++ does not.
- But C++ easily supports `Pack` and `Mask` types.
  - Bonus: Vectorization is roughly independent of compiler.
- SCREAM solution:
  - `Pack`: Multiple scalars packed together, respecting memory alignment and vector width.
  - `Mask`: Conditionals (e.g., `if` statements).

Methods: Manage Memory and Temporaries

- Moving data is expensive . . .
- . . . and becomes relatively more expensive with time.
- Must handle
  - Communication between devices
  - Global data on a device
  - Local data
    - Per team
    - Per thread

Temporaries implementation:

- Need reusable workspace shared among threads in a team.
- Minimize global memory footprint.
- SCREAM solution: `WorkspaceManager`.
  - Request and release column-friendly temporary arrays.
  - User-friendly and aggressive performance API options.
    - Start with user-friendly API.
    - When everything works, optimize with aggressive performance API.

Methods: PVM

Conversion strategy:

- Expose all Parallelism.
- Develop Vectorization strategy.
- Develop Memory, temporaries, MPI strategy.

Also:

- Maintain bit-for-bit against reference Fortran with a set of compiler flags and code configuration.
  - Cuda: `-fmad=false`
  - GCC: `-ffp-contract=off`
  - Intel: `-fp-model strict`
- Unit test everything.
  - `catch2`

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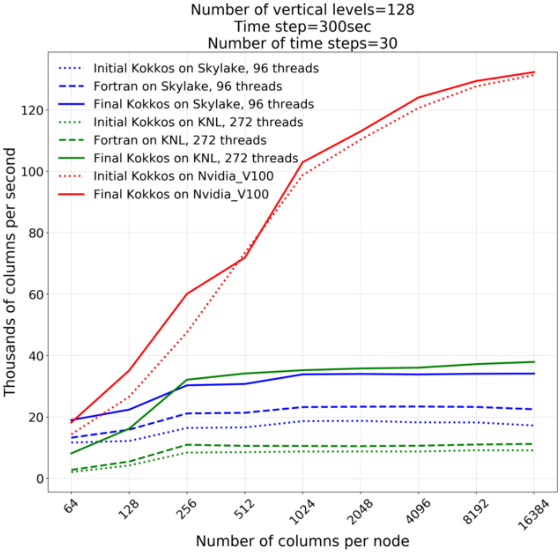
P3 mini-app overview

- To work through PVM for SCREAM, we made a mini-app implementing P3 rain sedimentation.
- Many intermediate versions.
- Final repo `master` has just a few.
- Docs to explain pieces.

P3 mini-app performance



- PVM:
  - Expose all Parallelism
  - Vectorize on Skylake and KNL
  - Memory and temporaries
- Performance and programmer convenience. Roughly,
  - Kokkos provides these for P.
  - Packs provide these for V.
  - Workspace provides these for M.
- Initial (performant) Kokkos: P
  - Also assure that V and M constructs don't decrease performance.
- Final Kokkos: PVM
- Comments:
  - On KNL, mostly V gives Final Kokkos a 2.9–3.4× speedup over the Fortran reference.
  - On SKX, mostly V gives a 1.4–1.5× speedup over the Fortran reference.
  - $n_e = 1024$ on full Summit: $\sim$2048 columns/GPU.

Next steps

SHOC has two algorithmic pieces plus a lot of code that has the same patterns as P3.
These two algorithmic pieces will likely be of use to others:

- Tridiagonal solve
  - Diagonally dominant $\Rightarrow$ no pivoting (great).
  - Two systems, one with 2 RHS, one with 3 + `num_tracer`. (But #RHS still much $<$ than number of threads in team: at most $\sim$43 vs 128.)
  - GPU: Combinations of two cyclic reduction variants and Thomas algorithm (standard elimination): thread across rows and RHS.
  - Non-GPU: Thomas algorithm, ideally with tracers `Pack`ed along `i` (not `k`).
- Linear interpolation
  - Many applications with the same grids $\Rightarrow$
    - Set up, probably $O(n \log n)$ and fully parallel.
    - Application, probably $O(n)$ and fully parallel.