Refactoring the Energy Exascale Earth System Model (E3SM) Super Parameterization for GPUs

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Energy Exascale Earth System Model (E3SM) – Multiscale Modeling Framework

• E3SM
  – Branched as “ACME” from CESM a few years ago
  – Changed names from ACME to E3SM recently
  – Coupling of five main models: Atm, Ocn, Land, Land Ice, Sea Ice
  – Targeted to hi-res DOE climate Grand Challenge questions

• E3SM Multi-Scale Modeling Framework (MMF)
  – Cloud resolving scales (dx=1km) will require about 22,000x more computation
  – MMF is a compromise: each global model column has its own hi-res Cloud Resolving Model (CRM) on a reduced domain
  – Global model nudges dynamical and moist variables in the CRM
  – CRM provided a single column of forcing to the global model
  – CRM retains a persistent internal state from one time step to the next
MMF vs Traditional Simulation

• Advantages
  – Traditional E3SM spends roughly 50% runtime in MPI in production runs
  – Traditional E3SM dynamics spends 90% runtime in latency-dominated MPI
  – CRMs do not communicate directly with one another
  – Thus, >90% of runtime has no MPI
  – Code is only about 30k lines

• Challenges
  – Original code was not well structured for correctness or threading
  – Most subroutines floated around outside modules (no parameter checking)
  – Most data was “use”d, not passed (hard to thread, dependencies unclear)
  – The loop over multiple CRM instances was outside the CRM code
  – SYPD throughput still enforces very little work per node (kernels are very small)
First Order of Business: Clean Up the Code

• Put all subroutines in modules, switch some “use” to parameters to avoid circular module dependency
  – Found several bugs with wrong number / type of parameters passed
• Allocate / deallocate module-level data to get off the stack
  – Some ghost in the machine bugs with PGI were resolved by this
  – Valgrind complained slightly less about the stacksize
• Replace “equivalence” statements with pointers
• F90-ize the borrowed ECMWF FFT routines
• Pass the entire E3SM-MMF code through valgrind
  – It now runs clean
Next: Create Fast, High-Coverage Test Suite

• Finding a bug is much faster if only 10 LOCs change could’ve caused it
• Created two low-res tests to cover all the code we care about
  – Both tests run at 80km grid spacing, 30 vertical levels for one model day
  – Test 1: 1-mom micro, 3-D CRM
  – Test 2: 2-mom micro, active aerosols, 2-D CRM
  – Compiling with GNU, total test time of 10 minutes on my desktop
• Create two baseline files per test
  – O0 and O3 to get the feel for how bit-level changes propagate over a model day
  – Then, compare refactored file against the diff between O0 and O3
Next: Push Loop Across CRMs Down the Callstack

• Requires redimensioning all module and high-level subroutine data to include another dimension ("ncrms")

• Chose to make ncrms the slowest-varying dimension
  – Makes performance impact on CPU minima
  – Makes certain sub-cycling easier to handle

• Changed 20K LOC in a single GitHub Pull Request
  – Passed bit-for-bit checks in the E3SM test system
  – We managed to stay off of the “gitlost” Twitter feed
Next: Find a Way to Unify OpenACC and OpenMP

- We cannot continue to be exposed to a single compiler’s bugs
- An OpenACC / OpenMP solution enables PGI, XL, Cray, and GNU*
- I’m not good with parsing or writing pseudo-compilers
  - So, we opted for a relatively simple solution using the CPP
- OpenMP 4.5 and OpenACC’s “parallel loop” share much in common
  - Ad hoc unified directive from the intersection of OpenMP 4.5 and OpenACC
- Requires variadic macro functions in CPP but nothing else
  - PGI anc XL support full CPP in .F* files; GNU doesn’t yet; Intel says “never!”
- Requires you to explicitly mention data flow in each kernel
  - This is tedious but useful for robustness
  - You don’t always know your routine will be called with data already on the GPU
### Mapping between OpenACC and OpenMP 4.5

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*Asynchronous behavior is very different*
Mapping between OpenACC and OpenMP 4.5

**OpenACC**
- !$acc parallel loop
- gang (Loop across GPU's SMs)
- worker (Outer loop within SMs)
- vector (Inner loop within SMs)
- copyin(), copyout(), copy()
- !$acc data, !$acc end data
- !$acc enter data, !$acc exit data
- create(), delete()
- !$acc update host(), !$acc update device()
- async(id), wait(id) *

**OpenMP 4.5**
- !$omp target teams
- distribute
- parallel do
- simd
- map(to:), map(from:), map(tofrom:)
- !$omp target data, !$omp end target data
- !$omp target enter data, !$omp target exit data
- map(alloc:), map(release:)
- !$omp target update to()
  !$omp target update from()
- nowait, taskwait *

*Asynchronous behavior is very different*
Differences b/t OpenMP 4.5 & OpenACC async Engines

- Likely the biggest difference between OpenMP 4.5 and OpenACC
- OpenACC mirrors the simplistic CUDA “stream” ideology
  - Everything is synchronized within streams, independent between streams
- OpenMP is more cumbersome, yet more capable
  - All asynchronous data and kernel clauses coordinate with “depend()” clauses
  - An op with depend(in:var) must wait for the previous op’s depend(out:var)
  - Theoretically, OpenMP compilers create GPU streams under the hood based on your explicitly given dependencies
- Since we decided to mention data per-kernel, our CPP-generated directives can use this info to create appropriate dependencies
- However, we must have separate data clauses between kernels and data statements (they have different dependencies)
Kernel Approaches for GPU porting

• Parallel dimensions
  – crm_nx, crm_ny, crm_nz (x,y,z dimensions of CRM)
  – ncrms (Number of CRM instances per compute node)

• In general, tightly nest and collapse all data-parallel loops
  – We don’t know a priori what nx, ny, nz, and ncrms will be
  – Collapsing gives the most flexible performance across configurations

• Use “atomic” for race conditions (mostly in the vertical dimension)
  – Atomic used to perform awfully on K20x, no hardware double precision atomics
  – But Volta does very well with them
  – Prefix / cumulative sum must still be isolated and extracted into its own loop

• Push intermittent if-statements down the loop stack to allow collapsing
  – This typically ruins vectorization on the CPU
Data and Asynchronous Approaches for GPU porting

• Allocate and deallocate data on the GPU in each routine
  – You can’t guarantee each CRM call will have the same “ncrms”

• Use “nested” data statements with the “present or” logic in Open*
  – All data statements have an implied “do this unless it’s present”
  – If the data is allocated, nothing happens, so you don’t have performance penalty

• Use asynchronous execution liberally
  – NOTE: This is not to overlap CPU and GPU computation
  – This is only to hide two things: (1) Kernel launch latencies; (2) cudaMalloc[Host]

• We have very small workloads in realistic simulations; high latencies
  – By launching asynchronously, we don’t see most of this latency

• Asynchronous launching makes correctness more difficult to maintain
Miscellaneous Stuff

• Managed memory performs poorly for small kernels with PGI
  – Allocations are excessively expensive, pool allocator is not performant
  – Gaps between kernels increase by 5-10x with Managed memory turned on

• XL currently cannot pin memory by default (poor CPU-GPU bandwidth)
  – You currently have to use the CUDA FORTRAN “pinned” attribute
  – They’re working on a compiler flag to fix this

• With all-asynchronous execution, cudaMalloc[Host] costs are hidden

• Currently redoing HOMME tracers/dynamics port with unified directives

• Going to complete RRTMGP radiation port in unified directives
  – RRTMGP is already ported to the E3SM-MMF code under ECP
Obligatory Performance Slide

- Previous OpenACC port gave expected GPU bandwidth improvement
  - IF we have enough work per GPU
  - We’ve since cleaned the code and are currently diversifying compiler support

- However, we do not have enough work per node in hi-res climate
  - In realistic simulations, we only got about 4x improvement on Summit
  - Since MPI isn’t involved, this is solely due to small workload issues
Current and Future Challenges for Climate Modeling

• Our 2,000x throughput requirement is starving hardware for work
  – Each 2x horizontal refinement needs 8x more work (time step reduction)
  – But we only have 4x more data to work on
  – Thus, workload per node cuts in half for each 2x refinement
  – Eventually MPI message time dominates, and accelerators starve for work

• We really need to consider creative ways to improve realism without reducing per-node workloads
  – MMF is helpful to overcome the MPI problem but doesn’t solve workload problem
  – Traditional numerics improvements can give 2-10x help but nothing fundamental
  – Deep Learning surrogate models and physics-based parameterizations may have a positive impact on intelligent dimensionality reduction
  – Simplified physics that directly target regional cloud-resolving grids
  – Direct ensemble-based approaches that relax the throughput requirement