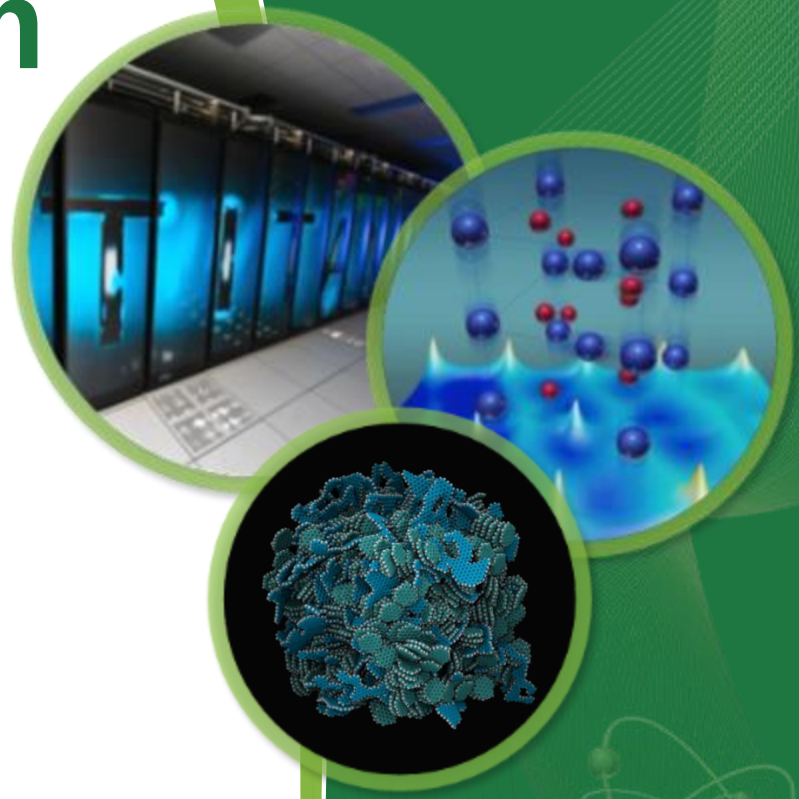
Refactoring the Energy Exascale Earth System Model (E3SM) Super Parameterization for GPUs



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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 Taditional 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 aovid 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

OpenACC	OpenMP 4.5
!$acc parallel loop	!$omp target teams
gang (Loop across GPU's SMs)	distribute
worker (Outer loop within SMs)	parallel do
vector (Inner loop within SMs)	simd
copyin(), copyout(), copy()	map(to:), map(from:), map(tofrom:)
!$acc data, !$acc end data	!$omp target data, !$omp end target data
!$acc enter data, !$acc exit data	!$omp target enter data, !$omp target exit data
create(), delete()	map(alloc:), map(release:)
!$acc update host(), !$acc update device()	!$omp target update to() !$omp target update from()
async(id), wait(id) *	nowait, taskwait *

*Asynchronous behavior is very different

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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 wih 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 asycnhronously, we don't see most of this latency
- Asynchronous launching makes correctness more difficult to maintain

Miscillaneous 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