Incorporating GPUs into Earth System Science

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BER E3SM Nonhydrostatic Atmosphere NGD
ASCR E3SM-MMF Exascale Computing Project
BER E3SM Performance Group
BER CMDV-SM project

Advanced Scientific Computing Advisory Committee
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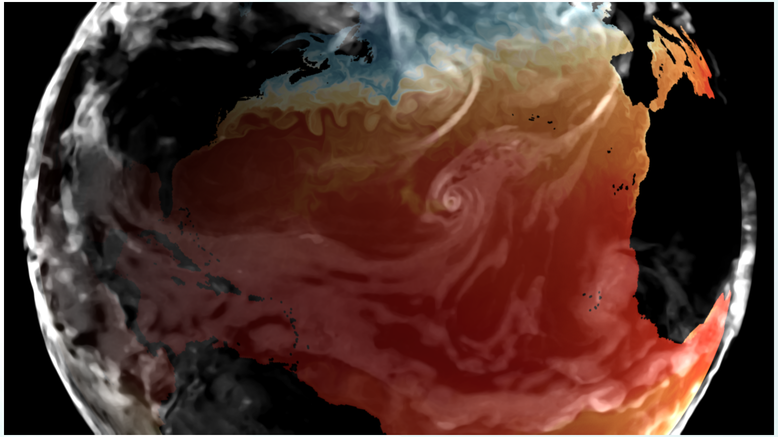
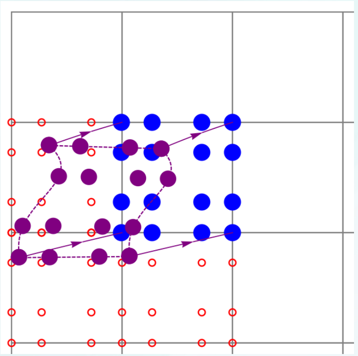
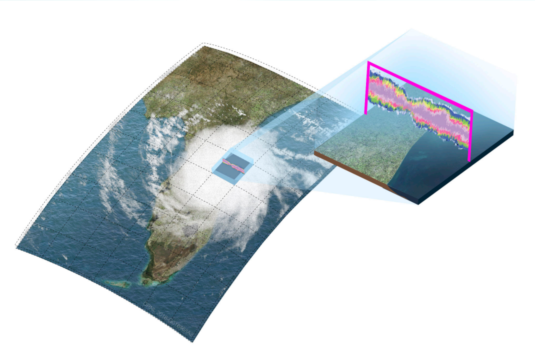
Earth System Modeling in DOE







- **BER: E3SM Project**
- ~70 FTEs, 8 labs + Universities
- **E**nergy **E**xascale **E**arth **S**ystem **M**odel
- DOE-SC science mission: Energy & water issues looking out 40 years
- Ensure E3SM will run well on upcoming DOE exascale computers

- **ASCR/BER SciDAC**
- ~10 FTEs over multiple projects
- Large focus on new algorithms

- **ASCR ECP Project**
- ~10 FTEs
- E3SM-MMF: ”superparameterization”

Three overarching science drivers

U.S. energy sector is vulnerable to:

- Decreasing water availability
- More intense storm events and flooding
- Increasing temperatures
- Sea level rise

- **Water cycle:** How does the hydrological cycle interact with the rest of the human-Earth system on local to global scales to determine water availability and water cycle extremes?
- **Biogeochemistry:** How does the biogeochemical cycle interact with other Earth system components to influence energy-sector decisions?
- **Cryosphere systems:** How do rapid changes in cryospheric systems evolve with the Earth system and contribute to sea level rise and increased coastal vulnerability?

Challenge: water cycle, biogeochemistry, and cryosphere systems interactions cannot be ignored for predictions or projections at longer time scales

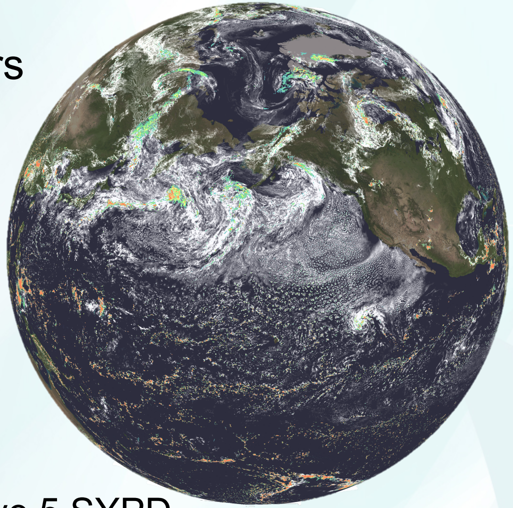
E3SM Exascale strategy: Running on GPUs

- All new DOE SC machines will be GPU based
- NERSC Perlmutter
- OLCF Frontier (and Summit)
- ALCF Aurora

Key Points for Earth System Models

- CPU performance (per watt) has nearly stagnated
  - 2x speedup over the last 6 years
- GPUs: 3x speedup (per watt) over today's CPUs
  - But only in the high-workload regime
  - Need major code rewrite or refactor
- Traditional climate simulation campaigns are run in the low-workload regime
- E3SM: Focus on several new types of simulation campaigns where GPUs will allow us to run simulations not possible on CPU systems

High Workload Simulations for GPUs



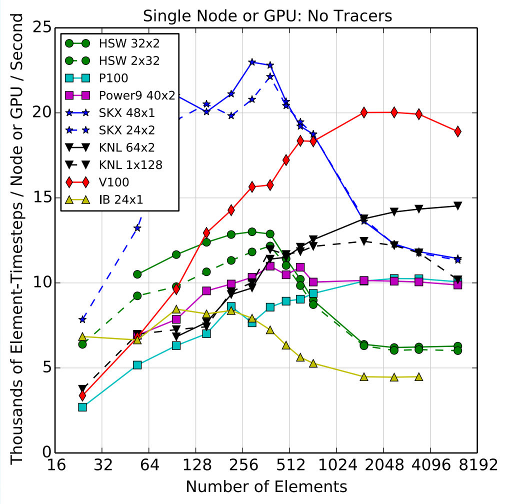
- Earth System Model running at 5 SYPD for ~300 simulated years
  - A $5M commodity CPU cluster is most efficient
- **Ultra high resolution “Cloud Resolving” model**
  - BER: E3SM’s ”SCREAM” project
  - On track for E3SM V3 (2021-2022)
  - Typical INCITE award: 10-30 simulated year
- **Increase “local” complexity**
  - ECP: E3SM-MMF project: “superparameterization”
  - Achieve many aspects of a cloud resolving simulation and also achieve 5 SYPD
  - Running on Summit since OLCF Early Access Program
- **Large Ensembles**
  - Each ensemble member is running slower but more efficiently on GPU systems.
  - E3SM V4 capability: large ensembles on GPU systems

Performance & Portability Strategy

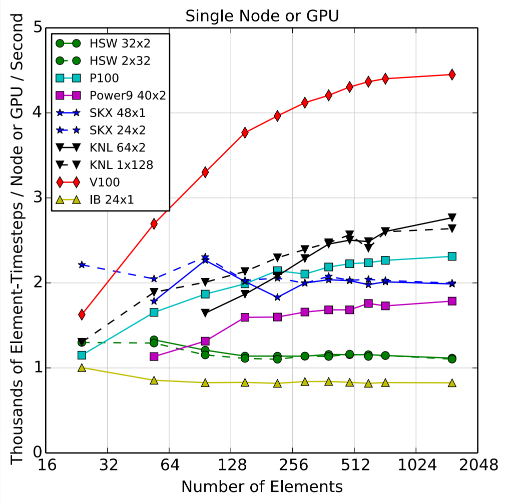
- Large investments in two approaches:
  - Fortran + OpenMP
  - C++ / Kokkos
- Both strategies require complete code refactor or rewrite, with careful coding to obtain competitive performance
- We are taking this opportunity to: replace legacy code, improve testing, software engineering and verification
- Takes several years per major component. Not simple code porting – requires computational science research along the way.

Detailed single node comparisons

- Atmosphere dynamical core with and without tracers (~1/2 the atmosphere mode)
- Shows slow improvement in CPUs going back to 2012
- Gives upper bound on possible performance: doesn't include. MPI and other overheads
- Dynamical core only: minimal benefit from GPUs
- Dynamical core + tracers: Large benefit from GPU, but only in high work load regime.
- Hope to soon add newer CPUs (Epyc, Fugaku ARM) and new GPUs



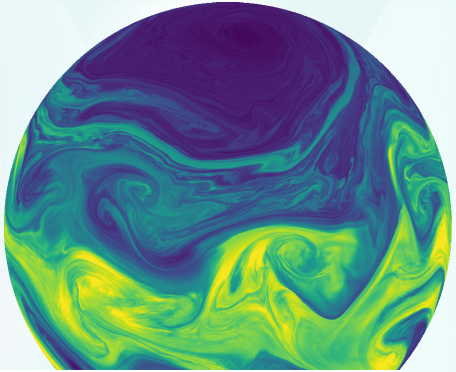
Atmosphere dynamical core



Atmosphere dynamical core with 40 tracers

Bertagna et al., *HOMMEXX 1.0: A Performance Portable Atmospheric Dynamical Core for the Energy Exascale Earth System Model*, GMD 2019

NGGPS cloud resolving (3km) benchmark
Scaling to all of Summit



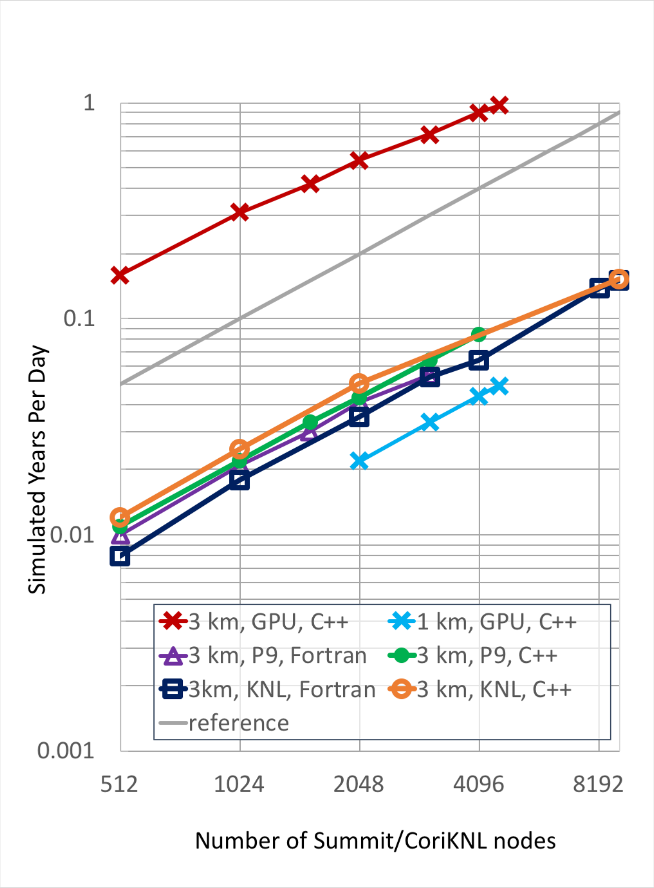
- Standardized benchmark from the National Weather Service
- Atmosphere model with realistic configuration and idealized physics
- Highlights from several generation of computers and Global clould resolving models (GRCMs)
- Double precision results (reported real*4 results ~1.6x faster)
- Results inline with Linpack/HPGC comparison

GCRM Model	Computer (Linpack rating)	NGGPS 3km Benchmark
NOAA FV3	Edison (2.6PF)	0.16 SYPD
HOMME (CESM)	TaihuLight (125 PF)	0.34 SYPD
E3SM's HOMMEXX_NH	Summit (200 PF)	0.97 SYPD

L. Bertagna et. al., SC '20: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, 2020

NGGPS 3km Benchmark: Strong scaling (per node)

- C++/kokkos and Fortran codes competitive IBM P9
- C++/kokkos code has hand-vectorized every loop, leading to excellent KNL performance.
- Summit node with 6 V100s obtains ~ 12x speedup (for ~6x more power?)
- 1km resolution also running well, but throughput is impractically low



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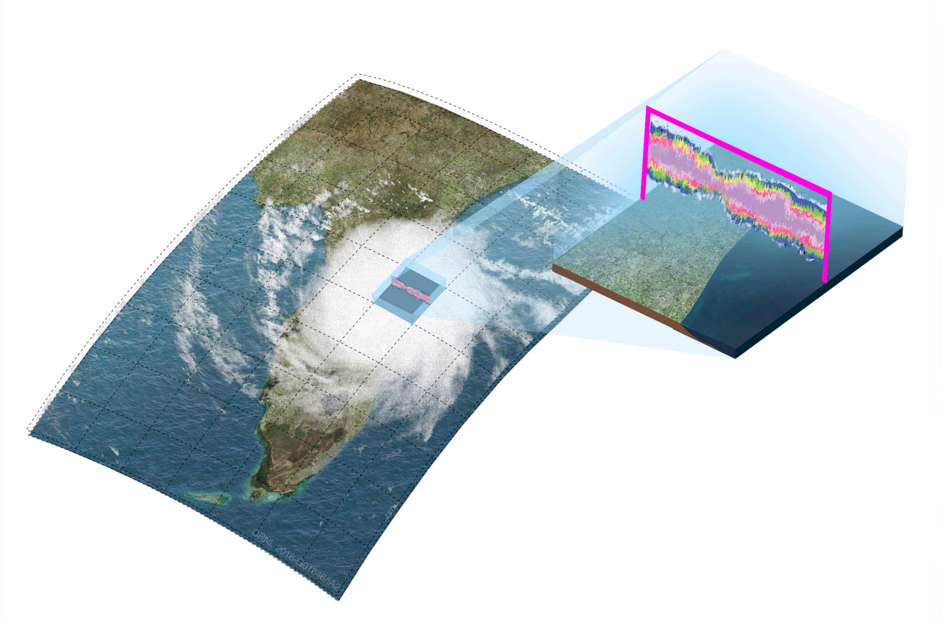
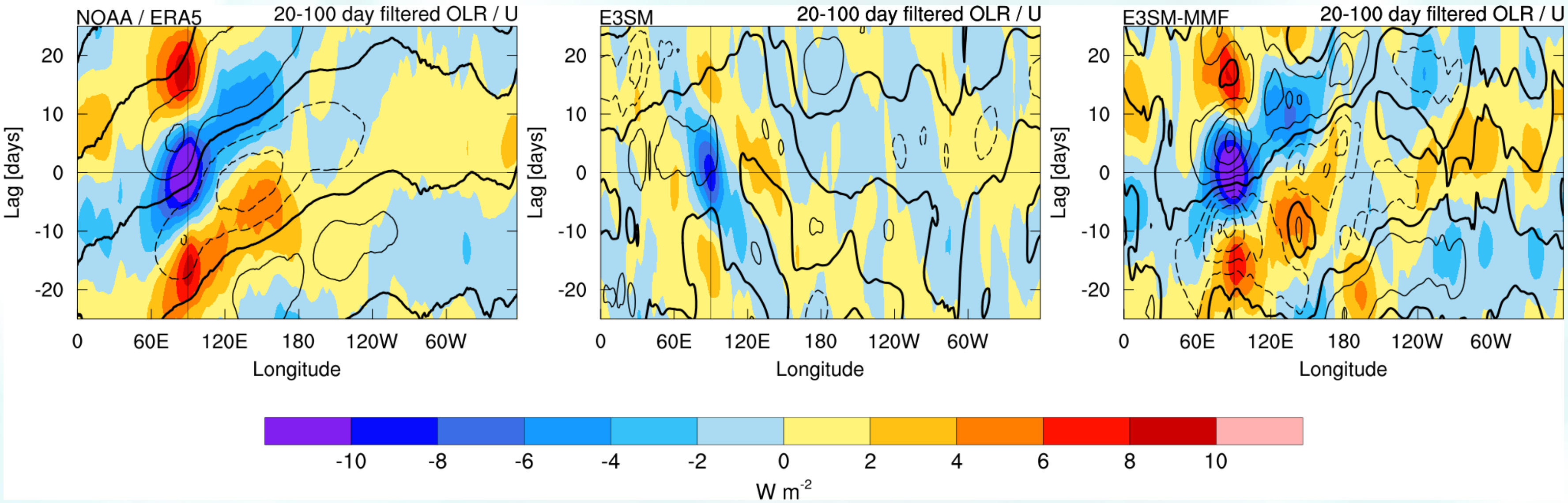
ECP Project: E3SM-MMF

- E3SM-MMF approach addresses structural uncertainty in cloud processes by replacing traditional parameterizations with cloud resolving “**superparameterization**” within each grid cell of global climate model
- Super-parameterization dramatically increases arithmetic intensity, making the MMF approach ideal for GPU acceleration.
- Exascale + MMF approach will make it possible for the first time to perform climate simulation campaigns with *some aspects* of cloud resolving resolutions.



ECP Project: E3SM-MMF



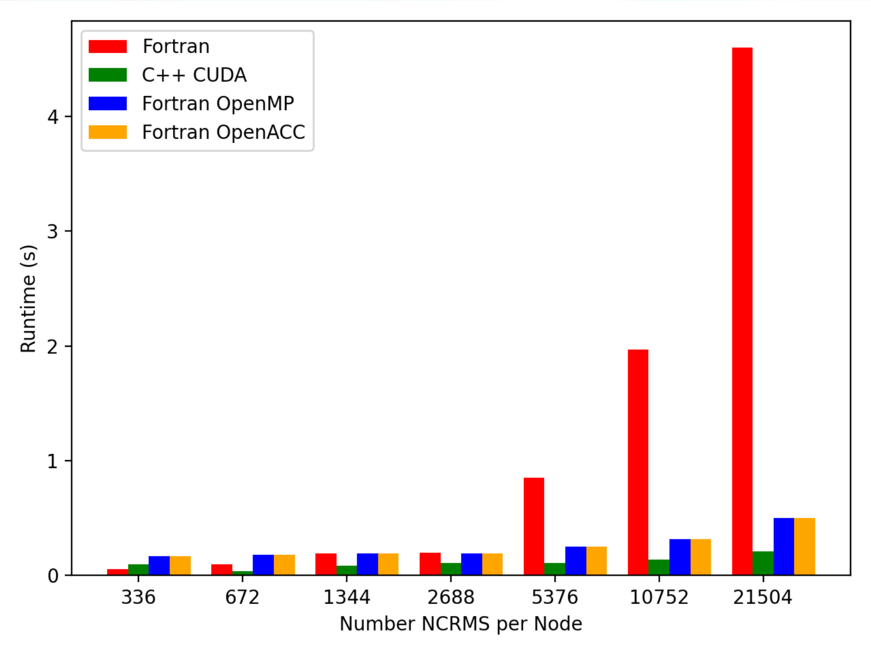
Cloud resolving resolution improves many aspects of our models, such as the Madden-Julian Oscillation, the dominant mode of sub-seasonal variability in the Tropics. Filtered outgoing longwave radiation and 850 mb zonal wind characterize the MJO eastward movement in time.

Compared to observations (left), E3SM-MMF (right) captures much of this eastward propagation, significantly better than the traditional resolution E3SM model (middle)

Analysis: W. Hannah (LLNL)

E3SM-MMF

- In the MMF, performance is dominated by the superparamertization, a 2D “CRM”
- Porting just the CRM to GPUs is sufficient to make effective use of GPU systems
- Performance of the CRM shows similar trends as before: in high workload regime (many CRMs per GPU), GPUs significantly outperform CPUs
- Fortran/OpenMP good but not competitive with C++ due to compiler maturity.



Closing thoughts

- CPU systems are getting better (Fugaku)
- GPU systems are getting better (Frontier, Aurora)
- E3SM V3: Two approaches to cloud resolving simulations made possible by GPU architectures
- E3SM V4 will run efficiently on *both* architectures
  - hopefully well prepared to adapt to post-Exascale hardware

Backup Slides

Summit Full Machine Benchmarks

Consider the E3SM v1 model running on Summit:

- Atmosphere dycore (25km, 40 tracers). GPU acceleration probably not as good for the rest of the model.
- In strong scaling limit, GPU systems cannot outperform CPUs
- If you are willing to run slower, GPUs provide significant advantage (18 nodes):
- E3SM v1 high-res model (projections)
  - 5 SYPD: no GPU benefit
  - 0.5 SYPD: GPUs more efficient
- How will this change in the future?