Progress toward an Earth System Model with Machine Learning Components

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Takeaways

• MPAS-A/GPU is the first operational GPU-accelerated *global weather forecast* model*. 

• We have conducted scaling studies on the MPAS-A/GPU dynamical core with tracers on 700 AC922 nodes on Summit (4200 V100’s!)

• The dycore has achieved 6.5 days/hour at 3 km resolution. This is still slow for climate studies, but close to what’s needed for seasonal forecasts.

• We have experimented with *overlapping calculations on heterogeneous nodes*.

• We’ve run a *machine learning component* in our climate model for nine simulated years with good results.

* MeteoSwiss has been running COSMO, a regional GPU model, in production for quite some time.
Global High-Resolution Atmospheric Forecasting System (GRAF)

Partnership between NCAR, IBM and the Weather Company
- NCAR’s MPAS-A global weather model capable of regional refinement
- Untapped data sources
- GPU-based MPAS forecast model

This talk will present details of the GPU acceleration of the MPAS-A model....
...and provide thoughts about building an Exascale Earth System Model
Simulation of 2012 Tropical Cyclones at 4 km resolution
– Courtesy of Falko Judt, NCAR
MPAS-A: the Algorithm

- Fully compressible non-hydrostatic equations written in flux form
- Finite Volume Method on staggered grid
  - The horizontal momentum normal to the cell edge \( u \) is sits at the cell edges.
  - Scalars sit at the cell centers
- Split-Explicit timestepping scheme
  - Time integration 3\textsuperscript{rd} order Runge-Kutta
  - Fast horizontal waves are sub-cycled
MPAS-A: The Grids

MPAS
Unstructured Voronoi (hexagonal) grid
- Good scaling on massively parallel computers
- No pole problems

Local Refinement

Vertical
MPAS
Height-based hybrid smoothed terrain-following vertical coordinate
- Improved numerical accuracy
There are ~350 halo exchanges / timestep!

Default time integration

Call physics

Do dynamics_split_steps
Do step_rk3 = 1, 3
compute large-time-step tendency
Do acoustic_steps
update u
update rho, theta and w
End acoustic_steps
End rk3 step
End dynamics_split_steps

Do scalar step_rk3 = 1, 3
scalar RK3 transport
End scalar rk3 step

Call microphysics

Allows for smaller dynamics timesteps relative to scalar transport timestep and main physics timestep.

We can use any FV scheme here (we are not tied to RK3)
Scalar transport and physics are the expensive pieces in most applications.
WEAK and STRONG Scaling of MPAS-A moist dynamical core on *Summit* and STRONG scaling on *Cheyenne* (dual, Intel 18c v4 Xeon)

**Weak Scaling MPAS-A Moist Dynamics:**
(SP, 56 levels)

**Strong Scaling MPAS-A Moist Dynamics:**
(56 levels, SP) at 3, 5 & 10 km

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1. Benchmarking on Summit supported by DoE via an OLCF Director’s Discretionary Allocation
2. Cheyenne is a 5.4 PF, 4032-node HPE system with EDR interconnect operated by NCAR
MPAS-A/GPU moist dycore scaling efficiency (Summit)
Current Design: Heterogeneous, Task-Parallel

Come see our in-situ vis demo in booth 401 (NCAR Booth)

EXASCALE NODE
- GPU-ranks
- CPU-ranks
- Linked-ranks

LAND SURFACE RADIATION
- Shown:
  - 4 GPUs/node
  - 5 ranks/GPU
  - 20 ranks for LS & RT

ON-LINE VIZ

ON-LINE ANALYSIS

Output

NetCDF
Full Physics MPAS-A on Summit (10 km, 56 levels, SP)

Configuration:
• 6 GPUs
• 40kpts/GPU
• 3 MPI ranks per GPU

Throughput
• 0.234 sec/step
• 3.2 days/hr @ 3 km (uniform)

Caveats
• Results for load-balanced RT
• Still room for improvement!
  • Halo exchanges (22%)
MPAS-A/GPU keys to success: Partnership

• Public-Private Partnership
• Open Source/Single Source
• Workforce development via student engagement

Come see our in-situ vis demo in booth 401 (NCAR)!

Key part of our team: University of Wyoming students and NVIDIA and PGI experts.
MPAS-A/GPU keys to success: *OpenACC*

- Exploiting **task parallelism** by
  - by overlapping CPU/GPU execution

- **Coalescing CUDA kernels** for MPI packs and unpacks in halo exchanges.

- **PCAST** auto-compare feature (PGI) for debugging GPU code.

- **Mixed execution** of OpenACC CPU threading and OpenACC GPU offload:
  - compile GPU files with “ta=tesla” flag;
  - compile CPU files with “ta=multicore” flag;
  - link all files together with “ta=tesla, multicore”
How close is MPAS-A to achieving a practical Cloud Resolving Model (CRM) capability?

\[ N^* = S \times L \times F \times R \]

\( N \) = speedup required
\( S \) = ratio of desired to observed throughput
\( L \) = vertical adjustment (number of levels/56)
\( F \) = floating point precision adjustment (i.e. SP->DP)
\( R \) = resolution adjustment (\( \Delta x/1 \) km)

* A “Drake Equation” for CRM?
How close is MPAS-A to achieving a practical Cloud Resolving Model (CRM) capability?

Goal: 1 simulated year per day in double precision and 100 levels at 1 km, then.

$$\begin{align*}
S &= 4.75 \\
L &= 1.8 \\
R &= 3 \\
F &= 1.5
\end{align*}$$

$$N = S \times L \times R \times F \sim 40x$$

What can we do besides just wait for 40x from HPC architectures?
How can we tackle the throughput gap?
A multi-prong approach...

\[ N = S \times L \times F \times R \]

- Parallelism, Optimization & Faster HW
- Machine Learning, Solvers, etc.
- Low-precision Physics

Various projects around the community are trying to tackle this:
- ESCAPE2
- E3SM
- CLIMA

A “Drake Equation” for CRM?

Credit: NRAO
Exascale Earth System Model Vision: Heterogeneous, Task-Parallel, In Situ, Intelligent

**EXASCALE NODE**
- GPU-based Connector
- CPU-based Connector

**MEDIATOR**
- ATM
- OCN
- ICE

**I/O**
- LAND
- ETC...

**RAW OUTPUT**
- ON-LINE ANALYSIS
- ML

**OUTPUT**
- OFF-LINE ANALYSIS
- ML

**SSD STORAGE**
- NetCDF
- Zarr Store

**DISK STORAGE**
- CPU
- GPU
Replacing cloud for rain processes with NNs

**ML TAU emulator:**
3 classifier networks, 4 regression networks
82,327 weights total
Dense Neural Network Hyperparameters
- 4 layers
- 60 neurons per hidden layer
- 11,761 total weights
- Rectified Linear Unit (ReLU) activation fns

**Bin Scheme (Tel Aviv University (TAU)):**
- Divide particle sizes into bins *(35)*
- Calculate evolution of each bin separately
- Better representation of interactions
- Much more computationally expensive than current bulk schemes used in climate models

Results after 9 simulated years
Offload to GPUs is, perhaps, a good step to getting ready for downstream innovation...
Thanks! Questions

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Cloud to Rain Processes

Cloud water mixing ratio ($q_c$)
Cloud water number concentration ($N_c$)
Rain water mixing ratio ($q_r$)
Rain water number concentration ($N_r$)

Cloud droplets grow into rain droplets through 3 processes:

**Autoconversion:** cloud droplets collide in a chain reaction to form rain drops
\[
\frac{dq_c}{dt} < 0, \quad \frac{dq_r}{dt} > 0
\]
\[
\frac{dN_c}{dt} < 0, \quad \frac{dN_r}{dt} > 0
\]

**Rain Accretion:** rain drops collide with cloud droplets
\[
\frac{dq_c}{dt} < 0, \quad \frac{dq_r}{dt} > 0
\]
\[
\frac{dN_c}{dt} < 0, \quad \frac{dN_r}{dt} = 0
\]

**Self-Collection:** rain drops collide with other raindrops
\[
\frac{dq_c}{dt} = 0, \quad \frac{dq_r}{dt} = 0
\]
\[
\frac{dN_c}{dt} = 0, \quad \frac{dN_r}{dt} < 0
\]

d: rain drop
c: cloud droplet
CCN: cloud condensation nuclei
Microphysics Emulation Recipe

- Run CESM2/CAM6 for two years and obtain instantaneous hourly output
- Filter and subsample data to find grid points with realistic amount of cloud water
- Transform and normalize inputs and outputs
- Train classifier deep neural networks to classify zero and non-zero
- Train regression deep neural networks to predict non-zero values
- Evaluate and interpret neural network predictions.
Extending Microphysics Emulator Work

Even more complex droplet process models exist – e.g. Superdroplet (right)

Such detailed codes (right) are ridiculously expensive for large scale models, so ML may be the only path forward.

Other complex interaction networks exist in Earth system models, including:
- Chemical reaction networks
- Ecological networks

Can lessons learned with droplet formation models be applied more broadly?

Superdroplet model output animation
Credit: Daniel Rothenberg