Accelerating wind energy simulations by reducing communication costs

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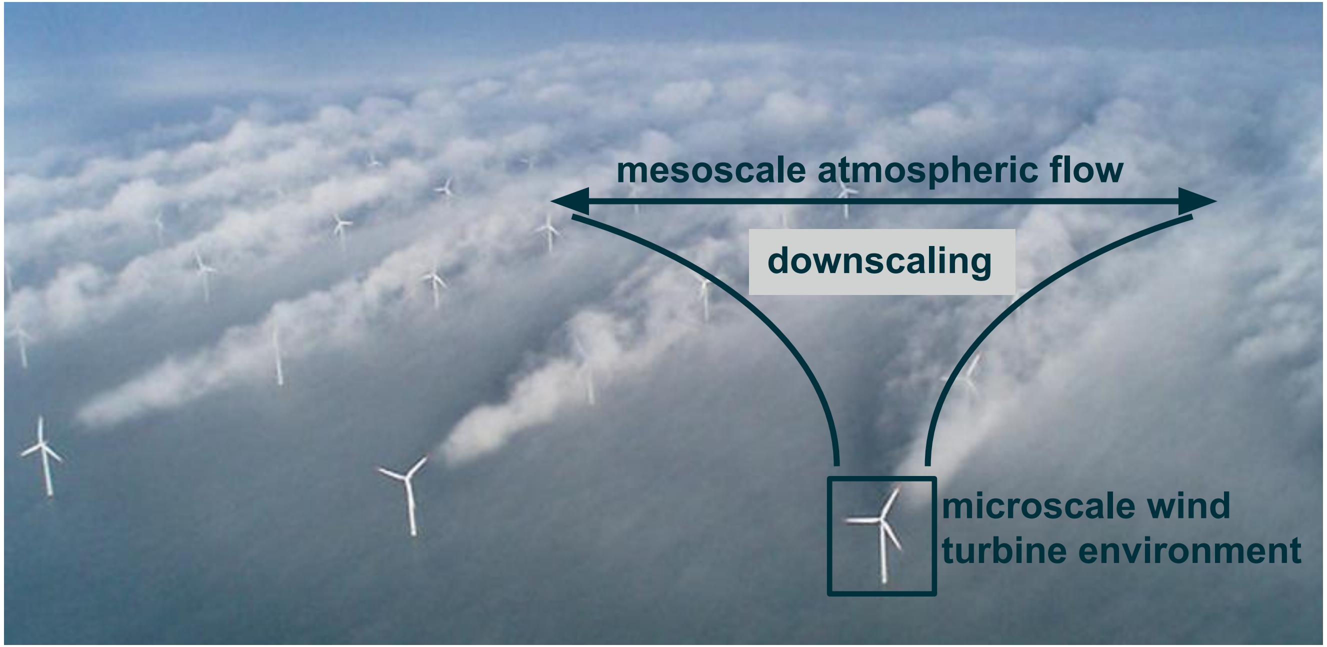
Wind farm simulations need atmospheric data as initial and boundary conditions

https://www.climate.gov/news-features/featured-images/wind-turbines-churn-air-over-north-sea

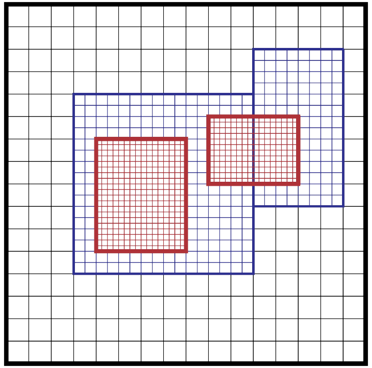


The physics important for the turbines have to be captured correctly in the atmospheric models while factoring in terrain/offshore conditions.

ERF code bridges the scale gap, based on the AMReX framework

Energy Research and Forecasting (ERF)

- is a modern C++ based, GPU-enabled alternative to the
    Weather Research and Forecasting (WRF) model.
- prioritizes accurate prediction of low-level winds.
- provides models for offshore and complex terrain environments.



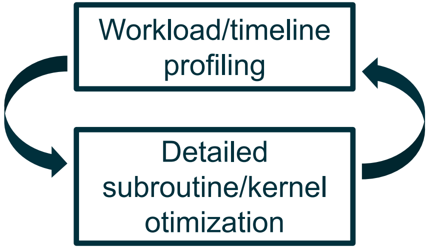
The **AMReX** framework provides

- block-structured adaptive mesh refinement.
- advanced data structures and memory management.
- interface for parallelism over CPUs and GPUs with efficient data transfer and load balancing.

How can we run the simulations faster?

- Profiling to find bottleneck ↔ detailed optimization.

  What if communication cost >> computational bottleneck?



- Systemic changes to data structures or memory management.
- Determining optimal run time settings: number of procs, affinity…

Run time settings or systemic changes can provide a significant boost when communication costs become the main bottleneck.

Reducing communication costs: a preview

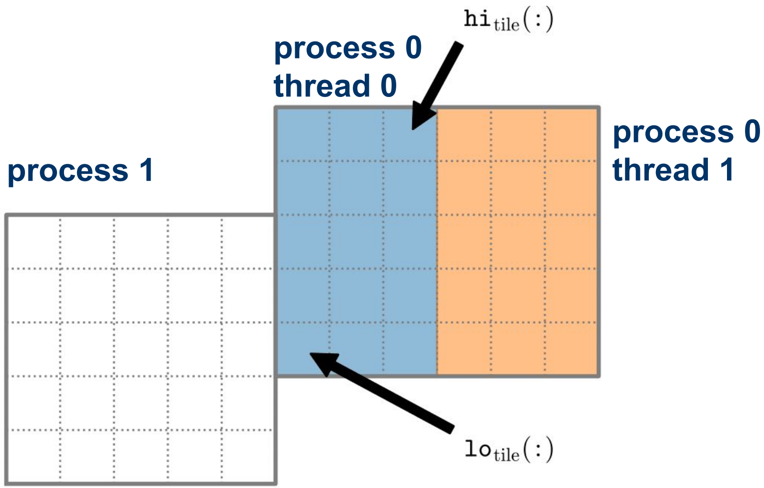
- OpenMP reduces communication cost within a node.
- GPU-aware MPI reduces communication cost between GPUs.
- A separate memory pool for communication buffers improves performance.

Directed and guided by:
Ann Almgren, Don Willcox, Weiqun Zhang, Aaron Lattanzi
Center for Computational Sciences and Engineering (CCSE), AMCR Division, Berkeley Lab

AMReX employs OpenMP multithreading to reduce intra-node communication costs

`MPI+X` strategy for parallelism

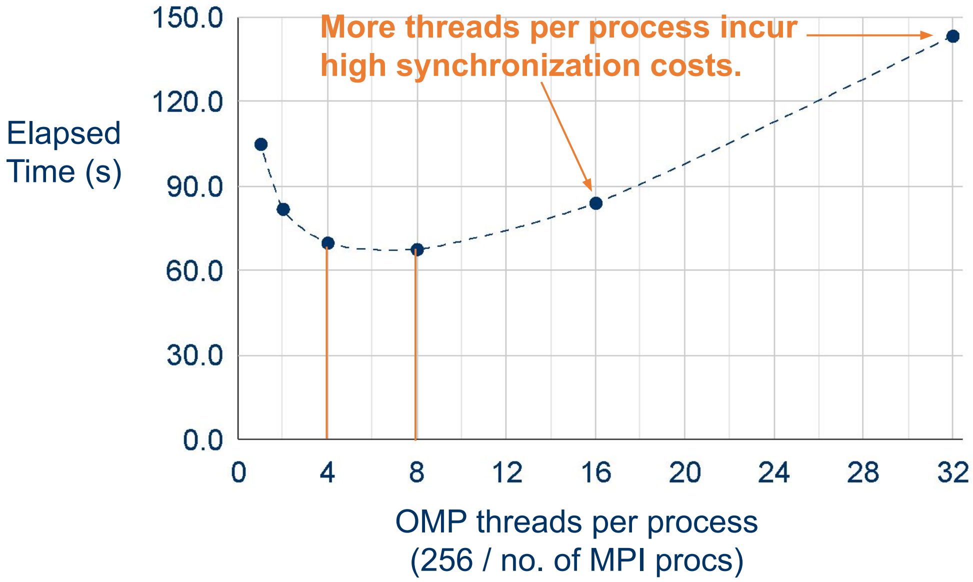
- Message passing interface (MPI) explicitly transfers data among distributed processes that provide coarse-grained parallelism over **grids**.
- `X = OpenMP` implements multiple threads on CPUs/cores within a node that compute **tiles** in parallel.
- Multiple threads can access the same memory space on a node (shared memory parallelism).



Running with 4-8 threads per process provides up to a 33% reduction in wall time

Atmospheric boundary layer (ABL) simulations

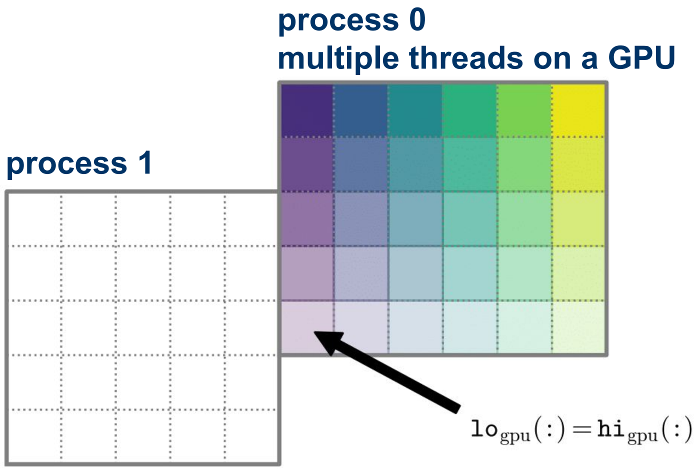
- 100 time steps, I/O and diagnostic calculations are turned off.
- Tested over **2 nodes (256 physical cores)** on NERSC's Perlmutter system. The problem size and number of cores are kept constant while varying the balance of MPI processes and OMP threads per process.



GPUs provide a 30x speed up for ERF by running thousands of threads in parallel

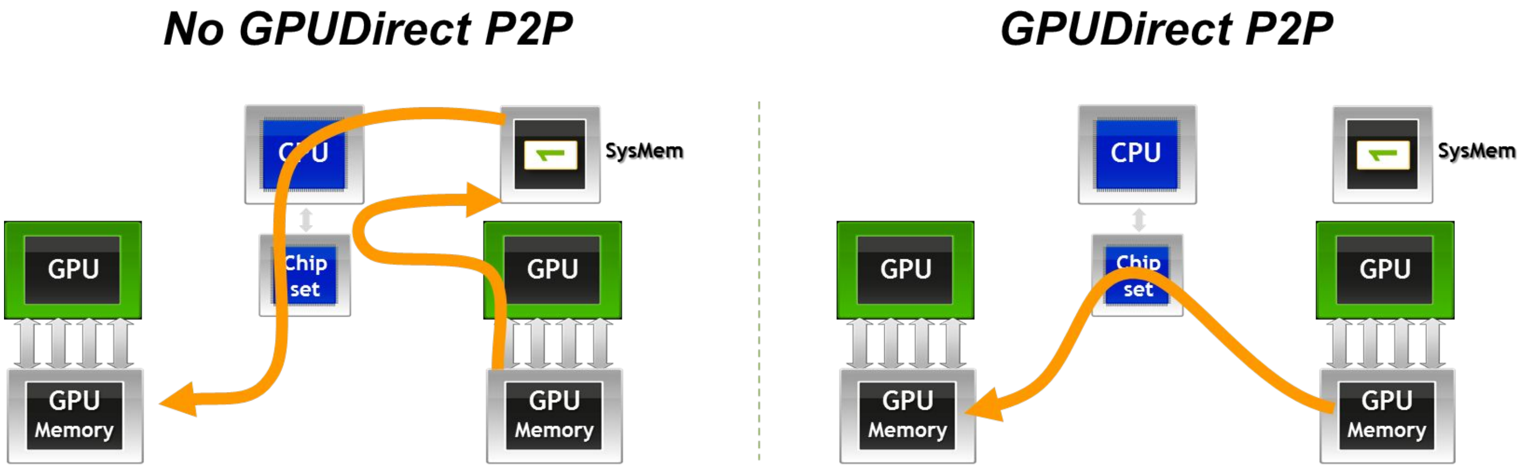
`MPI+X` strategy for parallelism

- `X = CUDA/HIP/SYCL` for GPUs based on the vendor.
- Each MPI process on a CPU “host” assigns work to a single GPU.



GPU-aware MPI can transfer data directly between GPUs, bypassing the host

This requires setting a specific process-GPU-NIC affinity.

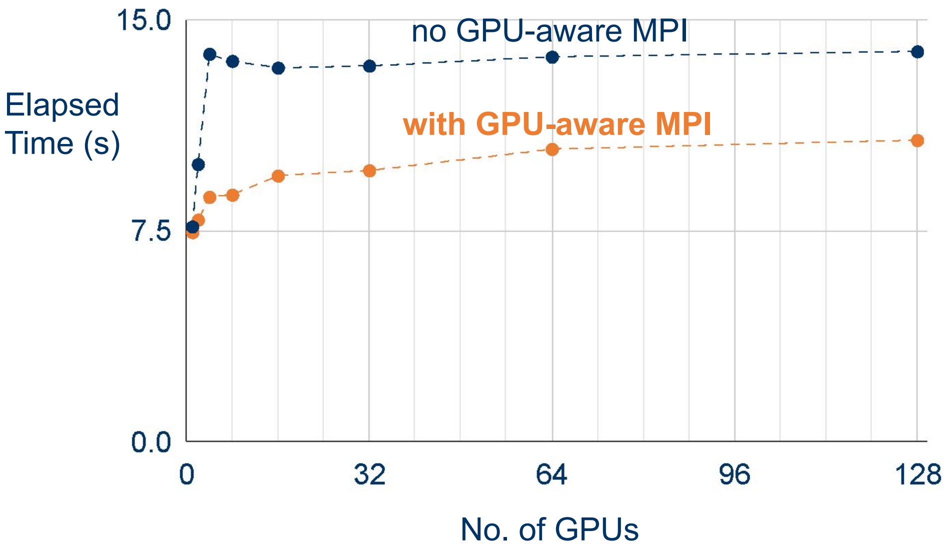


https://developer.nvidia.com/blog/introduction-cuda-aware-mpi/

Enabling GPUdirect results in a reduction of more than 20% in the wall times

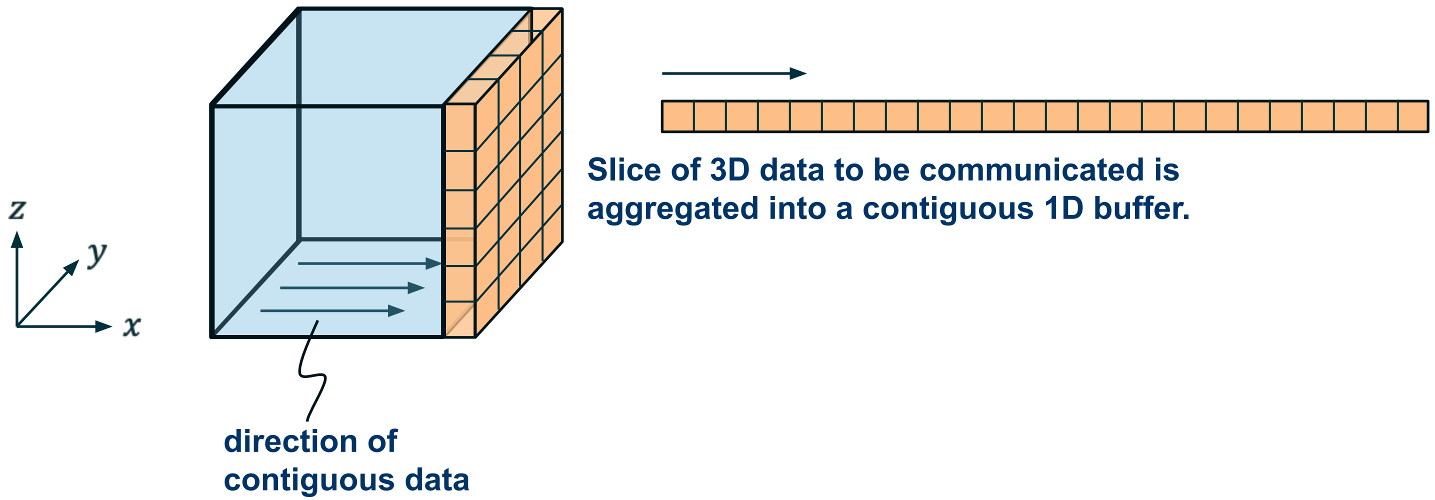
Weak scaling of the ABL application on Perlmutter

- The domain size is `128x128x512` for a single GPU;
- this is progressively scaled up to `2048x1024x512` for 128 GPUs (over 32 nodes).

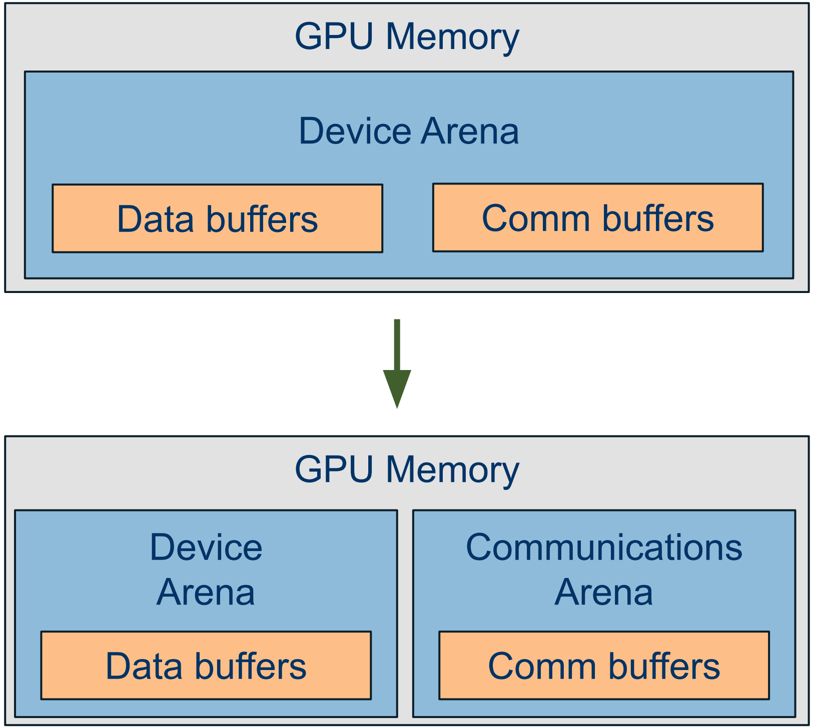


Communication buffers are used for efficient data transfer

Data aggregation reduces communication latency.



A distinct memory pool for comm buffers improves communication costs by 20% - 200%



Communication buffers sharing the same memory pool as data buffers degrades performance for a specific application.

Hypothesis: Comm buffers get assigned the same pointer in subsequent transfers, preventing the overhead of re-registering the address.

Summary: strategies to reduce communication costs

- ➢ Use of 4 - 8 OpenMP threads for shared memory parallelism over CPUs.
- ➢ Enabling direct data transfers between GPU - requires specific run time affinity settings.
- ➢ Implemented a distinct memory pool (arena) for communication buffers on the GPU.

These have a more significant impact than detailed profiling of the subroutines or kernels.

ERF is ready to be coupled with the wind turbine simulations

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FLOWMAS: Floating Offshore Wind Modeling and Simulation