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Preparing an Incompressible-Flow Fluid Dynamics Code for Exascale-Class Wind Energy Simulations

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Abstract

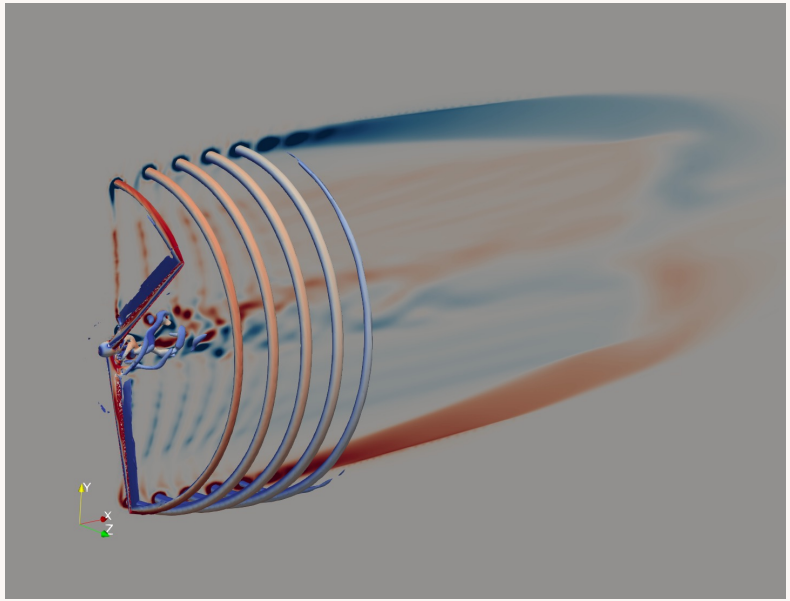
The U.S. Department of Energy has identified exascale-class wind farm simulation as critical to wind energy scientific discovery. A primary objective of the ExaWind project is to build high-performance, predictive computational fluid dynamics (CFD) tools that satisfy these modeling needs. GPU accelerators will serve as the computational thoroughbreds of next-generation, exascale-class supercomputers. Here, we report on our efforts in preparing the ExaWind unstructured mesh solver, Nalu-Wind, for exascale-class machines. For computing at this scale, a simple port of the incompressible-flow algorithms to GPUs is insufficient. To achieve high performance, one needs novel algorithms that are application aware, memory efficient, and optimized for the latest-generation GPU devices. The result of our efforts are unstructured-mesh simulations of wind turbines that can effectively leverage thousands of GPUs. In particular, we demonstrate a first-of-its-kind, incompressible-flow simulation using Algebraic Multigrid solvers that strong scales to more than 4000 GPUs on the Summit supercomputer.

Talk Outline

- Motivation
- Modelling strategy
- Linear solver innovations for GPUs
  - Assembly
  - AMG setup
  - Fast smoothers
- Computational results
  - Single-turbine, low-resolution performance
  - Single-turbine, high-resolution performance
  - Role of processor, compiler, and MPI-implementation on performance
- Emerging systems
- Looking forward

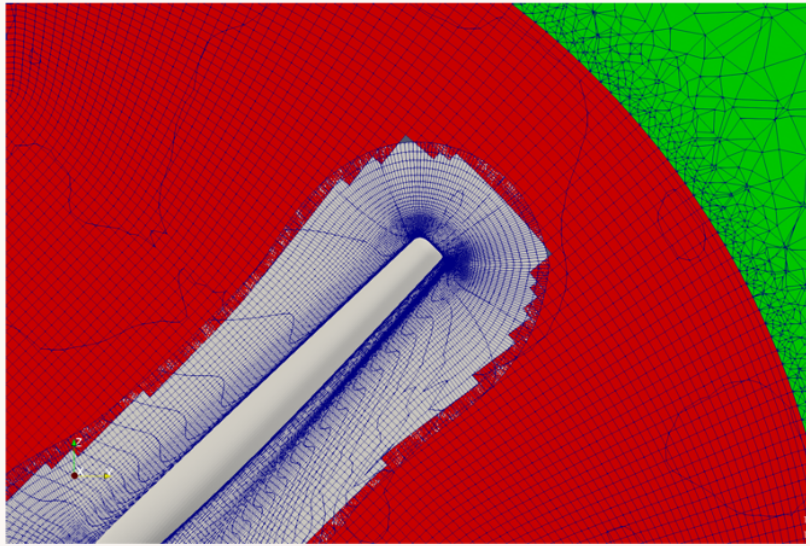
Motivation

- Exawind project goal is to build high-performance, simulation software capability of modeling entire wind farms.
- Algorithms must be able to resolve
  - micron-scale boundary layers around turbine blades
  - kilometer-scale atmospheric boundary layers in which the turbines operate
- Software must handle blade-deformation and turbine motion in a complex environment including offshore.
- Software must be high-performance for scientific exploration & engineering optimization.
- Nalu-Wind : unstructured blade-resolved solver (todays topic)
- AMR-Wind : structured background-solver



Modeling Strategy

- Decoupled overset mesh methodology used to model flow past turbine structure
- A Nalu-Wind mesh is a composition of multiple independent meshes that move with respect to one another.
- Mesh motion (i.e. blade rotation around the rotor) requires continuous connectivity updates.
- Primary benefits
  - Simple mesh creation process for wind farm simulations
  - Remove the need to reinitialize matrices at each time step
  - Enables a path to exascale AMR-Wind/Nalu-Wind coupling for many turbines

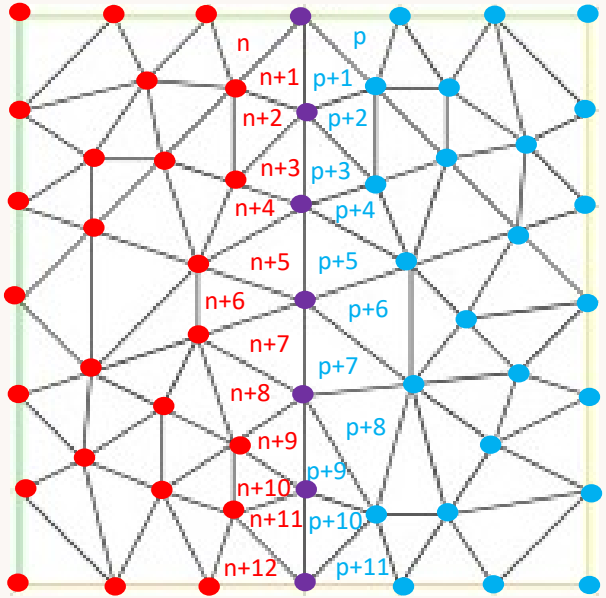


Nalu-Wind Software Stack

- STK (Sierra Toolkit) : handles the mesh data structures
- TIOGA : handles overset mesh capabilities
- Kokkos : Portable, parallel execution constructs
- Linear System Solvers :
  - Hypre : Boomer AMG, CUDA/HIP backends
  - Trilinos : Muelu, Tpetra, Kokkos
- Zoltan2 : Domain decomposition with ParMETIS, Scotch, RCB algorithms
- NetCDF/HDF5 : IO

Nalu-Wind Assembly

- Decoupled overset enables computation of the exact sparsity pattern for the global matrix for the entire simulation
- Each rank has an owned part, i.e. contributions to the matrix rows/rhs values on this rank
- Each rank might have a shared part, i.e. contributions to the matrix/rhs values on other ranks
- matrix/rhs contributions from mesh elements of same type (i.e. tetrahedron) are computed via atomics in a single Kokkos kernel



- Owned on rank 1
- Owned on rank 2
- Owned on rank 1, Shared on rank 2

Hypre Assembly

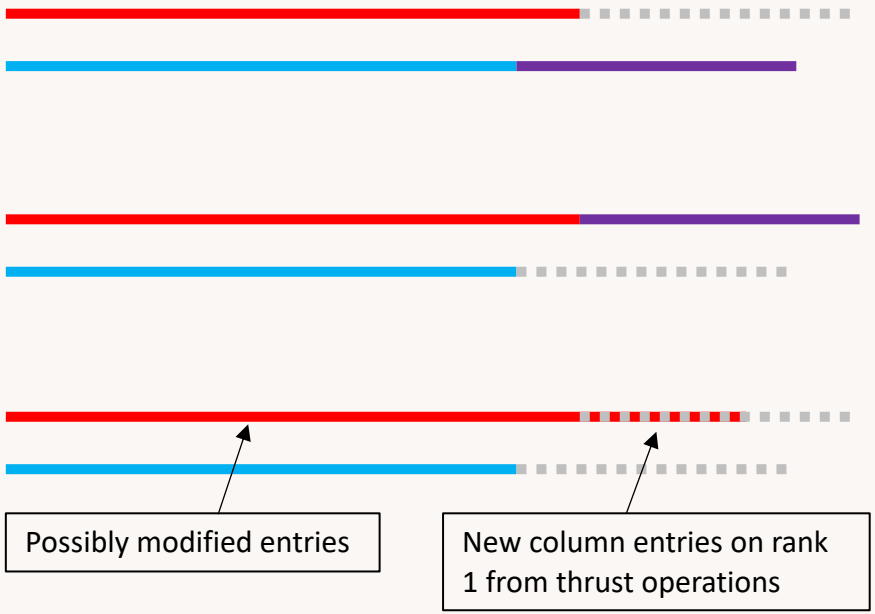
- Hypre Assembly API receives coordinate (coordinate) matrix with buffers of size $nnz_{local} = nnz_{owned} + \max(nnz_{shared}, nnz_{recv})$

  Before assembly (MPI Messaging), data are stacked with owned part followed by shared

- After MPI Messaging, shared elements are overwritten by the values received from other ranks

- *thrust::stable_sort_by_key* and *thrust::reduce_by_key* are used to complete the global matrix assembly

Matrix values memory schematic. Similar data structures for row and column indices
- Top line: rank 1
- Bottom line: rank 2
- Dotted line: space is allocated but not used



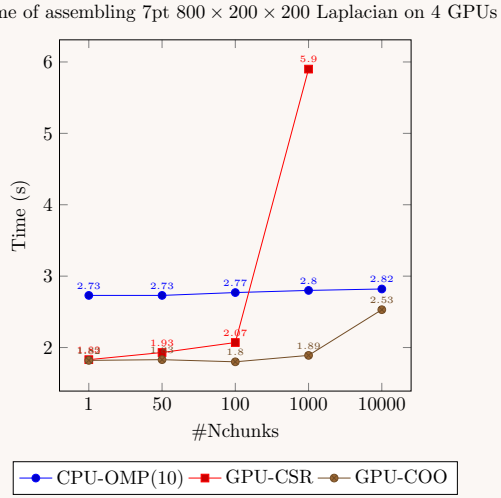
IJ interface on GPUs: the same interface as on CPUs

$$\begin{array}{c} \\ \text{rows} \end{array} \begin{array}{c} \text{column indices} \\ \begin{array}{cccccccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 4 & & -1 & & -1 & 4 & -1 & & -1 & \\ 5 & & & -1 & & -1 & 4 & & & -1 \\ 6 & & & & -1 & & & 4 & -1 & \end{array} \end{array}$$

```
HYPRE_IJMatrix A;
int nrows = 3, ncols[3] = {5, 4, 3}, rows[3] = {4, 5, 6};
int cols[12] = {1,3,4,5,7, 2,4,5,8, 3,6,7};
double values[12] = {-1,-1,4,-1,-1, -1,-1,4,-1, -1,4,-1};
/* set matrix coefficients several rows at a time */
HYPRE_IJMatrixSetValues(A, nrows, ncols, rows, cols,
values);
```

- Can use the same "CSR"-format input with all GPU pointers
- Alternatively, a more efficient "COO"-format input
- Assembly uses thrust: `sort_by_key, reduce_by_key`
- Set/AddTo matrix coefficients in big chunks for efficiency!

```
int nrows = 12, ncols = NULL;
int rows[12] = {4,4,4,4,4, 5,5,5,5, 6,6,6}; /* on GPU */
int cols[12] = {1,3,4,5,7, 2,4,5,8, 3,6,7};
double values[12] = {-1,-1,4,-1,-1, -1,-1,4,-1, -1,4,-
1};
/* set matrix coefficients several rows at a time */
HYPRE_IJMatrixSetValues(A,nrows,ncols,rows,cols,
values);
```

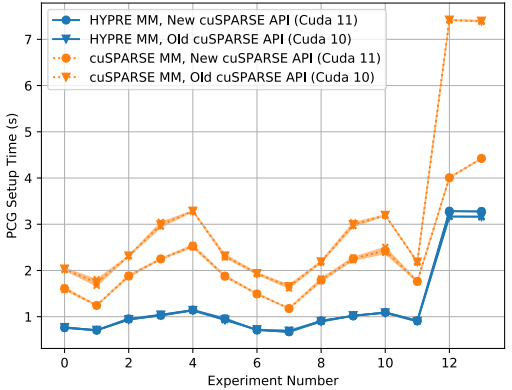


BoomerAMG setup on GPUs

- Coarsening algorithm: PMIS
  - massively parallel algorithm to find maximal independent set
  - uses cuRAND to generate random numbers on GPUs
- Aggressive coarsening to reduce the grid and operator complexity
  - corresponding two-stage interpolation
- Interpolation algorithms: direct interpolation and matrix-matrix based extended interp.
  - Bootstrap AMG (BAMG) direct interpolation by solving a local optimization problem
  - Distance-2 interp. in the form of mat-mat for better portability

$$-\left[\left(D_{FF}+D_{\gamma}\right)^{-1}\left(A_{FF}^{s}+D_{\beta}\right)\right]\left[D_{\beta}^{-1}A_{FC}^{s}\right]$$

  - More variants M-M ext+i/ ext+e
- Galerkin product RAP: use *hypre*'s SpGEMM kernel
  - Better performance than cuSPARSE



Boomer AMG Smoothers optimized for GPUs

- GMRES Krylov solver for momentum and pressure continuity
- Neumann Gauss-Seidel preconditioner and AMG smoother for pressure
- Based on the iteration for $Ax = b,\ \ A = D + L + U,\ r_k = b\ - Ax_k$

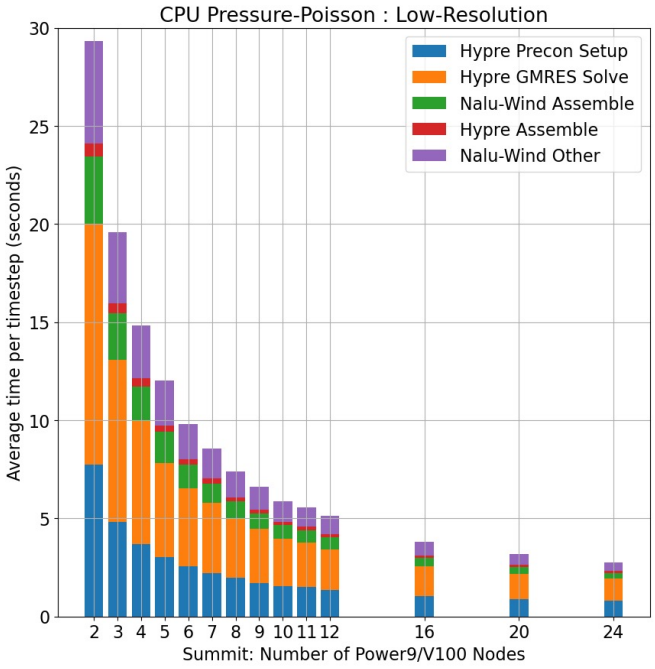
$$x_{k+1} = x_k + \sum_{k=0}^{n} (-DL)^k\, D^{-1}\, r_k$$

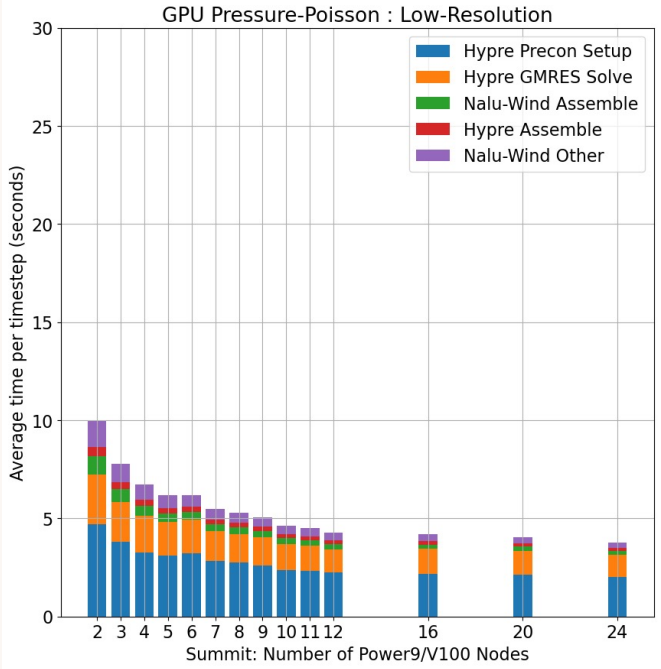
  - Exploits sparse matrix-vector products (SpMV)
  - SpMV are 25 to 50 times faster than direct triangular solver $Lx = b$ on GPU
  - Iterate for $k = 1, 2$
  - New smoother option in Hypre-BoomerAMG from LLNL

Computational Studies

- Results for 2 Turbines
  - Low-Resolution, Single-Turbine: 23 million mesh nodes
  - High-Resolution, Single-Turbine: 635 million mesh nodes
- Simulation parameters
  - 50 times steps
  - 4 Picard iterations per time step. Each picard iteration has
    - 1 pressure-Poisson solve, 3 momentum solves (decoupled), 2 scalar transport solves (TKE and SDR)
  - Solver residual tolerances set to 1.e-5
- All systems solved with Hypre
- Key Measurements
  - Per equation performance : average time spent solving each equation system
    - pressure-Poisson : Boomer AMG with 2 stage GS preconditioner
    - momentum and scalar transport : 2 stage GS preconditioner
  - Application-level performance : average time per time step

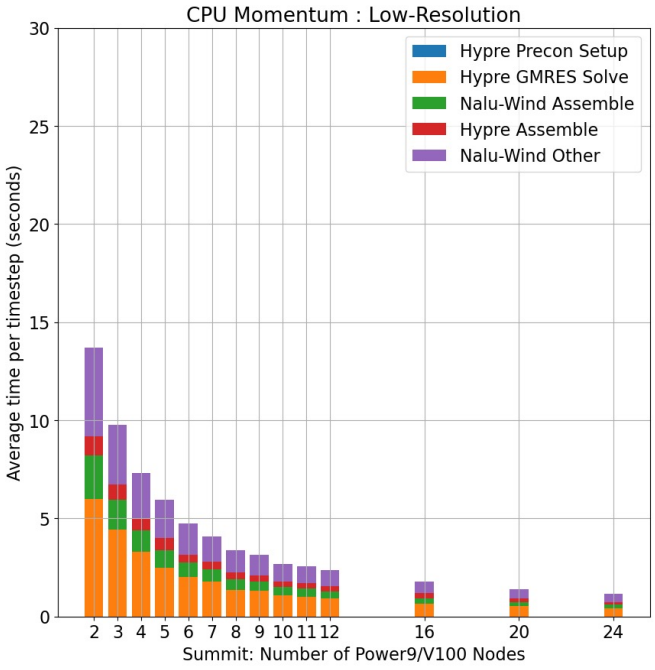
Pressure-Poisson/Hypre Boomer AMG

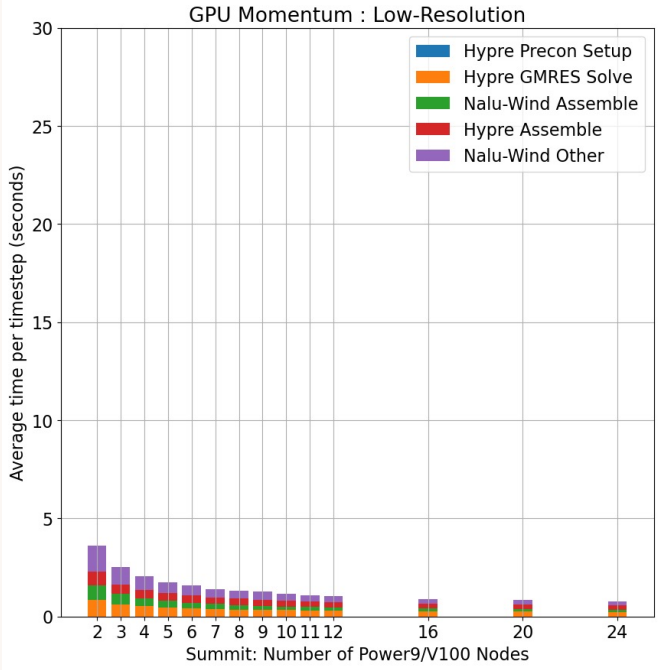




GPU implementation of Boomer AMG is substantially faster when there is substantial work per device!

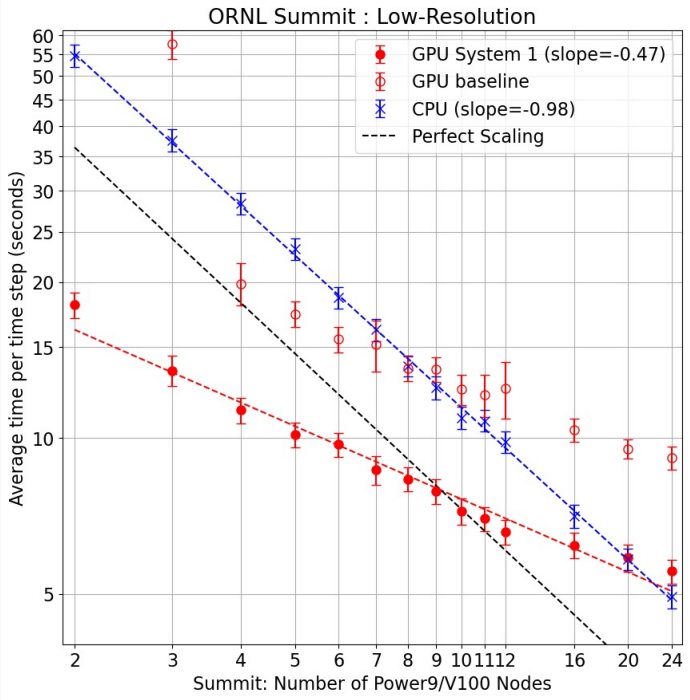
Momentum

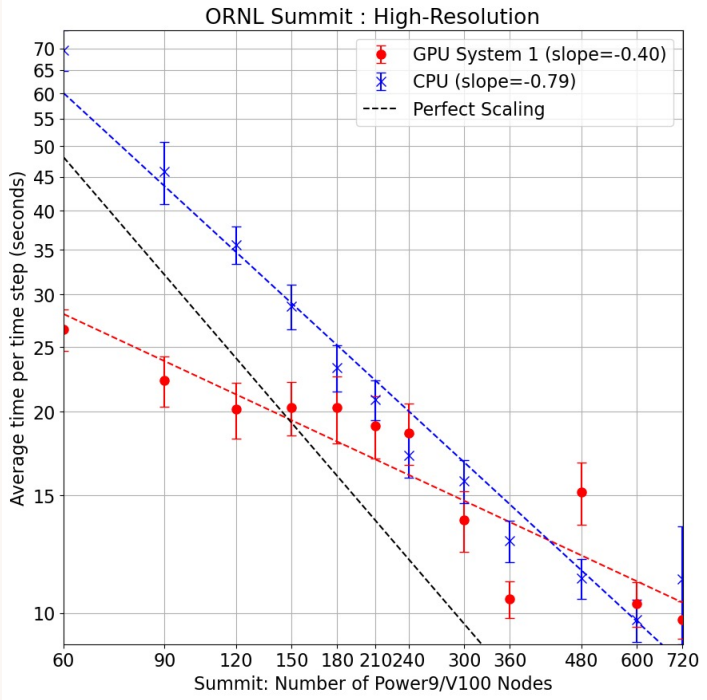




GPU accelerated Krylov solves with simple, but effective preconditioners are competitive with CPU implementations down to O(10^5) unknowns per device.

Low- vs High-Resolution Strong Scaling

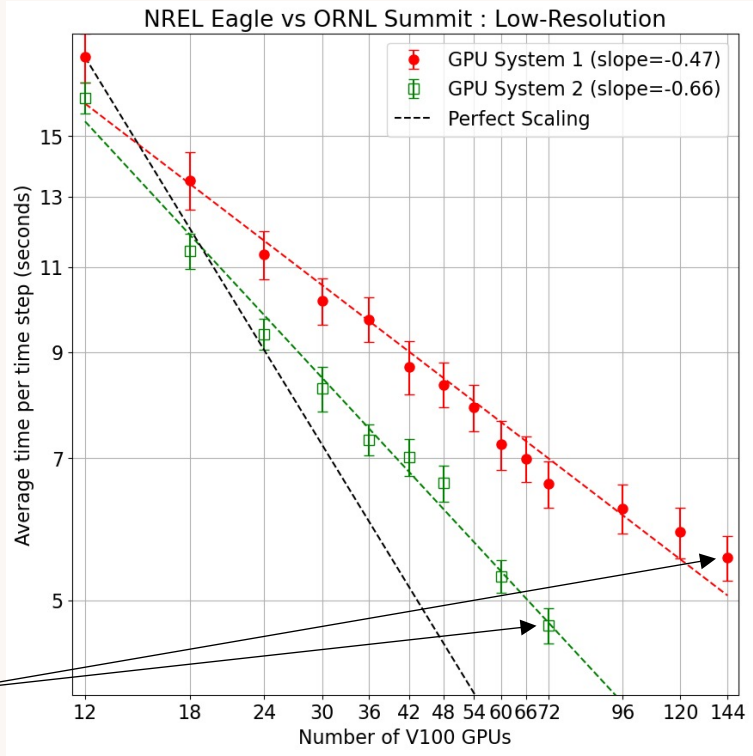




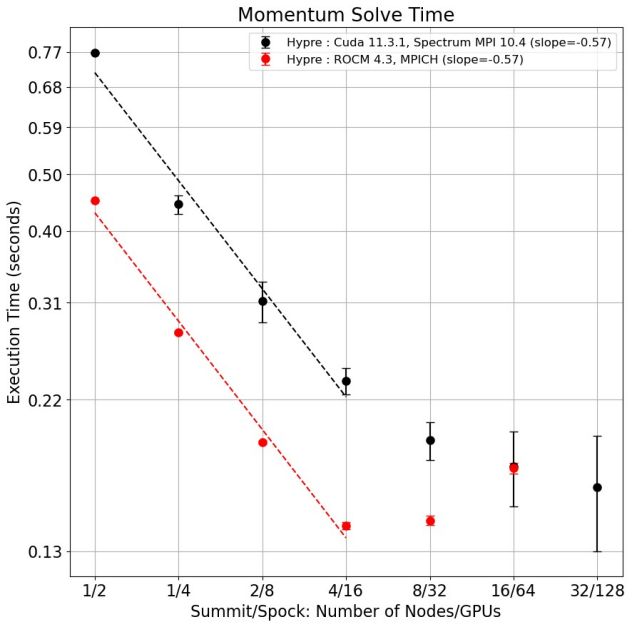
Application performance is good compared to CPUs when there is substantial work per device though the scaling is degraded.

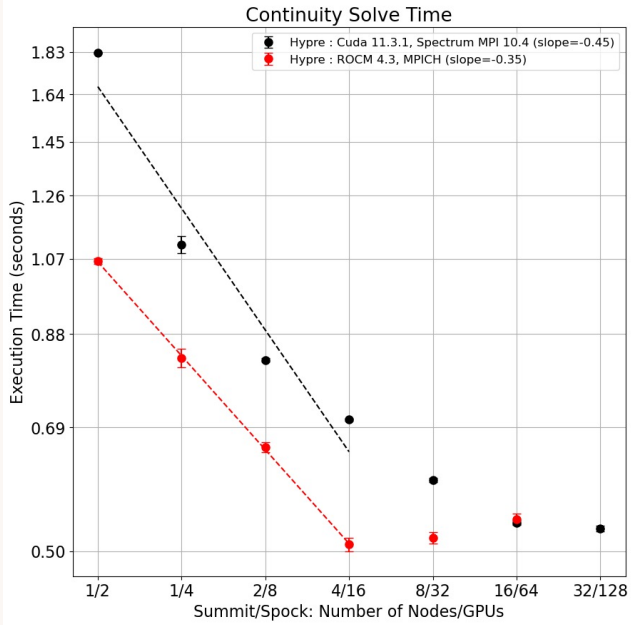
System Dependence

- NREL Eagle node configuration
  - 36 cores/Intel(R) Xeon(R) Gold 6150 CPU @ 2.70GHz
  - GCC 8.4.0
  - 2 NVIDIA V100 PCIE per node
  - MPI : HPE MPT
- ORNL Summit node configuration
  - 42 cores/POWER 9 @ 3.8 GHz
  - GCC 7.4.0
  - 6 NVIDIA V100 SXM2
  - Spectrum MPI 10.3
- All GPU resources per node utilized
- Eagle is 15% faster with half the number of GPUs. Most of the gain is achieved in pressure-Poisson preconditioner setup and solve



Emerging Architectures, Krylov Solve performance Summit vs Spock

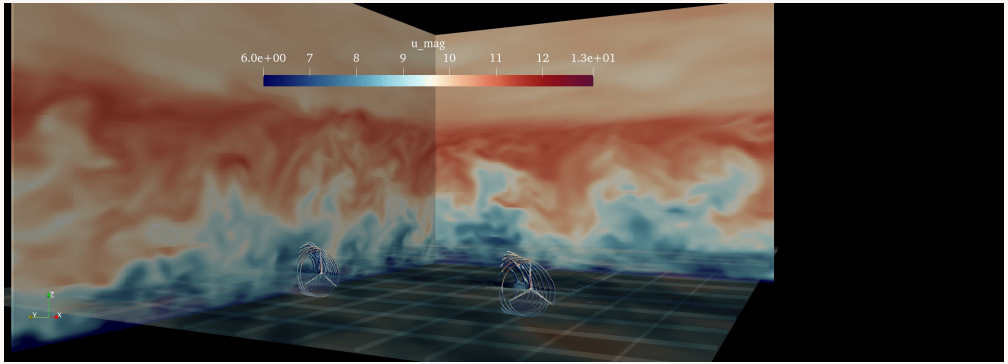




AMD M100 GPUs show substantial gains in performance over V100s. This bodes well for the Exawind software stack on Frontier!

Looking Forward

- In order to simulate entire Wind Farms, Exawind team is adopting a hybrid solver technique
  - Nalu-Wind around turbines
  - AMR-Wind everywhere else
  - TIOGA couples ALL the meshes
- Initial GPU version of the hybrid-solver nearly working
  - Loose coupling via TIOGA allows us to easily partition ALL compute resources (CPU/GPU)



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