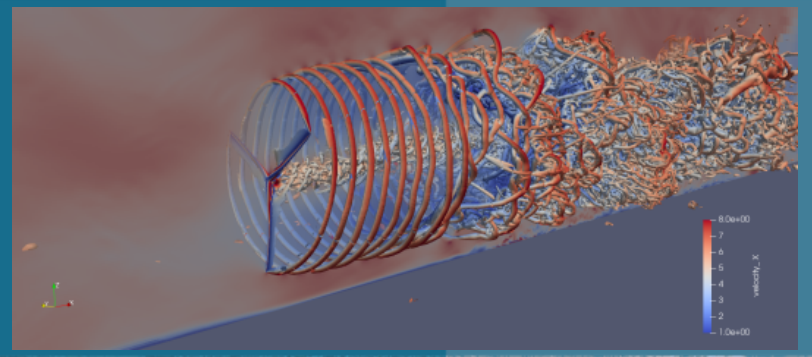
SAND2021-14238C

Sandia National Laboratories

Harnessing exascale for whole wind farm high-fidelity simulations to improve wind farm efficiency



Paul S. Crozier (co-PI), Christiane Adcock, Shreyas Ananthan, Luc Berget-Vergiat, Michael Brazell, Nicholas Brunhart-Lupo, Marc T. Henry de Frahan, Jonathan Hu, Robert Knaus, Jeremy Melvin, Bob Moser, Paul Mullowney, Jon Rood, Ashesh Sharma, Stephen Thomas, Ganesh Vijayakumar, Alan Williams, Robert Wilson, Ichitaro Yamazaki, Michael A. Sprague (PI)

Presented by: Paul S. Crozier, pscrozi@sandia.gov

November 17, 2021

Sandia Featured Presentation, DOE Booth (#2227) at SC21

U.S. DEPARTMENT OF ENERGY | NNSA

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ExaWind Funding & Development Team

U.S. Department of Energy Wind Energy Technologies Office

U.S. Department of Energy Exascale Computing Project

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ExaWind goals

- Create a multi-fidelity modeling and simulation environment for wind turbines and wind farms
- Enable simulations on current and next-generation supercomputers
- Enable a new understanding and ability to predict wind farm flows and turbine responses
- Create a foundation for next-generation lower-fidelity engineering models

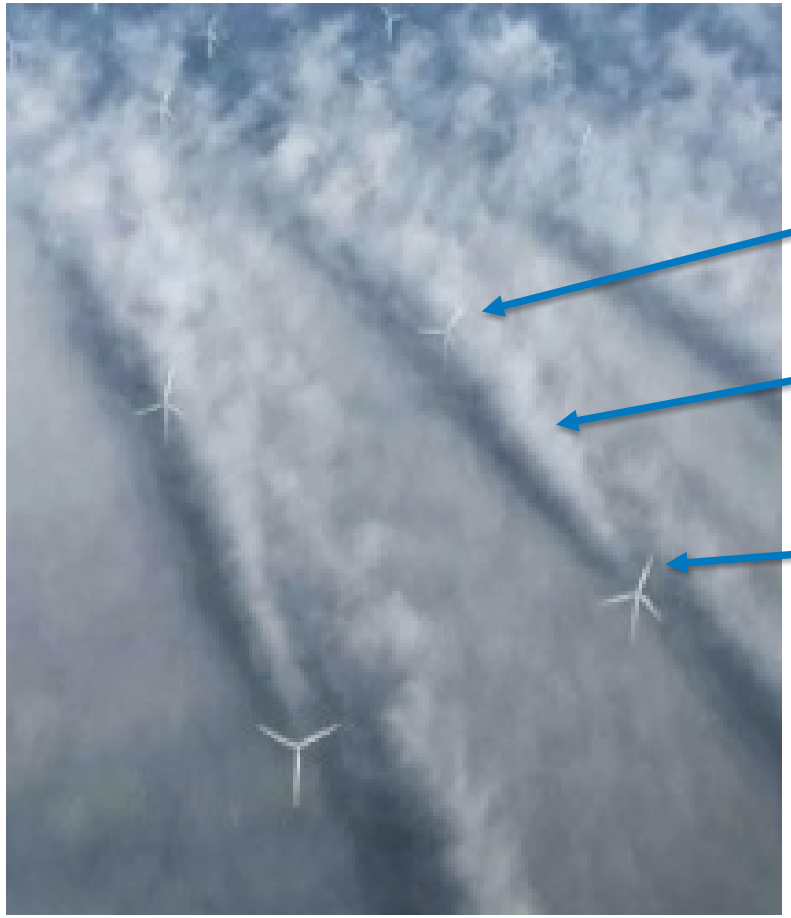


Photo by Gitte Nyhus Lundorff, Bel Air Aviation Denmark – Helicopter Services

Can we predict and understand:

Impact of wakes on downstream turbines?

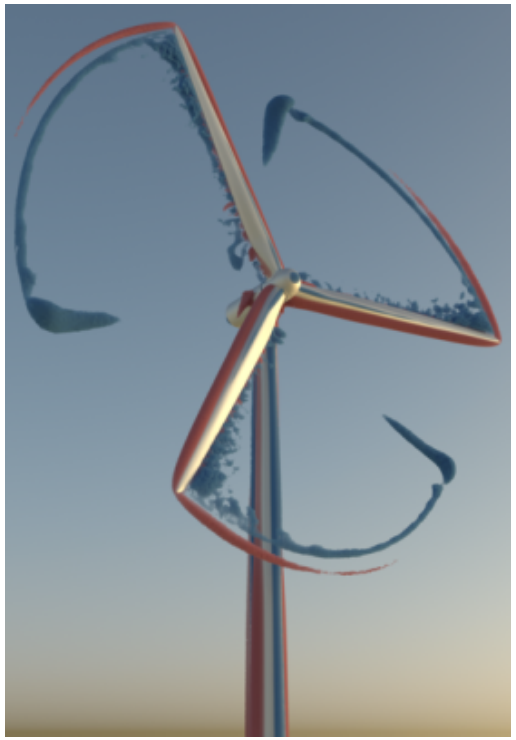
Evolution of the wakes?

Formation of the wakes?

… and all in a highly complex, dynamic metocean environment

ExaWind challenge problem: Baseline criteria

- **2 x 2 array of MW-scale turbines in a 3 x 3 x 1 km^3 domain**
  - NREL 5-MW reference turbine (126 m rotor diameter)
  - Simulation at rated wind speed (11.4 m/s for NREL 5-MW)
- Must resolve the viscous sublayer near the blades ($y^+ = 1$)
- Resolution must capture chord-scale atmospheric turbulent eddies, generation of near-blade vorticity, and propagation and breakdown of this vorticity; O(1) Courant number in wake (LES region); O(>>1) Courant number in RANS region
- Simulation will require at least **20B gridpoints**
- Demonstrate capability to complete a scientifically meaningful simulation of 500 s with one month of system time
- Simulation will be run near strong-scaling limit; use as much of exascale machine as possible to minimize time to solution

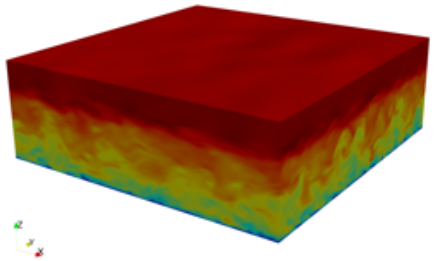


Blade-resolved simulation of NREL 5-MW turbine

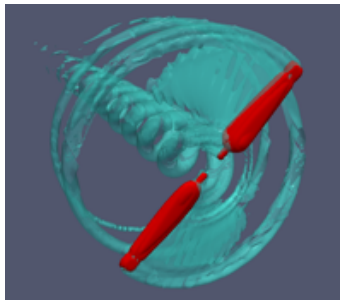
Challenge-problem details at https://confluence.exascaleproject.org/display/ADSE07/ADSE07+ExaWind+KPP-2+Challenge+Problem

The ExaWind software

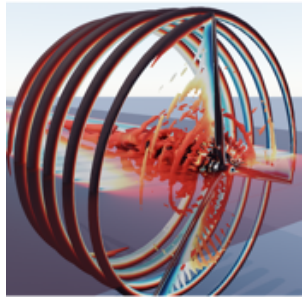
- Since 2016, we have been creating *ExaWind*:
  - An open-source collection of codes for wind turbine and wind farm simulations
  - https://github.com/Exawind
  - Multi-fidelity: Actuator-disk to highest-fidelity full-blade-resolved simulations
  - Backed by rigorous verification and validation
  - Established with modern software engineering, with a focus on performance portability
  - Funded by multiple projects and has a development team spanning multiple organizations
- Goals are to provide:
  - Pathways to understanding wind plant physics and reducing wind plant losses
  - Simulation-data and knowledge foundations for the next-gen design tools
  - The capability to explore disruptive technology innovations quickly and with confidence



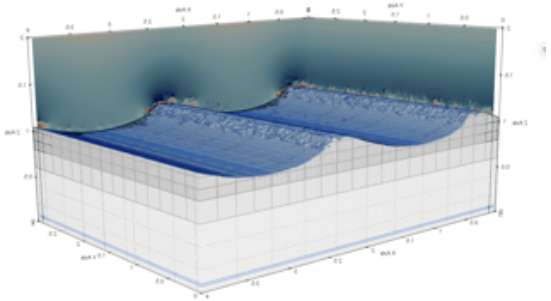
Atmospheric Boundary Layer Simulation



Actuator-Line Simulation



Blade-Resolved Simulation



Multi-Phase-Flow Simulation

The open-source ExaWind software stack

ExaWind: An open-source **multi-fidelity** modeling & simulation software stack designed to run on **laptops** and **next-gen supercomputers**

Nalu-Wind

- https://github.com/exawind/nalu-wind
- Incompressible-flow computational fluid dynamics (CFD)
- Unstructured-grid finite-volume discretization
- Built on Trilinos
- Leverages Trilinos and *hypre* linear-system solvers

AMR-Wind

- https://github.com/exawind/amr-wind
- Incompressible-flow CFD
- Structured-grid finite-volume discretization
- Built on AMReX, a framework for block-structured adaptive mesh refinement

TIOGA

- https://github.com/jsitaraman/tioga
- Library for overset-grid assembly

OpenFAST

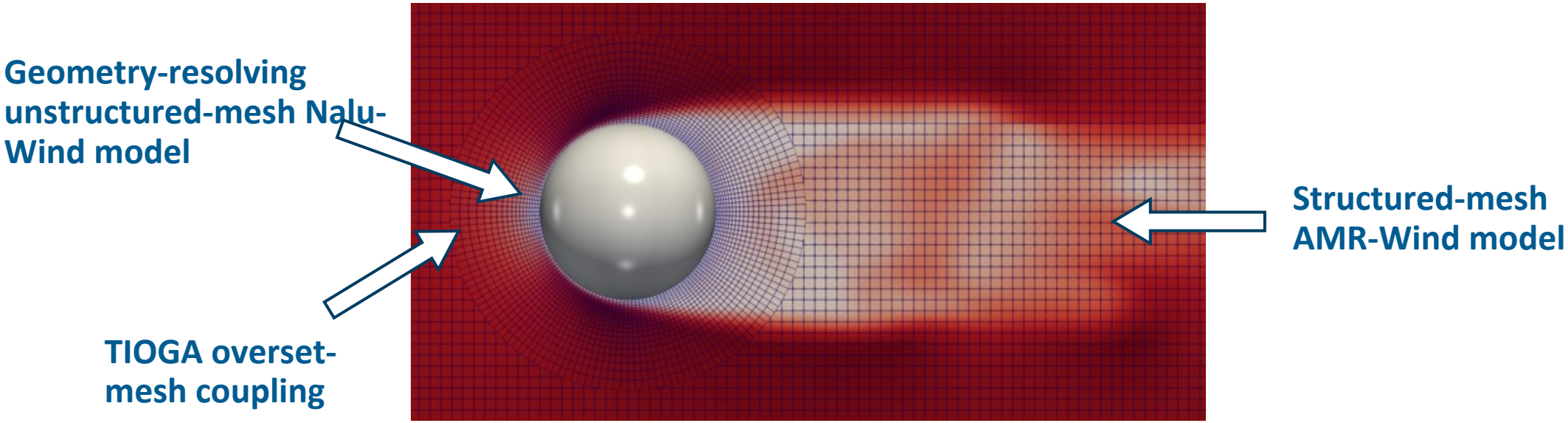
- https://github.com/openfast
- Whole-turbine simulation code

Software described in NAWEA 2019 paper

https://iopscience.iop.org/article/10.1088/1742-6596/1452/1/012071/pdf

ExaWind hybrid solver: AMR-Wind + Nalu-Wind

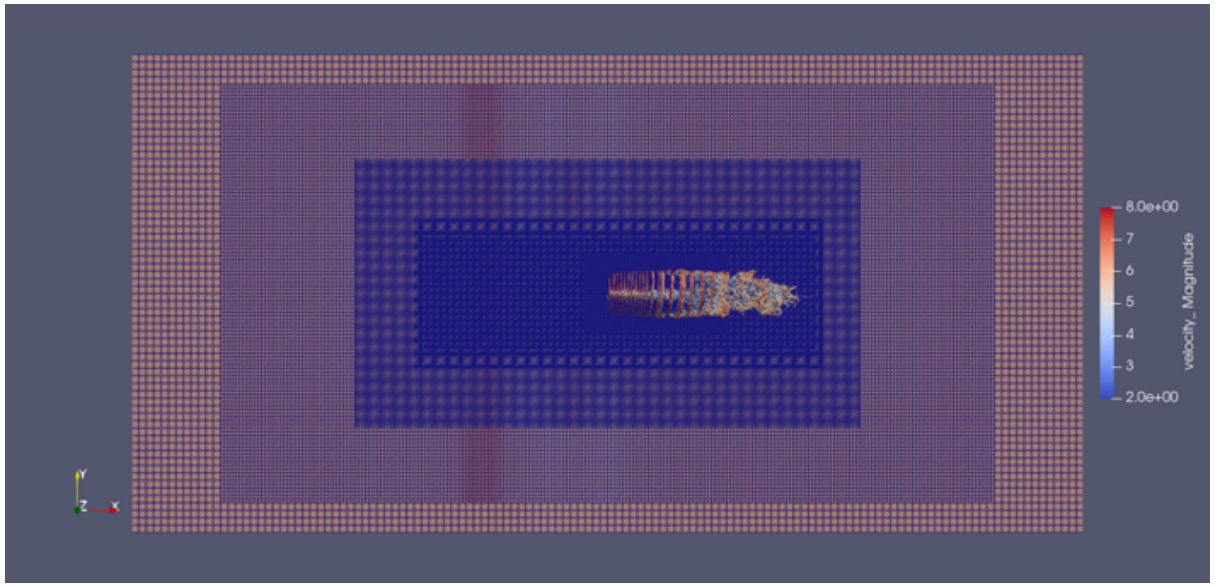
Nalu-Wind/AMR-Wind flow over a sphere

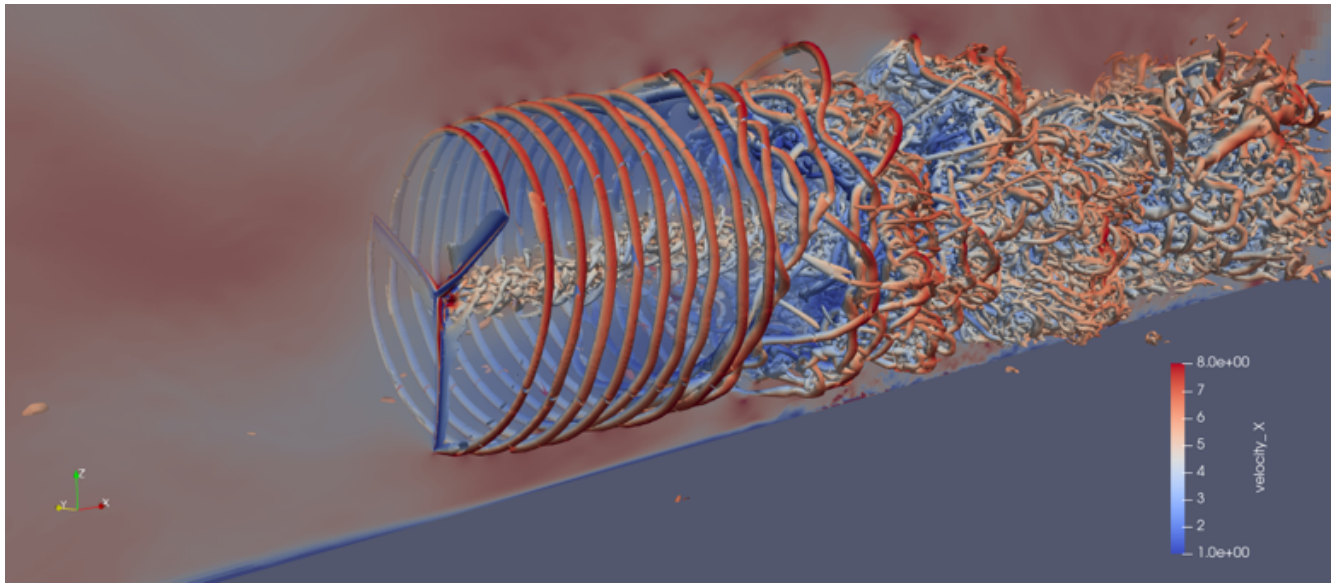


- Modeling approach for high-fidelity, blade-resolved simulations
- Relies on loosely coupled solves of global linear systems
- Provides ”optimal” solvers for the different grids

Actuator-Disk/Line simulations can be performed in either AMR-Wind or Nalu-Wind

ExaWind hybrid solver: Blade-resolved simulations





- AMR-Wind/Nalu-Wind CPU-only simulation on the NREL Eagle Supercomputer
  - NM-80 DanAero wind turbine rotor in turbulent flow with 122M grid points
  - Hybrid-RANS/LES coupling
  - Moving meshes with overset coupling
  - Simulation resolves 8 orders of magnitude in spatial scales:
    - $O(10^{-5})$ m boundary layer to $O(10^{3})$ m domain size
- Simulations performed as part of the IEA Task 29 validation

Key team members: Vijayakumar, Ananthan, Brazell, Sharma, Sitaraman

Source: Sprague, et al., 2021, ExaWind: Exascale Predictive Wind Plant Flow Physics Modeling, 2021 Exascale Computing Project Annual Meeting, NREL Tech. Report NREL/PO-5000-80015

HPC performance portability is central to ExaWind development

Supercomputer architecture is evolving rapidly

- U.S. Department of Energy supercomputers are increasingly relying on Graphical Processing Units (GPUs) for computational speed at low power
- The the first U.S. **exascale** supercomputers will have hybrid CPU-GPU architectures
  - Coming online in ~2022 (AMD & Intel GPUs)
  - Aiming for power requirements below 30 MW
- Hybrid CPU-GPU architecture is expected to become more common amongst HPC clusters
- **CFD codes will need to be able to utilize GPUs!**

https://www.flickr.com/photos/olcf/41941941904/in/album-72157683655708262/

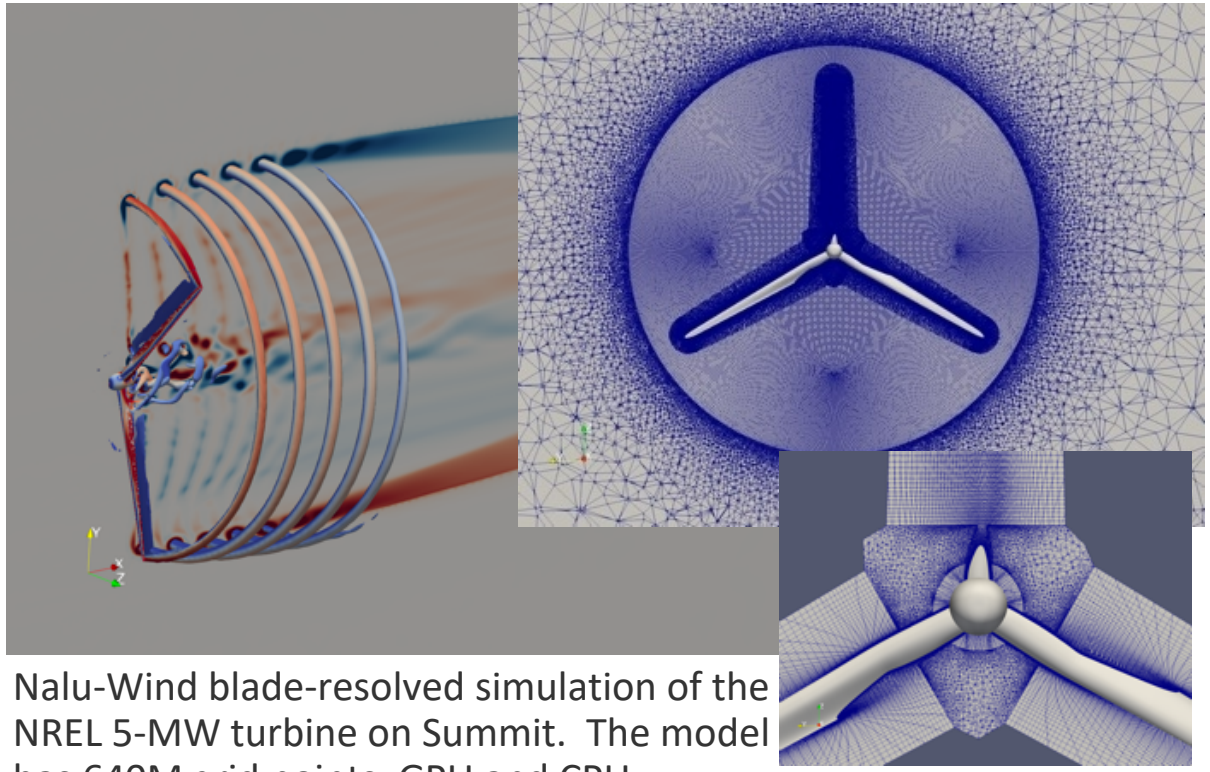
OLCF Summit:

- 200 x 10^{15} floating-point operations per sec.
- #2 fastest supercomputer (Top500; Nov. 2020)
- 4608 Nodes:
  - 2 IBM Power9 CPUs + **6 NVIDIA Volta GPUs**
- 10 MW system

Exascale systems will be at least 5 times faster

Nalu-Wind/*hypre* strong-scaling performance for CPUs and GPUs on Summit

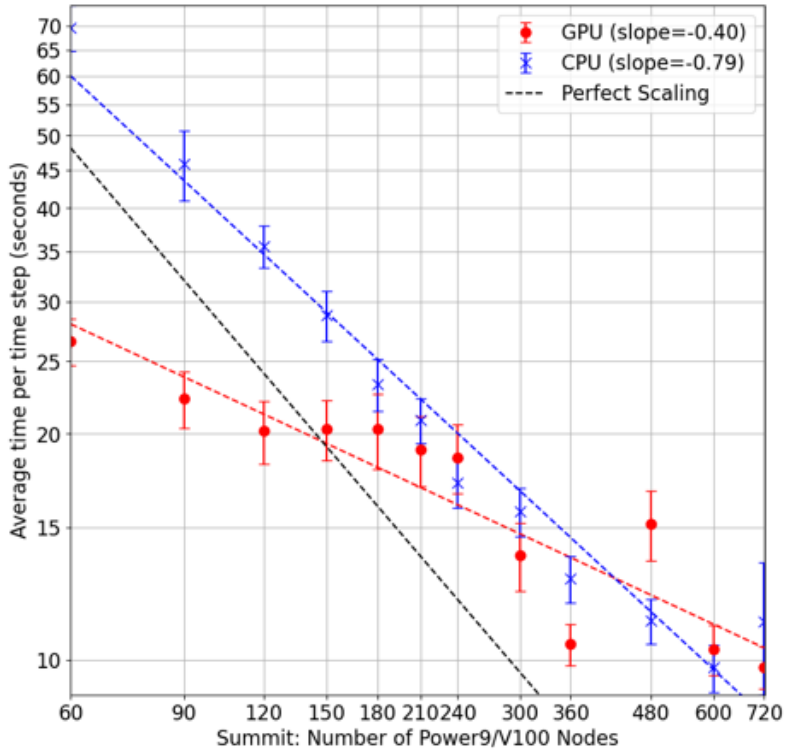
Blade-resolved Nalu-Wind turbine simulation with overset meshes



Nalu-Wind blade-resolved simulation of the NREL 5-MW turbine on Summit. The model has 640M grid points. GPU and CPU calculations used all GPUs and CPU-cores, respectively, on each node.

Key team members: Mullowney, Li, Thomas, Ananthan

Nalu-Wind/*hypre* strong-scaling

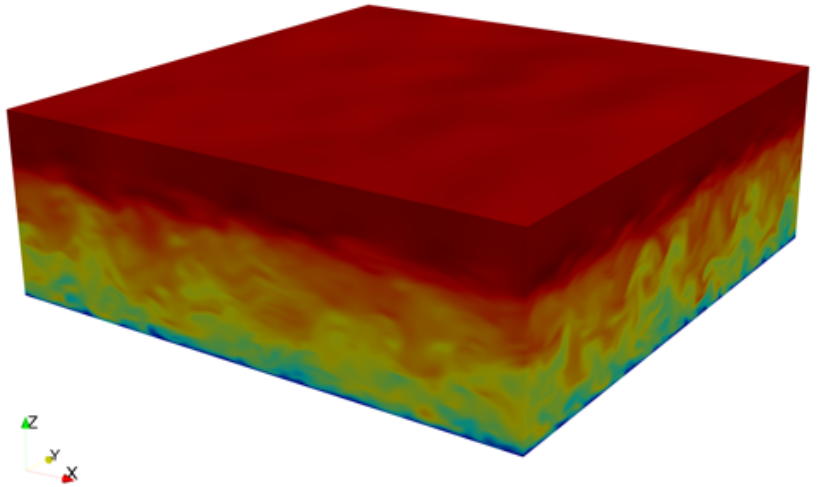


- GPUs can be faster than CPUs
- Preliminary observations show Nalu-Wind strong-scaling limits at about
  - 300,000 gridpoints per GPU, or
  - 26,000 gridpoints per CPU-core

Source: Sprague, et al., 2021, ExaWind: Exascale Predictive Wind Plant Flow Physics Modeling, 2021 Exascale Computing Project Annual Meeting, NREL Tech. Report NREL/PO-5000-80015

AMR-Wind strong-scaling performance for CPUs and GPUs on Summit

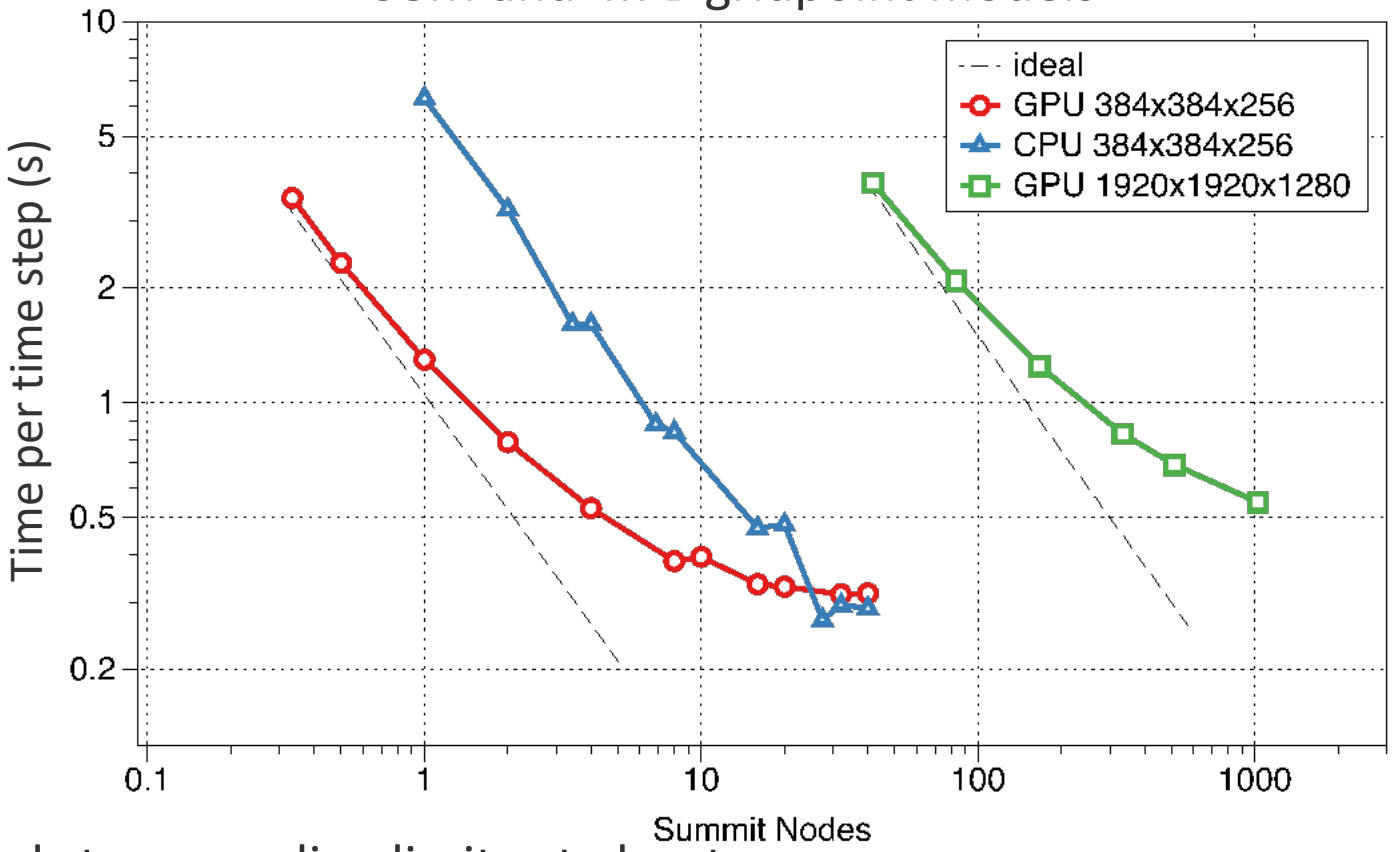
3D flow field from atmospheric boundary layer (ABL) simulation



ABL LES *precursor* simulation on a 3 km x 3 km x 2 km domain with uniform mesh resolution on ORNL Summit. GPU and CPU calculations used all GPUs and CPU-cores, respectively, on each node.

AMR-Wind Strong-scaling performance

38M and 4.7B gridpoint models



- GPUs can be faster than CPUs
- Preliminary observations show AMR-Wind strong-scaling limits at about
  - 1.2M gridpoints per GPU, or
  - 30,000 gridpoints per CPU-core

Key team members: Brazell, Ananthan, Rood, Almgren, Mullowney, Thomas

Source: Sprague, et al., 2021, ExaWind: Exascale Predictive Wind Plant Flow Physics Modeling, 2021 Exascale Computing Project Annual Meeting, NREL Tech. Report NREL/PO-5000-80015

Spock and Summit strong scaling performance for the ABL 20M momentum solve using Trilinos (Belos/Ifpack2)

Trilinos solver stack

- Main-line branch
- Open source & available now
- Belos GMRES
- Ifpack2 w/ Gauss-Seidel preconditioner
- Changes needed to Kokkos-Kernels

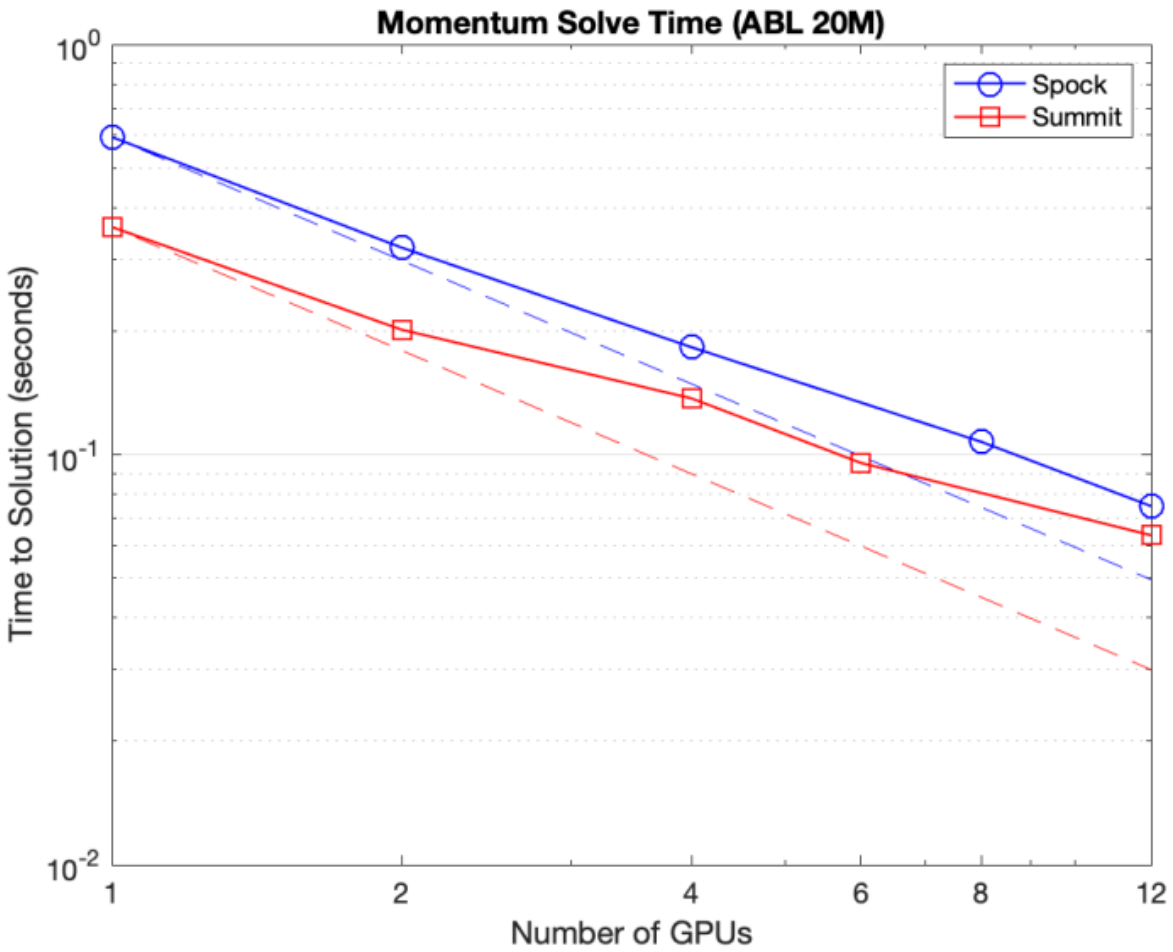
Spock

- Frontier precursor
- 36 compute nodes, each with:
  - 1x 64-core AMD EPYC 7662 “Rome” CPU
  - 4x AMD MI100 GPUs
- Used the HIP backend without UVM
- No TPL support for rocBLAS/rocSPARSE, yet

Summit

- 4608 compute nodes, each with:
  - 2x IBM POWER9 CPUs w/ 42 cores
  - 6x Nvidia V100 GPUs
- Used CUBLAS TPL

Key team members: Hu, Berget-Vergiat, Yamazaki



Results

- Decent scaling up to 12 GPUs
- Orthogonalization time about the same
- Iteration time 3x slower on Spock; working on improving this

Trilinos linear solve time per timestep on 360 GPUs of Summit

Problem description

- NREL 5-MW turbine
- Overset mesh
- Refined mesh
  - 634 M nodes
  - 719 M elements
- Nalu-Wind
- Trilinos solver stack
  - Tpetra
  - Ifpack2
  - Zoltan2
  - MueLu
  - (UVM removed)
- 10 timesteps
- 1 nonlinear iteration per timestep

Max time (in seconds) over all MPI ranks

Nalu-Wind Timer	Momentum	Continuity
init	7.54	6.77
assemble	0.62	0.28
load complete	1.22	1.12
solve	10.77	5.58
precond setup	0.02	16.33
misc	0.63	0.53
Total solver time	20.7	30.63
Linear iterations	6.9	30.3

Improvements made to the Trilinos solver stack

- UVM removed
- Issue in multigrid algorithm resolved
- Optimized the construction of the filtered matrix used in prolongator smoothing

Key team members: Hu, Berget-Vergiat, Yamazaki

Summit and Eagle strong scaling performance for NREL-5-MW using *hypre*

hypre solver stack

- Core algorithm results published at SC21

Summit

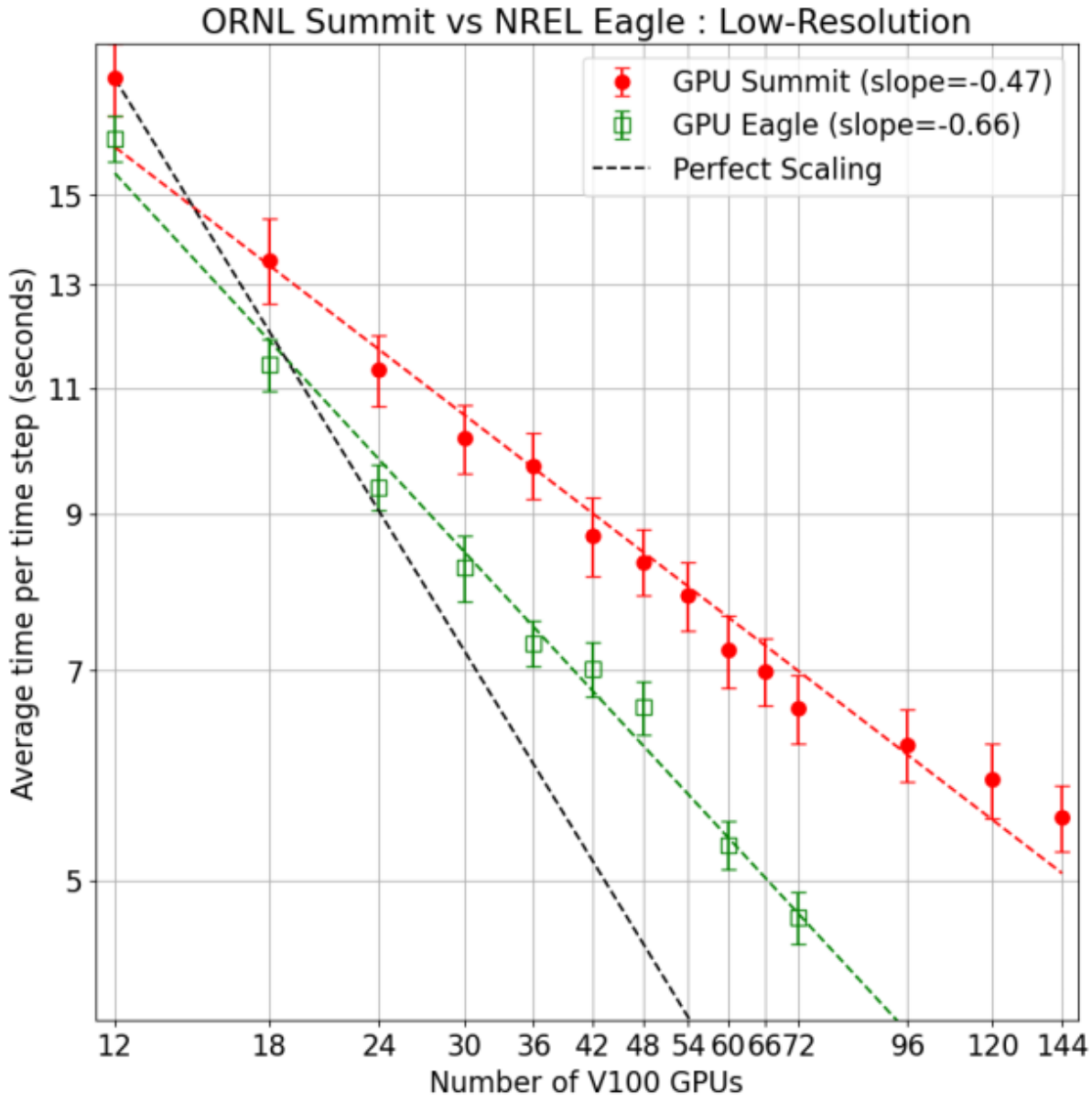
- 4608 compute nodes, each with:
  - 2x IBM POWER9 CPUs w/ 42 cores
  - 6x Nvidia V100 GPUs

Eagle

- 2618 compute nodes, each with:
  - 1x x86-based CPU w/ 36 cores
  - 2x Nvidia V100 GPUs

Results

- 72 GPUs on Eagle 15% faster than 144 GPUs on Summit
- Hardware-software configuration plays a critical role for implicit solvers on unstructured grids.
  - MPI implementations different
  - Base compilers different



Key team members: Thomas, Mullowney

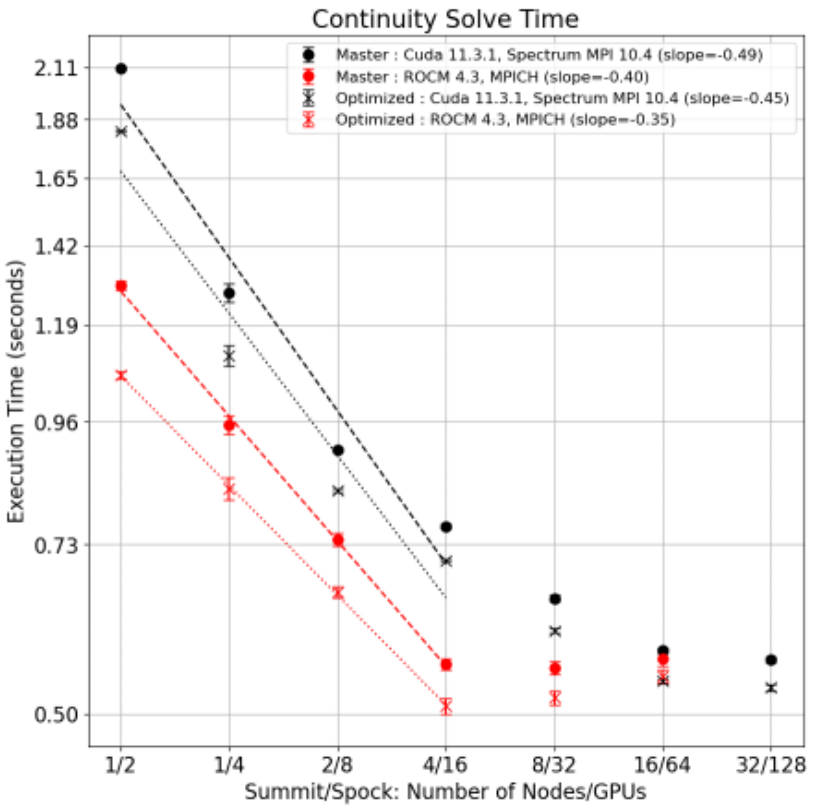
Strong scaling for continuity and momentum solves on Summit and Spock

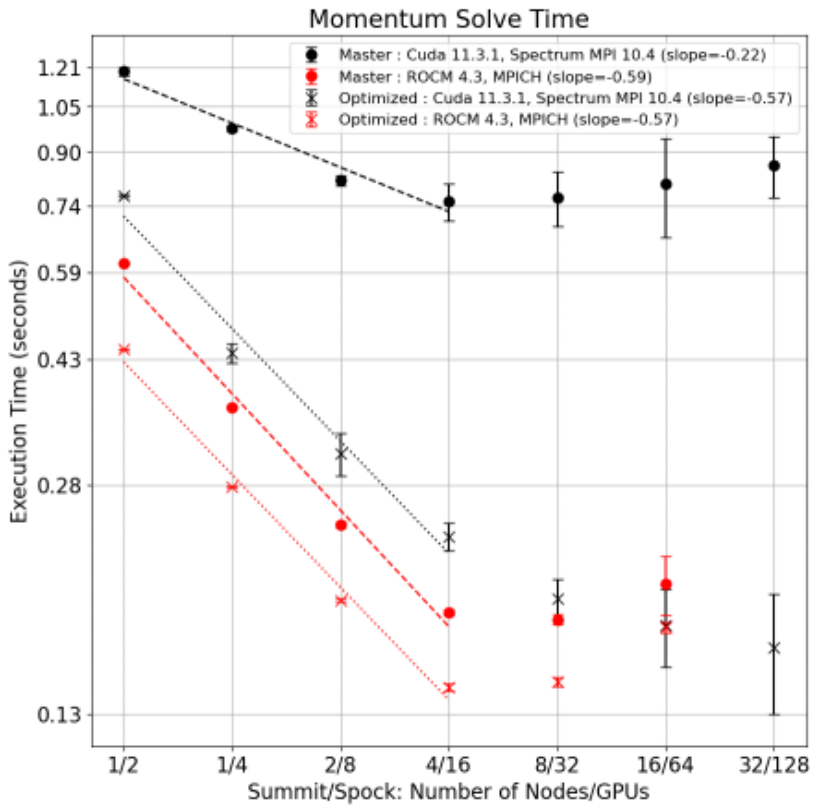
hypre solver stack
- Core algorithm results published at SC21
- Main-line and optimized branch shown

Spock
- Frontier precursor
- 36 compute nodes, each with:
  - 1x 64-core AMD EPYC 7662 “Rome” CPU
  - 4x AMD MI100 GPUs
- Using HypreBoomer AMG preconditioner

Summit
- 4608 compute nodes, each with:
  - 2x IBM POWER9 CPUs w/ 42 cores
  - 6x Nvidia V100 GPUs

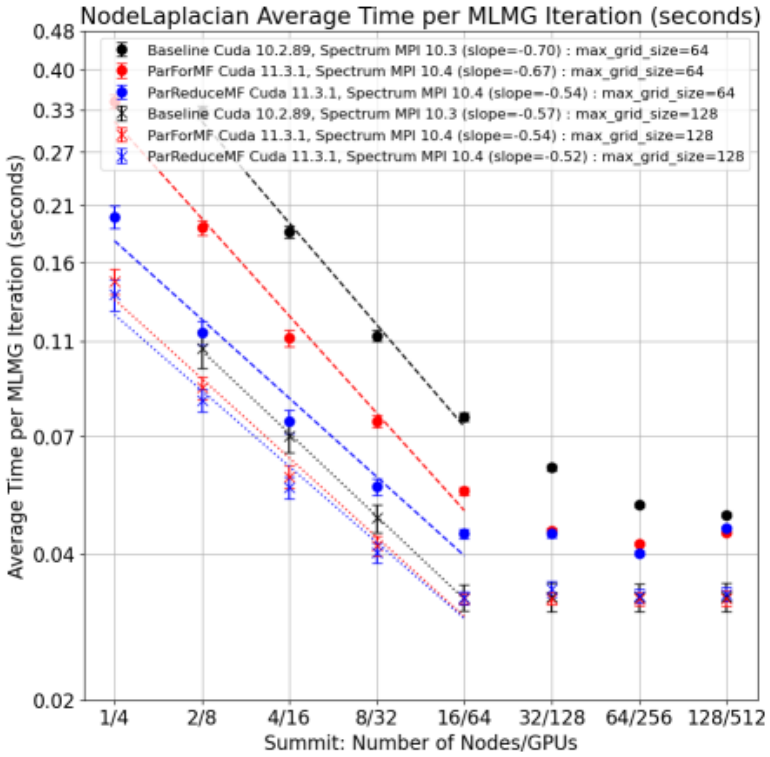
Results
- Spock faster per GPU
- Poor scaling beyond 16 GPUs
- HypreBoomer AMG needs to be optimized for HIP
- Ongoing work to further accelerate momentum solves
  - Prototype block GMRES iteration method ready
  - Hope to better exploit proc-level parallelism

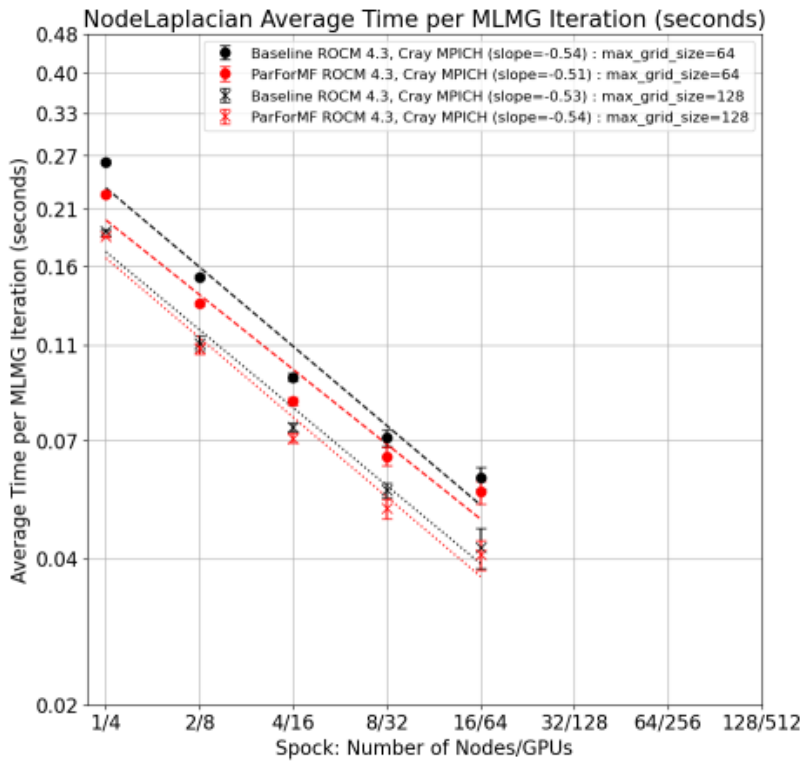


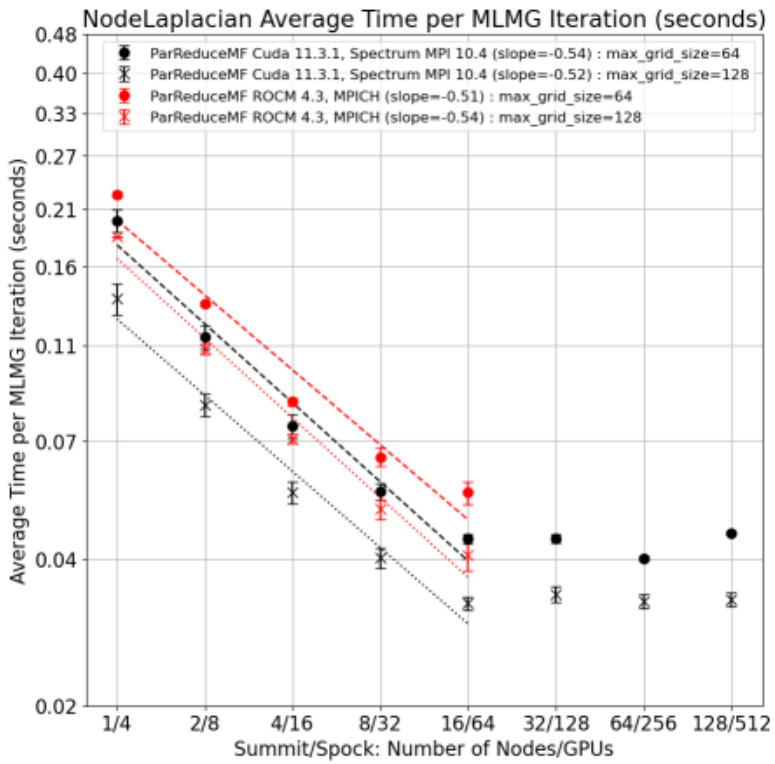


Key team members: Thomas, Mullowney

Nodal Poisson solves on Summit and Spock
AMReX linear solver improvements







Problem description

- Poisson solve on 512^3 domain
- Multi-Level Multi-Grid (MLMG) solver
- AMReX software, 3 versions:
  - Baseline
  - ParForMF (Parallel For improvements)
  - ParReduceMF (Parallel Reduce improvements)
- max_grid_size is the block size; bigger saturates GPUs

Key team members: Thomas, Mullowney

AMReX improvements

- Multiple kernel launches fused
- Parallel For
  - Kernels applied ind. across block data
  - Stencil operations
  - Interpolations
- Parallel Reduce
  - Results combined across the entire domain
  - 2-norms of gridded quantities

Results

- AMReX improvements helped
- Larger blocks faster
- Bigger gain for smaller blocks
- Summit gains more than Spock
- Summit faster than Spock
- Tune kernels for AMD?
- Improve boundary cell messaging?

AMR-Wind vs. Nalu-Wind

Problem description

- ABL, neutral atmospheric boundary layer problem
- 5 x 5 x 1 km^3
- 10 m grid spacing
- Nalu-Wind grid has 25 M nodes
- AMR-Wind grid has 52 M nodes
- Linear solver tolerance of 10^{-12}

Summit

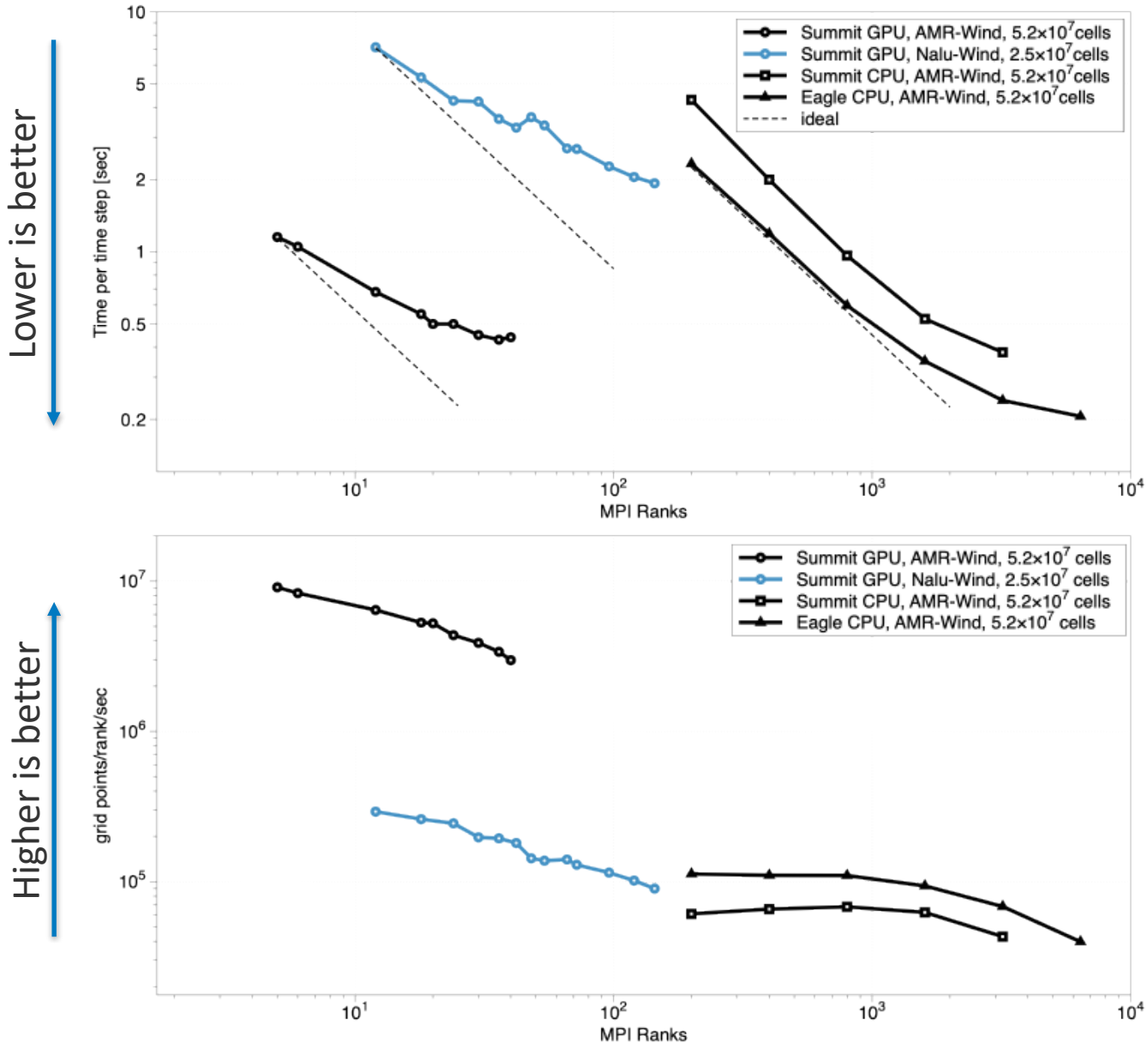
- 4608 compute nodes, each with:
  - 2x IBM POWER9 CPUs w/ 42 cores
  - 6x Nvidia V100 GPUs

Eagle

- 2618 compute nodes, each with:
  - 1x x86-based CPU w/ 36 cores
  - 2x Nvidia V100 GPUs

Results

- AMR-Wind ~10x faster than Nalu-Wind
- AMR-Wind able to process ~20x more grid points/s
- GPUs more efficient and faster than CPUs
- Eagle faster than Summit for this setup



Key team members: Brazell, Mullowney

Hybrid AMR-Wind / Nalu-Wind solver NREL 5-MW demonstration problem on Summit

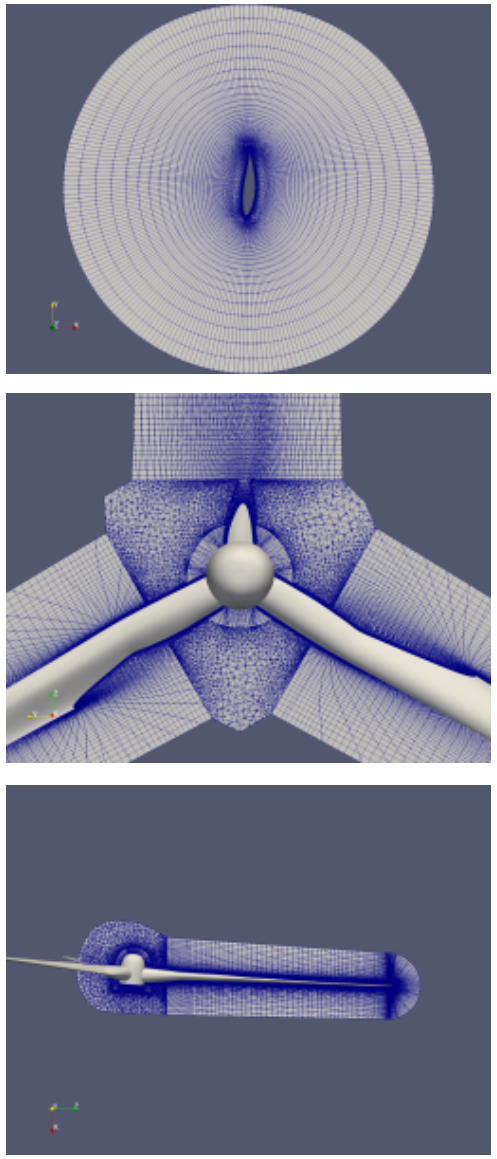
Problem description

- Small wind farm (1 or 2 turbines)
  - Domain size of O(10) km^3 (depends on ABL type)
  - Turbines spaced 3.6D apart
- NREL 5-MW turbines
  - 126 m dia reference turbine
  - Targets offshore wind
- Hybrid AMR-Wind / Nalu-Wind solver
- 870,000 elements; 741,000 nodes
- Turbulence models
  - $k - \omega$ SST near-body
  - Blended $k - \omega$ and $k - \varepsilon$ elsewhere
- Solvers
  - Trilinos / Tpetra / GMRES / G-S for momentum
  - *hypre* for continuity solves and AMR-Wind MLMG
- Overset coupling via TIOGA

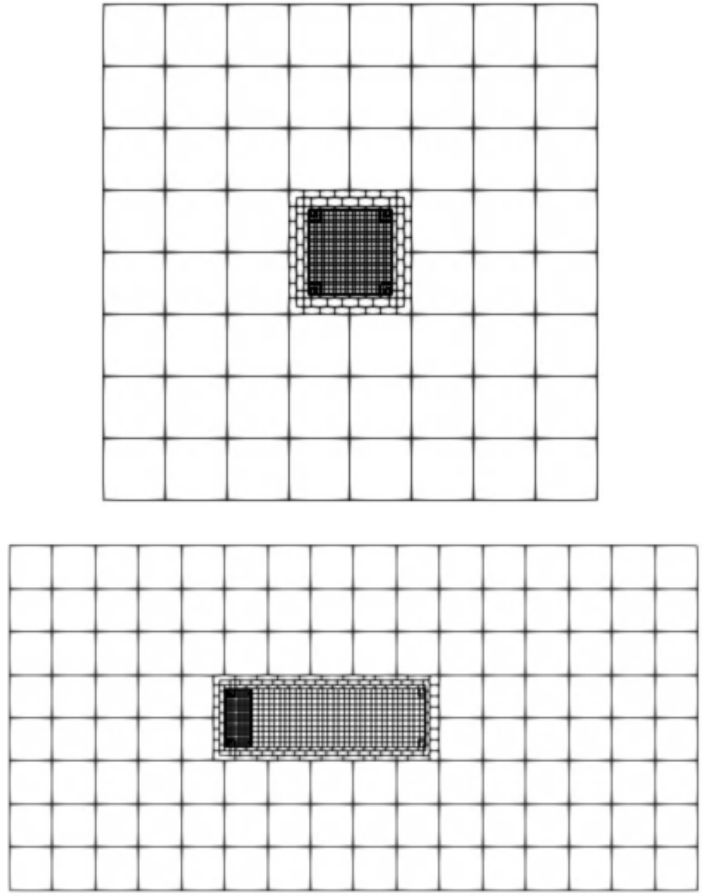
Summit

- 4608 compute nodes, each with:
  - 2x IBM POWER9 CPUs w/ 42 cores
  - 6x Nvidia V100 GPUs

Key team members: Sharma, Ananthan

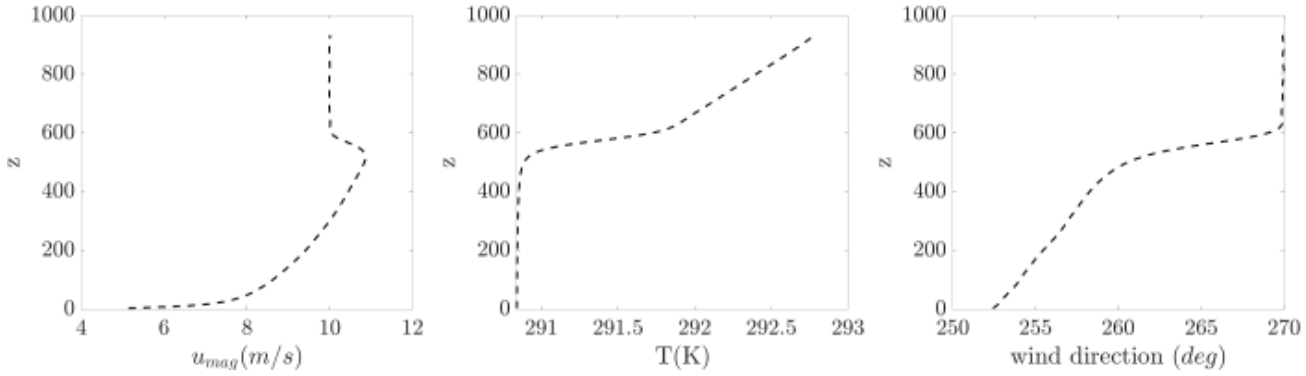


The near-body mesh used to model the NREL 5-MW rotor with Nalu-Wind. The mesh consists of structured, hyperbolically extruded mesh on the rotor blades and a fully unstructured mesh block around the hub and the hub-blade transition region.

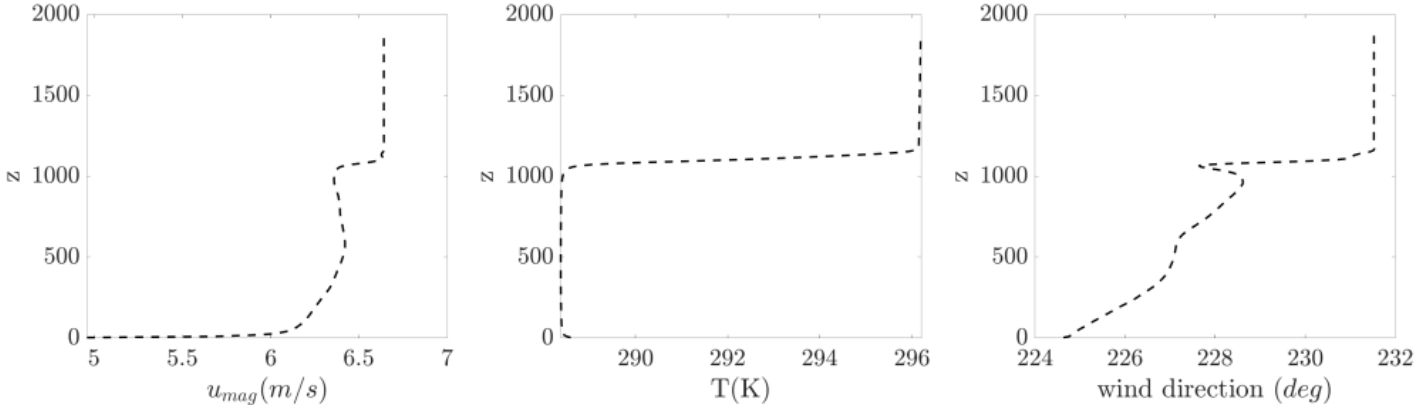


Outline of AMReX grids and local refinement boxes for NREL 5-MW turbine operating under uniform inflow.

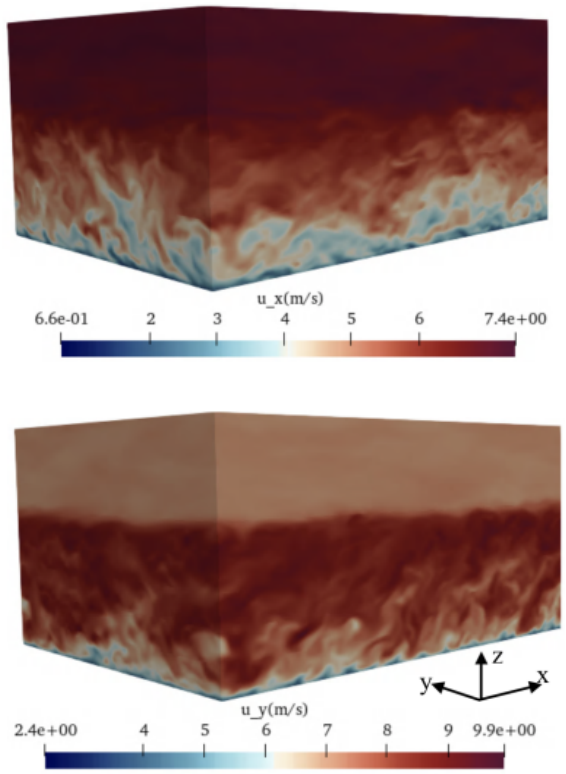
Hybrid AMR-Wind / Nalu-Wind solver NREL 5-MW demonstration problem on Summit (continued, slide 2)



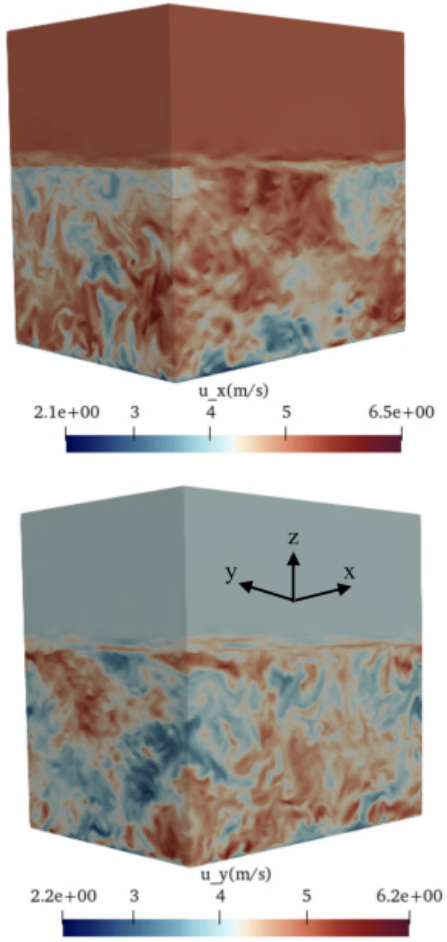
Case 1. Vertical-distribution statistics for a neutrally stable atmospheric boundary layer.



Case 2. Vertical-distribution statistics for a weakly unstable stable atmospheric boundary layer.



Case 1. Velocity profiles obtained from the neutral ABL precursor simulation.



Case 2. Velocity profiles obtained from the weakly unstable ABL precursor simulation.

Results

- ABL develops as expected
- Successful simulations using hybrid solver
- Case 1: neutral ABL, 31 hours of physical time
- Case 2: weakly unstable ABL, 5 hours of physical time

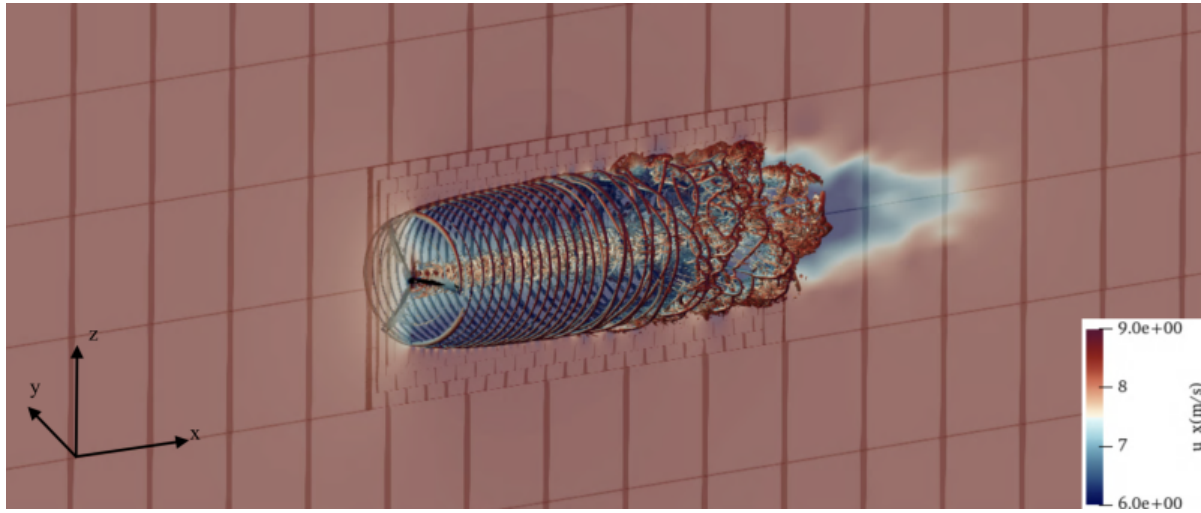
Key team members: Sharma, Ananthan

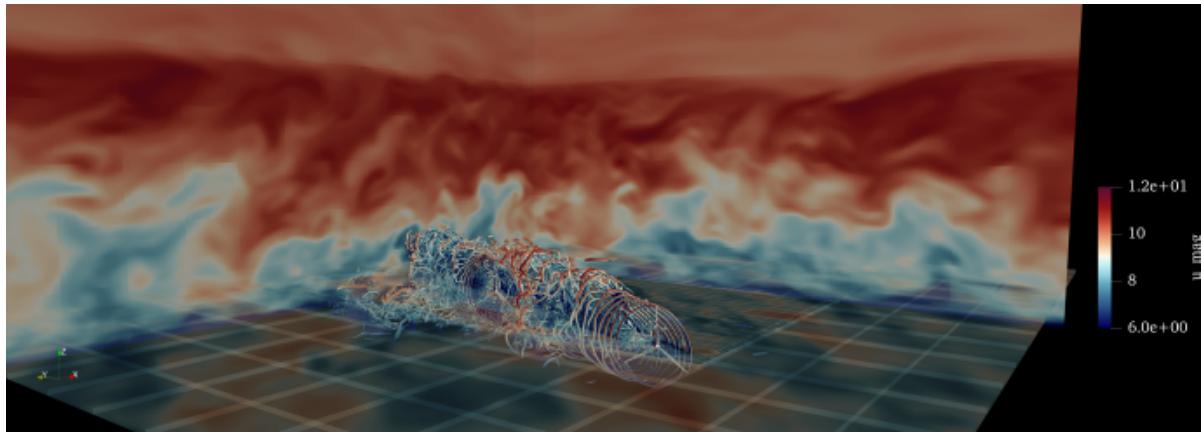
Hybrid AMR-Wind / Nalu-Wind solver NREL 5-MW demonstration problem on Summit (continued, slide 3)

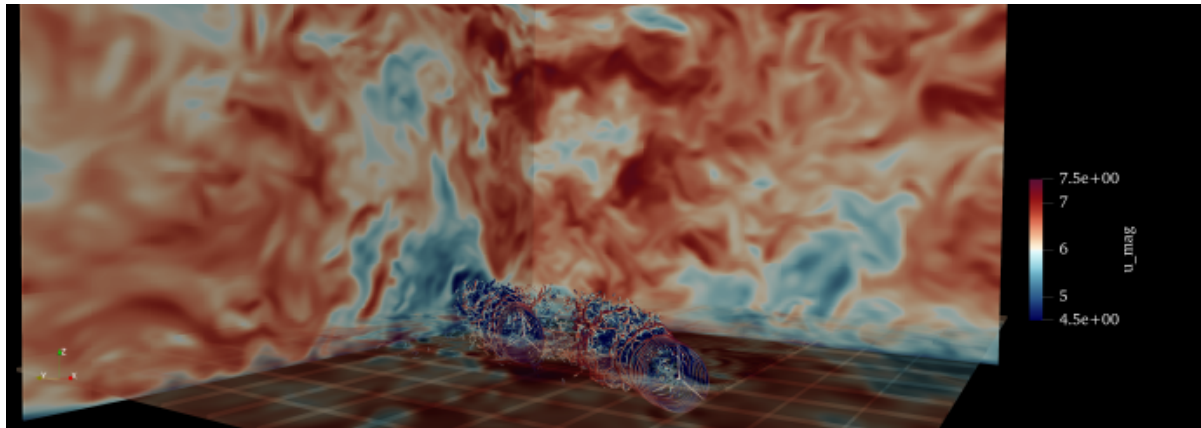
Results

- Successful demonstration of ExaWind solver stack on Summit, including:
  - Nalu-Wind
  - AMR-Wind
  - TIOGA
  - C++ driver code

- First demonstration of multiple wind turbines using the hybrid solver







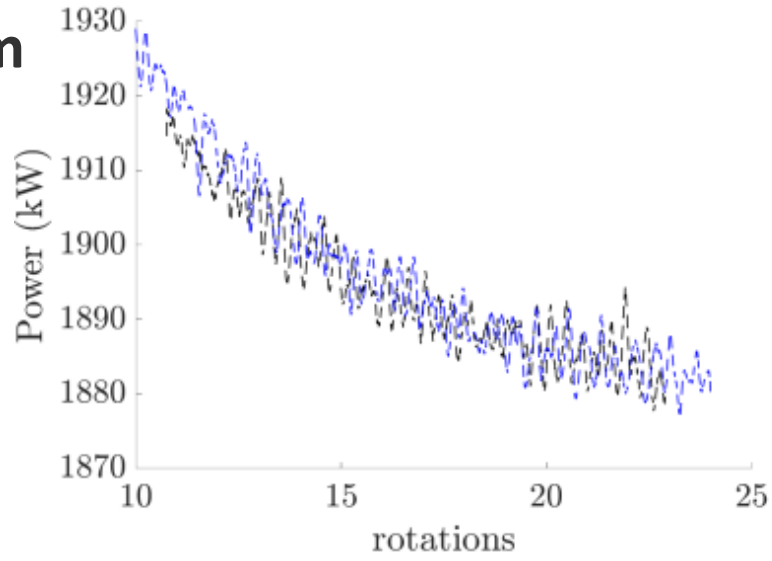
Isocontours of Q-criterion with velocity visualized in the wake for NREL 5-MW turbine(s) operating under uniform inflow wind speed of 8 m/s.

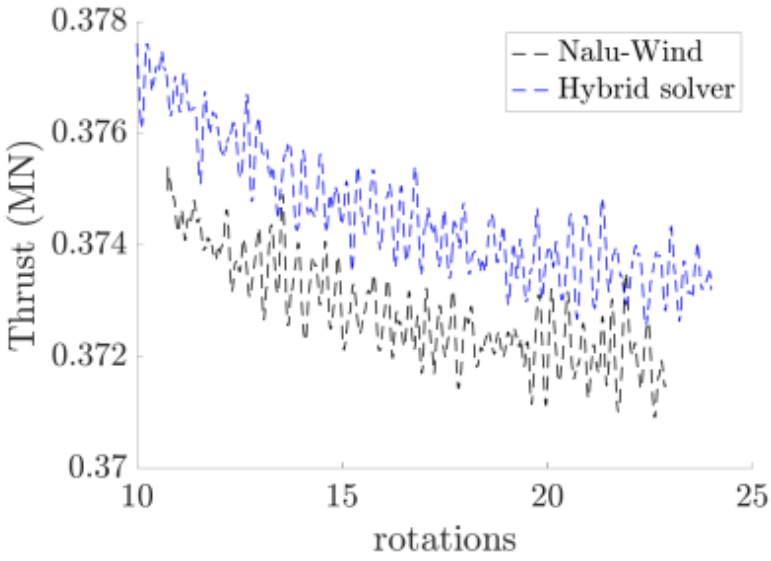
Key team members: Sharma, Ananthan

Hybrid AMR-Wind / Nalu-Wind solver NREL 5-MW demonstration problem on Summit (continued, slide 4)

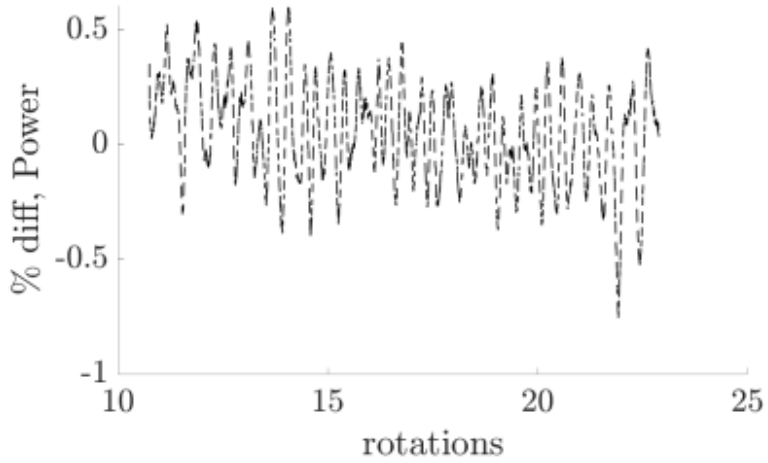
<u>Results</u>

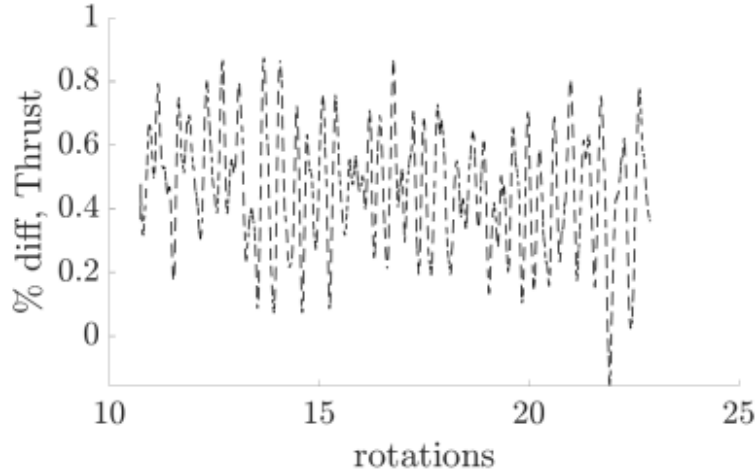
- Hybrid solver produced correct QoIs
- Efficient hybrid solver compares favorably to Nalu-Wind-only simulations
- Excellent agreement obtained
  - 0.2% difference in predicted power
  - 0.45% difference in predicted thrust





Hybrid solver vs Nalu-Wind only. Comparison of turbine power and thrust for NREL 5-MW turbine operating under uniform inflow wind speed of U = 8 m/s for time-step sizes corresponding to 0.25.





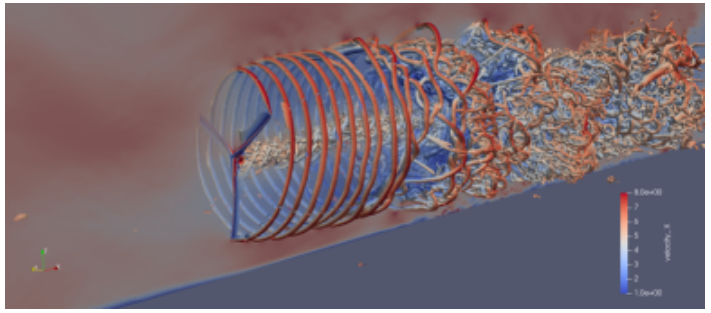
Difference in steady-state power predicted using hybrid AMR-Wind/Nalu-Wind solver with respect to stand-alone Nalu-Wind runs.

Key team members: Sharma, Ananthan

Conclusions and Future Work

Conclusions

- ExaWind software stack will enable harnessing of exascale HPC for high-res simulation of wind farms
- ExaWind team is creating an exascale-ready open source CFD software stack for the wind energy research community
- Will empower community with tools for better wind turbine and farm designs, and optimized performance to maximize electricity generation



Future work

- Meet ECP challenge problem in 2023
  - Scale up to whole wind farms
  - Push on Nalu-Wind/AMR-Wind hybrid solver
  - Include FSI, better BCs, better turbulence models
  - Improve underlying Trilinos & *hypre* solvers
- Prepare ExaWind software for exascale
  - Improve performance on Summit, Eagle, Spock
  - Better leverage GPUs
  - Port to, and prepare for, Frontier (& Aurora)
- Continue V&V and credibility improvement activities
- Add offshore wind and complex terrain capabilities
  - Floating platforms
  - Ocean waves
  - Whole turbine motion

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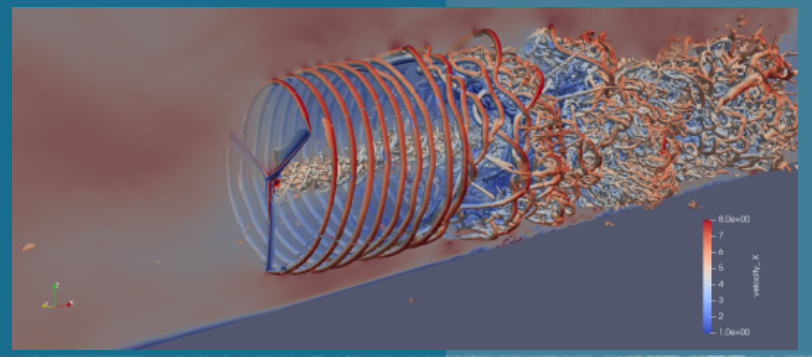
Harnessing exascale for whole wind farm high-fidelity simulations to improve wind farm efficiency



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