Towards Exascale for Wind Energy Simulations

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Abstract

We examine large-eddy-simulation modeling approaches and computational performance of two open-source computational fluid dynamics codes for the simulation of atmospheric boundary layer (ABL) flows that are of direct relevance to wind energy production. The first is NekRS, a high-order, unstructured-grid, spectral element code. The second, AMR-Wind, is a block-structured, second-order finite-volume code with adaptive-mesh-refinement capabilities. The objective of this study is to co-develop these codes in order to improve model fidelity and performance for each. These features will be critical for running ABL-based applications such as wind farm analysis on advanced computing architectures. To this end, we investigate the performance of NekRS and AMR-Wind on the Oak Ridge Leadership Facility supercomputers Summit, using 4 to 800 nodes (24 to 4,800 NVIDIA V100 GPUs), and Crusher, the testbed for the Frontier exascale system using 18 to 384 Graphics Compute Dies on AMD MI250X GPUs. We compare strong- and weak-scaling capabilities, linear solver performance, and time to solution. We also identify leading inhibitors to parallel scaling.

Keywords

Exascale, Scalability, Large-Eddy Simulation

Introduction

Atmospheric boundary layer (ABL) flows are an important part of everyday life. Aside from being a primary driver of vertical exchanges in moisture, aerosols, and atmospheric gases, the ABL affects practical aspects of life—including the transportation system, renewable energy generation, pollution dispersion, noise propagation, and transmission of electromagnetic signals. ABL flows are turbulent, and the state of the turbulence is affected by density stratification that arises in large part from surface heating and cooling. Additionally, Coriolis effects caused by planetary rotation and curvature complicate the flow. Furthermore, regional-scale weather patterns and terrain add complexity to the ABL. Significant research effort is applied to ABL flows because of their importance and complexity Moeng (1984); Berg and Kelly (2020); Beare et al. (2006); Sullivan et al. (2008); Kosović and Curry (2000); Pedersen et al. (2014); Mirocha (2020); Churchfield and Moriarty (2020). This work focuses on numerical computation of ABL flows using large eddy simulation (LES), where the governing physics equations are solved in filtered form such that the larger, energy-containing eddies are directly resolved, and the remaining “subgrid-scale” (SGS) turbulence is modeled. LES was born out of ABL research roughly five decades ago Lilly (1962); Smagorinsky (1963), and continues to evolve and improve.

Wind energy is a prime example of an application driven by the ABL. Generation of electrical energy from farms of wind turbines at night in the stable ABL is a particularly interesting situation. The winds tend to be stronger, so generation is higher. With decreased turbulence, wind turbine wakes persist for longer distances, significantly affecting wind farm efficiency and fatigue loads on waked wind turbines. With this example in mind, researchers wish to increase grid resolution to reduce reliance on the SGS turbulence model, but they also wish to increase the overall domain size to encompass the wind farm, which commonly extends many kilometers horizontally. Increased domain size is desirable in many other applications besides wind energy. For example, LES can be used to study deep convection, which happens over a large geographical extent many kilometers into the atmosphere, and there is a push toward LES of regional-scale weather.

High-fidelity LES of the turbulent ABL is dependent on massively parallel high-performance computing (HPC). HPC architectures are evolving from traditional homogeneous x86-CPU-based computing. For example, the world’s second-fastest computer (as of June 2022), the Supercomputer Fugaku at the RIKEN Center for Computational Science Fugaku, is built around Fujitsu’s custom ARM A64FX processor and does not use a GPU. Alternatively, the U.S.

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Department of Energy (DOE) has embraced a hybrid CPU-GPU approach for its leadership-class computing. Summit, the world’s fourth-fastest computer, has nodes that house two IBM POWER9 CPUs (each with 22 cores) and six Nvidia V100 GPUs and is capable of \(200 \times 10^{15}\) floating-point operations per second (FLOPS). Similarly, DOE’s first exascale-class supercomputers, i.e., those capable of at least \(10^{18}\) FLOPS, will be a hybrid CPU-GPU based systems. Frontier, the world’s first exascale class supercomputer at the Oak Ridge Leadership Computing facility, has nodes that house one AMD CPU and 4 AMD MI250X GPUs Frontier.

As described in a 2015 DOE workshop report Sprague et al. (2017), the transition to exascale computing brings many opportunities in computational fluid dynamics (CFD), as well as significant challenges. Two of the grand challenge opportunities described in that workshop report are relevant to this paper: the simulation of boundary layer turbulence over large areas and the simulation of an entire wind farm under realistic atmospheric flow conditions. The transition to GPU-accelerated computing is significant for those performing CFD for numerical weather forecasting or for LES of ABL flows. While hybrid CPU-GPU processing potentially enables dramatically faster computing (at low power), legacy CPU-based codes need significant overhauls or rewrites to run effectively in a CPU-GPU environment Sprague et al. (2017); Robinson and Sprague (2020).

Several groups have introduced CFD codes for LES of atmospheric flows with an emphasis on GPU calculations. While early efforts in weather forecasting on GPUs focused at \(O(100)\) m resolution (see, e.g., Schalkwijk et al. (2015)), more recent efforts have performed high-fidelity GPU-based LES on \(O(1)\) m grid sizes. Van Heerwaarden et al. Van Heerwaarden et al. (2017) introduced the MicroHH 1.0 incompressible-flow solver directed at atmospheric flow; the solver is based on finite-difference spatial discretization and a split-operator time integration. The authors showed that for problem sizes that fit, a single GPU had performance similar to that of 32 CPU cores. Sauer and Múnoz-Esparza Sauer and Muñoz-Esparza (2020) introduced the FastEddy LES model that was created for CPU and GPU systems. FastEddy solves the fully compressible Navier–Stokes equations using finite-difference spatial discretization and explicit Runge–Kutta time integration. The authors showed excellent scaling on up to 32 GPUs and argued that one GPU provides performance similar to that of 256 CPU cores. Recent high-order incompressible flow codes using fast tensor-product operator evaluation include ExaDG Arndt et al. (2020) and SPECHT_Fs Huismann et al. (2019) and deal.ii Krank et al. (2017). ExaDG and deal.ii use a discontinuous Galerkin formulation, whereas SPECHT_FS uses a continuous Galerkin formulation similar to that in Nek5000/RS.

In this paper we examine LES modeling approaches and computational performance of two open-source, incompressible-flow, GPU-oriented CFD codes that employ fundamentally different spatial discretization and data structures. The first is NekRS NekRS; Fischer et al. (2021a, 2020), which is an updated version of the Nek5000 code Nek5000. Nek5000/RS is a high-order, unstructured-grid, spectral-finite-element CFD code. The second is AMR-Wind AMR-Wind, which is part of the ExaWind simulation suite Sprague et al. (2020). AMR-Wind is a block-structured, second-order, finite-volume-method CFD code with adaptive mesh refinement (AMR) capabilities and is built on the AMReX library, a software framework for massively parallel, block-structured applications AMReX-Codes. Both of these codes are part of the U.S. DOE Exascale Computing Project, which is supporting the development of GPU-ready applications for exascale-class supercomputers ECPAlexander et al. (2020).

We compare NekRS and AMR-Wind predictions and performance on the well-known GEWEX (Global Energy and Water Cycle Experiment) Atmospheric Boundary Layer Study (GABLES) stably stratified benchmark LES case Beare et al. (2006), which is illustrated in Fig. 1. The flow comprises a quiescent mean flow above \(\approx 200\) m (going to the right and into the page in Fig. 1) with a sheared turbulent boundary layer (going to the right and out of the page) over the 0–200 m vertical range. The flow is coupled with thermal buoyancy effects. The computational domain is \(400 \times 400 \times 400\) m and doubly periodic in the streamwise \((x)\) and cross-flow \((y)\) directions. Potential temperature distributions at Reynolds number \(Re = 50 M\) and \(\approx 6\) hours are illustrated in Fig. 2 along with profiles in Fig. 3.

In addition to investigating these codes’ ability to represent ABL physics, an objective of this study is to co-develop these codes in order to improve model fidelity and performance, features that will be critical for running ABL-based applications such as wind farm analysis on advanced computing architectures. By careful cross-comparison, both codes have made significant advances. This article focuses on performance. A separate article addresses subgrid-scale modeling for LES of the ABL. Here we investigate the scalability of NekRS and AMR-Wind on the Oak Ridge Leadership Computing Facility supercomputer Summit, using 4 to 800 nodes (24 to 4,800 NVIDIA V100 GPUs). We provide iteration counts, average-time per step, and the real-time ratio (ratio of wall-clock time to physical time), as well as detailed performance metrics. We additionally include a limited set of timing data for the two codes on Crusher, using up to 384 Graphics Compute Dies (GCDs) on AMD MI250X GPUs (one MPI rank per GCD).

The paper is organized as follows. Section II describes the codes and gives an overview of the numerical approaches used. Section III discusses the numerical setup of the simulations. Section IV provides studies comparing the codes’ performance and scaling. Section V presents a brief summary.

### Description of Codes

The numerical results are based on LES, which requires enhanced dissipation to provide an energy drain at the grid scale. Consequently, the incompressible Navier–Stokes (NS) and potential temperature equations are solved in a spatially filtered resolved-scale formulation, expressed in
where the angle brackets $\langle \rangle$ is an "isotropy factor," which accounts for variability in the SGS constants due to anisotropy of the mean flow. In Sullivan et al. (1994), the fluctuating eddy viscosity, $\nu_s$, is obtained by using an eddy viscosity model based on the SGS turbulent kinetic energy equation, in which the shear production term is computed from the fluctuating velocities as suggested by Schumann (1975a).

Here, the fluctuating (isotropic) part is taken into account through the use of either a high-pass filter (HPF) Stolz et al. (2005) or a Smagorinsky (SMG) model based on the fluctuating strain rate. For the former model, which is not eddy-viscosity based, $\nu_t$ in Eq. (7) is by definition equal to zero. On the other hand, the expression for $\nu_T$ is derived so that the law-of-the-wall behavior can be recovered in the absence of any resolved turbulence.

The SGS modeling in AMR-Wind is based on Smagorinsky (1963), where a single partial differential equation for subgrid-scale kinetic energy is solved, and from that a subgrid-scale eddy viscosity is computed. The Boussinesq eddy viscosity hypothesis is then invoked to obtain the subgrid-scale stress tensor and heat flux vector.

In the following subsections we discuss the details of the numerical approaches of Nek5000/RS and AMR-Wind. For simplicity, we use $u_i$, $p$, and $\theta$, dropping the overbar notation from $\bar{u}_i$, $\bar{p}$, and $\bar{\theta}$ in the remaining sections.

**Nek5000/RS**

Nek5000 Nek5000 is a spectral element code that is used for a wide range of thermal-fluids applications. It employs high-order spectral elements Patera (1984) in which the solution, data, and test functions are represented as locally structured $N$th-order tensor-product polynomials on a set of $E$ globally unstructured curvilinear hexahedral brick elements. The approach yields two principal benefits. First, for smooth functions such as solutions to the incompressible NS equations, high-order polynomial expansions exhibit rapid convergence with approximation order, often yielding a significant reduction in the number of unknowns ($n \approx EN^3$) required to reach engineering tolerances. Second, the locally structured forms permit local lexicographical ordering with minimal indirect addressing and, crucially, the use of tensor-product sum factorization to yield low $O(n)$ storage costs and $O(nN)$ work complexities Orszag (1980).

NekRS Fischer et al. (2021a) is a GPU-accelerated version of Nek5000 that is targeting high performance on forthcoming exascale platforms. For performance portability, NekRS is written in C++/OCCA Medina et al. (2014).
Several key kernels are based on highly tuned OCCA kernels coming from the development work of Warburton and co-workers in the libParanumal library Chalmers et al. (2020). Specific attention in NekRS has been given to ensure scalability to $P = 10^5–10^6$ ranks and beyond Fischer et al. (2021b). NekRS retains access to the standard Nek5000 interface, which allows users to leverage existing user-specific source code such as statistical analysis tools for turbulence.

Time integration in Nek5000/RS is based on a semi-implicit splitting scheme using $k$th-order backward differences (BDF$k$) to approximate the time derivative coupled with implicit treatment of the viscous and pressure terms and $k$th-order extrapolation (EXT$k$) for the remaining advection and forcing terms. This approach leads to independent elliptic subproblems comprising a Poisson equation for the pressure, a coupled system of Helmholtz equations for the three velocity components, and an additional Helmholtz equation for the potential temperature. The pressure Poisson equation is obtained by taking the divergence of the momentum and forcing terms. This approach leads to independent elliptic subproblems comprising a Poisson equation for the pressure, velocity, and temperature. Velocity and temperature Helmholtz equations are obtained once $p^n$ is known:

$$\frac{\partial}{\partial t} \frac{\partial}{\partial x_j} p^n = q^n, \quad (8)$$

$$\beta_0 \Delta t \frac{\partial}{\partial x_j} \left( \frac{1}{Re + \gamma \nu} \right) 2S^n_{ij} = - \frac{\partial}{\partial x_i} p^n + r^n_i, \quad (9)$$

$$\left[ \frac{\beta_0}{\Delta t} - \frac{\partial}{\partial x_j} \left( \frac{1}{Pe + \gamma \nu} \right) \frac{\partial}{\partial x_j} \right] s^n = s^n, \quad (10)$$

where $\beta_0$ is an order-unity constant associated with BDF$k$, Fischer et al. (2017); $S^n_{ij}$ is the resolved-scale strain-rate tensor as described in (5); $q^n$, $r^n_i$, and $s^n$ represent the sum of the values from the previous timesteps for the contributions from BDF$k$ and EXT$k$. Also included in $r^n_i$ and $s^n$ are eddy diffusion terms coming from the mean-field eddy diffusivity mentioned above. The fully coupled system of Helmholtz equations for the three velocity components (9) is used only when the fluctuating (isotropic) part of the SGS stress tensor is modeled using an SMG model based on the fluctuating strain rate. When this part is modeled through the use of a high-pass filter (HPF) Stolz et al. (2005), the resulting Helmholtz equations for the three velocity components are not coupled.

With the given time-splitting, we recast (8)–(10) into weak form and derive the spatial discretization by restricting the trial and test spaces to be in the finite-dimensional space spanned by the spectral element basis. The discretization leads to a sequence of symmetric positive definite linear systems for pressure, velocity, and temperature. Velocity and temperature are diagonally dominant and readily addressed with Jacobi-precondition conjugate gradient iteration. The pressure Poisson solve is treated with GMRES using $p$-multigrid as a preconditioner. Details of the formulation can be found in Fischer and Lottes (2004); Fischer et al. (2017); Phillips et al. (2022).

NekRS supports several features to accelerate performance, including overlapped communication and computation during operator evaluation, which yields a $10–15\%$ performance gain for NS simulations; FP32 local-operator inversion and residual evaluation for the Chebyshev-accelerated Schwarz-based $p$-multigrid; and projection of the velocity and pressure solutions onto the space of prior solutions to generate an initial guess, which can yield a $1.5–2$-fold NS performance gain Fischer (1998). On the NVIDIA A100, the OCCA-based kernels are close to the bandwidth-limited roofline and are sustaining $2.1–2.2$ TFLOPS (FP64) for the Poisson operator, and $3.1–3.8$ TFLOPS (FP64) for the advection operator. In the pressure preconditioner, the forward Poisson operator on the coarsest multigrid levels realizes $2.5–3.9$ TFLOPS (FP32) and the Schwarz smoother sustains $2.5–5.1$ TFLOPS (FP32). (The lower values are for smaller values of $N$ that are used in the $p$-multigrid V-cycle.) Comparable values are realized on the NVIDIA V100s on Summit, save that they are $\approx \frac{1}{2}$ times lower than those on the A100. Sustained flop rates for the full NS solver are $\approx 470$ GFLOPS per V100 on Summit, as discussed in Section.

**AMR-Wind**

AMR-Wind is a spatially and temporally second-order accurate finite-volume code. Important aspects of the discretization are discussed below; for more details readers can see Almgren et al. (1998) since the discretization is similar to the incompressible-flow solver IAMR. Velocity, scalar quantities, and gradients of pressure are located at cell centers, whereas pressure is located at nodes. Partial staggering combined with an approximate projection method yields linear systems that are well studied, have small-bandwidth stencils, and can be efficiently solved with standard techniques such as geometric multigrid. These discretization choices give a well-balanced mix of both efficiency and accuracy. In addition to the spatial staggering there is also staggering in time similar to a Crank–Nicolson formulation. The time discretization is

$$\frac{c_k^{n+1} - c_k^n}{\Delta t} + \left[ \frac{\partial c_k u_j}{\partial x_j} \right]^{n+1/2} = \frac{1}{\rho^{n+1/2}} \frac{\partial q_k^{n+1}}{\partial x_j} + G_k^{n+1/2}, \quad (11)$$

$$\frac{u_j^n - u_j^n}{\Delta t} + \left[ \frac{\partial u_j u_j}{\partial x_j} \right]^{n+1/2} = \frac{1}{\rho^{n+1/2}} \left( \frac{\partial p^{n+1/2}}{\partial x_i} - \frac{\partial p^{n-1/2}}{\partial x_i} \right) + F_i^{n+1/2}, \quad (12)$$

where $c$ indicates a scalar quantity and $u$ denotes velocity. The index $n$ represents a time step, the index $i$ runs over the three momentum equations, the index $k$ runs over the scalar equations, and the repeated index $j$ indicates summation. $F_i^{n+1/2}$ and $G_k^{n+1/2}$ are source terms and are evaluated at time step $n + 1/2$. $\rho$ is density, which in these simulations is constant in time and space, but we leave the time level to show at what point in time density is evaluated if the code is run in variable-density mode.

The advection term is formed by extrapolating in time by using a Godunov method Almgren et al. (1998). Specifically, the velocity is first extrapolated in space (to the faces) and in time to $n + 1/2$ in a predictor step. MAC projection Bell
et al. (1991) is applied to ensure that the face velocities are divergence free, which takes the form
\[ P^{\text{MAC}}(u^f) = u^f - \frac{1}{\rho^f} \left( \frac{\partial \psi}{\partial x_i} \right), \]
where \( u^f \) represents a face velocity and \( \psi \) is a Lagrange multiplier located on the cells. Setting the divergence equal to zero forms a variable coefficient Poisson equation:
\[ \frac{\partial}{\partial x_j} \left( \frac{1}{\rho^f} \frac{\partial \psi}{\partial x_j} \right) = \frac{\partial u^f}{\partial x_j}. \]
The Poisson equation is discretized by using a cell-centered seven-point stencil in 3D, which is efficiently solved by using multilevel multigrid as a linear solver Zhang et al. (2019). Once the velocity on the faces is divergence free, the advection terms are formed. Options for discretizing these advection terms include Godunov PLM Van Leer (1977), PPM Colella and Woodward (1984), and WENO-Z Motheau and Wakefield (2020). The Godunov schemes are high-order accurate and use an extended stencil. The scalar equations (e.g., potential temperature) are advanced one at a time by solving a Helmholtz problem. This Helmholtz problem is discretized by using a cell-centered finite-difference method forming a 7-point stencil in 3D Almgren et al. (1998). The momentum equations are saved for last to allow the advection terms to be evaluated at \( n + 1 \) by using the previously updated scalar equations. A good example is the Boussinesq buoyancy term, which adds a source term at time \( n + 1 \) to the momentum equation. The Boussinesq buoyancy term is a function of the already advanced potential temperature, which is averaged to time \( \frac{t^{n+1}}{\Delta t} = (n + 1) \Delta t \). The Boussinesq buoyancy term is a function of the already advanced potential temperature, which is averaged to time \( \frac{t^{n+1}}{\Delta t} = (n + 1) \Delta t \). The scalar equations and momentum equations can be solved by using geometric multigrid or, if diagonally dominant enough, a Krylov method such as bicgstab (biconjugate gradient stabilized) is sufficient. In this work, because of the small time step, we use only bicgstab in all of the Helmholtz solves.

The intermediate velocity \( u^* \) is advanced by solving a Helmholtz problem in tensor form. However, this velocity vector \( u^* \) is not guaranteed to be divergence free. An approximate projection method is used to solve for the velocity at time \( t^{n+1} = (n + 1) \Delta t \):
\[ u^{n+1} = P(u^*), \tag{13} \]
where the nodal projection \( P \) is defined to be
\[ P(u^*) = u^* + \frac{\Delta t}{\rho^{n+1/2}} \left( \frac{\partial p}{\partial x_i} - \frac{\partial \phi}{\partial x_i} \right). \tag{14} \]
This approximate projection is different from the algorithm in Almgren et al. (1998) and more similar to the projection in Almgren et al. (2000) labeled version 2. Taking the divergence of (14) and setting it equal to zero, we have
\[ \frac{\partial}{\partial x_j} \left( \frac{\Delta t}{\rho^{n+1/2}} \frac{\partial \phi}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left( u^*_j + \frac{\Delta t}{\rho^{n+1/2}} \frac{\partial p}{\partial x_j} \right), \tag{15} \]
where \( \phi \) is a Lagrange multiplier related to the pressure field and solved on the nodes. To solve the nodal projection in (15), a variational form is used, which leads to a 27-point stencil Almgren et al. (1998). The right-hand side of (15) is formed by taking finite differences across cells and averaging them to each node. Each node has four contributions in each coordinate direction. Once the solution \( \phi \) is obtained, the velocity is updated by using (14), and the pressure and its gradient are updated by using
\[ p^{n+1/2} - \phi, \frac{\partial p^{n+1/2}}{\partial x_i} \leftarrow \frac{\partial \phi}{\partial x_i}. \]

The gradient \( \frac{\partial \phi}{\partial x_i} \) is approximated by taking finite differences of \( \phi \) along edges and averaging each edge to the cell center. For each coordinate direction four edges contribute to the value at the cell center.

**Simulations**

We consider a stable ABL in which the ground temperature (at \( z = 0 \)) is cooler than the air temperature and where the ground temperature continues to cool over the duration of the simulation. Here we give full details of the numerical setup. The simulation domain is \( \Omega = L_x \times L_y \times L_z = 400 \ m \times 400 \ m \times 400 \ m \), with \( x \) the streamwise direction, \( y \) the spanwise direction, and \( z \) the vertical direction. Simulations are initialized (at \( t = 0 \)) with constant velocity in the streamwise direction equal to geostrophic wind speed of \( U = 8 \ m/s \). The initial potential temperature is \( 265 \ K \) in \( z \leq 100 \ m \) and linearly increased at a rate of 0.01 K/m in 100 m \( \leq z \leq 400 \ m \). The reference potential temperature is \( 263.5 \ K \). The Reynolds number is \( Re = U L_b / \nu \), where \( L_b = 100 \ m \) is the thickness of the initial thermal boundary layer and \( \nu \) is the molecular viscosity. An initial perturbation is added to the temperature with an amplitude of 0.1 K on the potential temperature field for \( 0 \leq z \leq 50 \ m \).

Periodic boundary conditions (BCs) are used in the streamwise and spanwise directions. At the top boundary, \( z = 400 \ m \), a stress-free, rigid lid is applied for momentum, and the heat flux for the energy equation is set consistent with the 0.01 K/m temperature gradient initially prescribed in the upper region of the flow. At the bottom boundary, we perform simulations with impenetrable traction BCs for the velocity where the specified shear stress comes from Monin–Obukhov similarity theory Monin and Obukhov (1954). For the energy equation, a heat flux is applied that is derived from the same theory and a specified potential temperature difference between the flow at a height, \( z_1 \), and the surface. The surface temperature is from the GABLS specification following the rule \( \theta_b(t) = 265 - 0.25 t \), where \( t \) is in hours. Because the boundary conditions are periodic (lateral), or the mass flow rate through the boundaries is zero (top and bottom), pressure boundary conditions are not needed.

In Nek5000/RS, the implementation of the traction BCs for the horizontal velocity components is performed in the context of the log-law for which we follow the approach of Grotjans and Menter (1998) and Kuzmin et al. (2007), which is appropriate for finite element methods based on a weighted residual formulation. The traction BCs imposed on the tangential velocity are based on the horizontally averaged slip velocity that develops at the boundary and the law of the wall and is effected through the use of the mean-field eddy viscosity model of Sullivan et al. (1994). The approach
Figure 2. NekRS(HPF, SMG) and AMR-Wind at three grid-refinement levels for potential temperature at time 6 h.

Figure 3. NekRS (HPF, SMG) and AMR-Wind: velocity magnitude and potential temperature at each hour, 1 h, 2 h,...,9 h.
originally used by Schumann (1975b) is used to convert the horizontally averaged traction to local values based on the local slip velocity in each of the horizontal directions.

In AMR-Wind, the periodic BCs in the \( x \) and \( y \) directions and the slip boundary on the top wall are applied. On the bottom wall, Dirichlet BCs in the normal direction and inhomogeneous Neumann BCs in the \( x \) and \( y \) directions are applied. The inhomogeneous Neumann BC is set using the expression for \( \tau \), the total wall shear stress, and \( q \), the total wall heat flux, in (16). The stresses are specified at the terrain boundary following Moeng Moeng (1984). The wall stress vector is defined as

\[
\tau_{i3} = \frac{u_i s + \bar{\theta} (u_i - \bar{u}_i)}{s^2} u^2_x, \tag{16}
\]

where \( u_i \) is the velocity at the first cell height, \( s \) is the wind speed \( s = \sqrt{u_x^2 + u_y^2} \), and \( u_x \) is the friction velocity computed by using the Monin–Obukhov similarity law Monin and Obukhov (1954); Etling (1996). The overbar indicates a horizontal plane average at the first cell height. The heat flux is defined as

\[
q = \left[ (\theta - \bar{\theta}) s + (\bar{\theta} - \theta_w) s \right] \frac{u_x K}{\bar{s} \phi_h}, \tag{17}
\]

where \( \theta \) is the temperature, \( \theta_w \) is the wall temperature, \( \kappa \) is the von Karman constant, and \( \phi_h \) comes from the Monin–Obukhov similarity law.

The range of scales in these simulations is evident in Fig. 2, which shows variations in potential temperature on a horizontal \( x-y \) slice at the height \( z = 100 \) m. For resolutions \( \Delta x = 3.12 \) m, \( 1.56 \) m, and \( 0.78 \) m, respectively from left to right, for the differing codes/models. For NekRS, \( \Delta x \) represents the average grid spacing given by \( 400 \) m/(\( E_0^x N \)), where \( E_0 \) is the number of elements in the \( x \), \( y \), or \( z \)-direction and \( N \) is the local polynomial order. The number of elements is \( E = E_0^x = 16^3, 32^3 \), and \( 64^3 \) for the stated resolutions. The top row in Fig. 2 shows NekRS results using MFEV and HPF; the middle row shows NekRS results using MFEV and Smagorinsky, as described in Section ; and the bottom row shows AMR-Wind results. At a height of \( z = 100 \) m, the temperature variations around the horizontally averaged value are small, between \( 264.40 \) K and \( 264.80 \) K. One can see that as the grid scale is decreased from \( \Delta x = 3.12 \) m to \( 0.78 \) m, both codes capture increasingly finer scales. We remark that direct numerical simulation at the given Reynolds number, \( Re = 5 \times 10^7 \), would require \( \approx 10^{15} \) grid points, which is two orders of magnitude beyond current state of the art simulations of \( n = 18000^3 \) for isotropic turbulence Ravikumar et al. (2019). The importance of the SGS model is that it potentially allows one to account for the effects of small-scale motions without needing to resolve all of them.

Figure 3 shows profiles of the horizontally averaged streamwise, \( \langle u \rangle \), and spanwise, \( \langle w \rangle \), wind velocities (top) and potential temperature, \( \langle \theta \rangle \), (bottom) at 1-hour time intervals between 1 h and 10 h for a mesh resolution of \( n = 512^3 \) (\( \Delta x = 0.78 \) m) for each code. The left figures show NekRS results using MFEV and HPF, the center figures show NekRS using MFEV and Smagorinsky, and the right figures show the results for AMR-Wind. As can be observed, the time evolution of the mean velocity and temperature profiles obtained from the two codes agree well despite using very different numerical methods and subgrid-scale models. The agreement between AMR-Wind and NekRS improves when using MFEV and Smagorinsky (i.e., between the center and right figures). Specifically, the height of the low-level jet peak velocity during quasi-steady evolution in the GABLS problem (after approximately 7 h) is between \( 150 \) and \( 160 \) m, and its maximum value is between \( 9.5 \) and \( 9.7 \) m/s. An outgrowth of these comparative simulations has been a concerted effort to carefully validate and cross-check the SGS models. The improvement in the NekRS SGS model, realized by moving away from the HPF model to using the Smagorsnky model for the isotropic stress term, is a direct outcome of this collaborative effort.

**Performance**

Here we compare performance and tuning for the two codes. For each case, the codes use the same spatial resolution, \( \Delta x \), and timestep size, \( \Delta t \). Each code uses iteration tolerances of \( 10^{-4} \) and \( 10^{-6} \) for the respective 2-norm residuals of the pressure-Poisson and velocity-Helmholtz problems. For purposes of timings, we use the solution at 6 hours as an initial condition in each case in order to ensure that performance studies are done over a timeframe in which the solutions have a representative turbulent flow. Table 1 provides a summary of the test parameters, in physical units, that are used for the strong- and weak-scaling studies. The spectral element cases use 8th-order polynomial basis (\( N = 8 \)) with a number of gridpoints given by \( n = E N^3 \). For these cases we take \( \Delta x \) to be the average grid spacing in each direction (i.e., \( 400 \) m/\( n \)). For the weak-scale study, the domain height is fixed at \( 400 \) m while the dimensions are increased in the \( x \) and \( y \) directions as \( n \) is increased. In order to avoid initial transient behavior, the average (wall) time per step, \( t_{\text{step}} \), in seconds is measured over steps 101–200.

**Performance Tuning and Profiling**

We begin with performance optimization, profiling analysis, and CPU versus GPU comparisons.

NekRS GPU performance tuning on Summit is demonstrated in detail in Fischer et al. (2021a,b). The base libParanumeral kernels have their origins in the work of Warburton and co-workers Chalmers et al. (2020); Świrydowicz et al. (2019); Chalmers and Warburton (2020); Abdelfattah et al. (2021). A key algorithmic component is the Chebyshev-accelerated Schwarz-based \( p \)-multigrid for the pressure solve Phillips et al. (2022), which is performed in 32-bit precision (e.g., as in Fehr et al. (2018)) to reduce injection-bandwidth pressure on the Summit network interface cards. Communication for the nearest-neighbor communication (direct-stiffness summation in the finite element or spectral element context Deville et al. (2002)) is overlapped with computation whenever it proves to be effective, which can yield as much as 10–15% savings in NS applications. At the strong-scale limit of \( \approx 2 \) M points per GPU, there are enough points interior to each rank’s subdomain to balance out the communication overhead for the gather-scatter exchanges, at least at the fine-mesh level evaluations. For the coarser \( p \)-multigrid levels, it is not always the case that one can
AMR-Wind: Performance progress with AMReX library updates

|                | Old Version | Intermediate Version | New Version |
|----------------|-------------|----------------------|-------------|
|                | Wall time per timestep |               |             |
| Advection      | 3.3200e-01 (s)  | 2.4100e-01 (s)  | 2.5600e-01 (s) |
| MAC Projection | 6.2582e-02 (s)  | 6.0782e-02 (s)  | 6.0000e-02 (s) |
| Pressure Solve | 7.3671e-02 (s)  | 7.3481e-02 (s)  | 7.3000e-02 (s) |
| Velocity Solve | 1.1401e-01 (s)  | 1.1300e-01 (s)  | 1.1200e-01 (s) |
| Scalar Solve   | 3.4827e-02 (s)  | 3.4827e-02 (s)  | 3.4827e-02 (s) |
| Fillpatch      | 1.5538e-02 (s)  | 1.5538e-02 (s)  | 1.5538e-02 (s) |

Here, SS10 indicates Slingshot 10, and SS11 indicates Slingshot 11, which shows about a 1.5× improvement over SS10. The listings also show which communication mode was used. We see that pw+device, which stands for pairwise device-to-device exchange (i.e., via GPU-direct) is used in most instances. The pw+host, which indicates the use of pairwise exchanges via the host, is used only in the case of many short messages, which is typically the scenario at the coarsest levels of the p-multigrid solver.

Over the course of the collaboration, AMR-Wind realized a 1.4× speedup with some improvements derived through AMReX library updates. The performance progress is demonstrated in Table 2, where the rows present a timing breakdown of a typical flow time step. Advection involves predicting and forming the advection term using Godunov PPM WENO. MAC projection is a Poisson equation linear solve with a 7-point stencil that ensures that the face velocities are divergence free. The pressure solve is a Poisson equation linear solve with a 27-point stencil that approximately corrects the cell velocity to be divergence free at the end of the time step. Velocity and scalar solve are Helmholtz equations with a 7-point stencil, and Fillpatch performs all communication within and across processors outside of the linear solver communication. In the table, the old version is AMR-Wind using AMReX from April 2021. The intermediate version is the same source code but with improvements to the linear solver settings. In particular, the components of the momentum equations are solved separately instead of as a coupled tensor solve. The velocity and scalar (temperature) linear systems are solved by using bi-conjugate gradient iteration instead of a full geometric multigrid approach. In Table 2 we see that these optimizations reduce the velocity solve time by almost 3× (.114 s to .039 s) and the scalar solve time by 1.5× (.035 s to .022 s). The new version is AMR-Wind based on AMReX from 2022 with the same improved linear system settings. Here the scalar solve improves by another factor of 1.5, and the pressure solve is reduced from .0073 s to .0063 s per step.

For AMR-Wind, Table 3 more clearly indicates the elliptic solves as leading cost contributors. This cost is also reflected in Fig. 4, where the two largest contributors to run time are the pressure solve and the MAC projection onto a divergence-free space. In fact, these plots show that the requirement of two Poisson-like solves for AMR-Wind is the principal cause for discrepancy in run-time between the two codes. MAC projection is solved using geometric multigrid. While not necessary, it does provide more robustness and increases the stability of the scheme to CFL=2. If it did not require the MAC step, AMR-Wind would be faster on 4 nodes than NekRS, pressureSolve is a Poisson solve that is used at the end of the timestep to form an approximate divergence-free velocity at the cell center; it is a node-based 27 point stencil, and the linear system is solved using geometric multigrid. scalarSolve and velocitySolve are both Helmholtz solves that are cell-based 7 point stencils, the scalarSolve advances in time the potential Temperature

Table 1. Problem setup for strong and weak scaling studies.

| Domain size | Grid Points (n) | Δx (m) | Δt (s) |
|-------------|----------------|--------|--------|
| 400 m³      | 512 × 512 × 512 | 0.78   | .025000 |
| 400 m³      | 1024 × 1024 × 1024 | 0.39  | .01250 |
| 400 m³      | 2048 × 2048 × 2048 | 0.19  | .015625 |
| 3200 m³     | -               | -      | -      |

| Domain size | Grid Points (n) | Δx (m) | Δt (s) |
|-------------|----------------|--------|--------|
| 400 m × 400 m × 400 m | 512 × 512 × 512 | 0.78   | .025000 |
| 800 m × 800 m × 400 m | 1024 × 1024 × 512 | 0.78   | .025000 |
| 1600 m × 1600 m × 400 m | 2048 × 2048 × 512 | 0.78   | .025000 |
| 3200 m × 3200 m × 400 m | 4096 × 4096 × 512 | 0.78   | .025000 |

Table 2. AMR-Wind performance optimization.
### Table 3. CUDA kernel statistics from NVIDIA® Nsight™ profiler using nsys profile --stats=true -t nvtx,cuda.

| AMR-Wind | NekRS |
|----------|-------|
| **Time [%]** | **Total Time (ms)** | **Instances** | **Average (µs)** | **Name** | **Remark** |
| 15.0 | 1890.142 | 142823 | 13.234 | fab_to_fab | array box local copy |
| 9.9 | 1256.128 | 12800 | 98.148 | MLNodeLaplacian::Fsmooth | multigrid smoother |
| 6.9 | 873.629 | 24800 | 35.227 | amrex::Copy | multiple array box parallel copy |
| 5.9 | 738.200 | 5600 | 131.821 | MLABecLaplacian::Fapply | Laplacian op. eval. |
| 4.5 | 564.742 | 43200 | 13.072 | MLPoisson::Fsmooth | multigrid smoother |
| 3.5 | 438.271 | 6800 | 64.451 | MultiFab::LinComb | vector-vector addition |
| 3.1 | 394.024 | 3200 | 123.132 | MLABecLaplacian::normalize | normalize solution |
| 3.0 | 384.391 | 800 | 480.488 | godunov::compute_fluxes | advection momentum |
| 2.9 | 359.910 | 800 | 449.887 | godunov::compute_fluxes | advection scalar |
| 2.7 | 344.575 | 11800 | 29.201 | MultiFab::Xpay | vector-vector addition |
| 2.4 | 303.2 | 29850 | 11.085 | FabArray::setVal | set value of array box |

### Figure 4. NekRS vs AMR-Wind GPU cost breakdown on Summit (top) and Crusher (bottom), using $n = 512^3$ and 2000 steps.

NekRS-Compute Profiling: CUDA Kernel Statistics

11 nodes (66 GPUs), $n/P = 2.03M$, $n = 512^3$, 2000 steps

**NekRS**

| Time [%] | Total Time (ms) | Instances | Average (µs) | Name | Remark |
|----------|-----------------|-----------|--------------|------|--------|
| 7.2      | 1438.604        | 3327      | 432.402      | subCycleStrongCubatureVolumeHex3D | dealiased vel. adv. |
| 6.6      | 1320.502        | 8002      | 165.021      | gatherScatterMany_doubleAdd | FP64 local gather-scatter |
| 5.1      | 1017.806        | 8144      | 124.976      | packBuf_doubleAdd | FP64 packing for gs |
| 5.0      | 1009.247        | 3533      | 285.663      | subCycleStrongCubatureVolumeHex3D | dealias scalar adv. |
| 4.7      | 935.298         | 251       | 3726.289     | scatterMany_double | FP64 scatter |
| 4.4      | 879.495         | 8144      | 107.993      | unpackBuf_doubleAdd | FP64 gather |
| 3.3      | 667.776         | 3192      | 209.203      | subCycleRKUpdate | RK4 vector update |
| 2.9      | 577.150         | 850       | 679.000      | ellipticStressPartialAxCoeffHex3D | viscous op. eval. |
| 2.4      | 480.331         | 2788      | 172.285      | ellipticPartialAxHex3D | pressure op. eval. |

Equation and velocitySolve is three separate solves to advance each of the momentum equations in time. BiCG is used to solve all of the linear Helmholtz subproblems. The advection terms in the governing equations are discretized using a Godunov WENO-Z scheme to provide these terms on the cell faces at time $t^{n+\frac{1}{2}}$. Other function calls comprise source term calculations, boundary conditions, planar averaging, communication (excluding linear solve communication), linear solve setup, and copying solution arrays.

For AMR-Wind on both Summit and Crusher, the time per step, $t_{\text{step}}$, decreases with increasing node count as each component of the timestep takes less time. Both Poisson solves, however, take a higher percentage of the time step as $P$ is increased, which reflects the communication-intensive nature of the Poisson problem. Overall, Crusher is providing better performance than Summit. This is partly because there
For NekRS, we start the GPU analysis with NVIDIA's profiling tools. Table 3 summarizes the kernel-level metrics for the critical kernels, which are identified with NVIDIA's Nsight Systems. At this granularity, the table indicates that the bulk of the time for NekRS is spent evaluating the dealiased advection operator (subCycleStrongCubatureVolumeHex3D) both for the velocity vectors and for the temperature. Other leading consumers are the gather-scatter operations. Largely missing from this table for NekRS is the pressure. Other leading consumers are the gather-scatter operator (subCycleStrongCubatureVolumeHex3D) both for the velocity vectors and for the temperature. Other leading consumers are the gather-scatter operations. Largely missing from this table for NekRS is the pressure preconditioner. Figure 4 shows the cost breakdown for this type of analysis over node counts ranging from 4 to 16. At lower node counts, the bulk of the NekRS time is spent in the pressure preconditioner, which is separated across many kernels for the various levels of p-multigrid.

Each NekRS job tracks basic runtime statistics using a combination of MPI Wtime and cudaDeviceSynchronize or CUDA events. These are output every 500 time steps unless the user specifies otherwise. From these, we collect aggregate timing breakdowns, roughly following the physical substeps of advection, pressure, and viscous-thermal-updates, plus tracking of known communication bottlenecks such as the pMG coarse-grid solve for the pressure preconditioner. Figure 4 shows the cost breakdown for this type of analysis over node counts ranging from 4 to 16. At lower node counts, the bulk of the NekRS time is spent in the makef and makeq (advection) routines, which are respectively responsible for setting up the right-hand-sides for the momentum and energy equations. To allow a larger CFL, the ABL simulations use characteristics-based timestepping, which involves solving a sequence of hyperbolic subproblems on the interval $[t^{n-2}, t^n]$ (one for each velocity component and one for temperature).

Table 4 gives a detailed breakdown of the per rank kernel performance for NekRS in the 4-node case of Fig. 4. The kernels are the advection subroutine (advSub), with either 3 components (velocity) or 1 (temperature); the Poisson/Helmholtz matrix-vector product (Ax) for the elliptic solves; and the fast-diagonalization method (fdm) for the Schwarz smoother (Lottes and Fischer (2005)). For each kernel, $N$ indicates the polynomial order. To leading order, the amount of tensor-contraction work for each operation scales as $CE_p(N+1)^4$ and the number of memory references as $CE(N+1)^3$, with $E_p$ the number of elements on each rank and $C \approx 12$–30 a kernel-dependent constant. FP indicates the working floating-point precision; GB/s the sustained streaming bandwidth on the device; GFLOPS the number of billions of floating-point operations per second sustained on the device for that particular kernel; and KV the kernel version identified as the fastest entry in each runtime benchmark test. The 32-bit precision kernels are used in the lower levels of p-multigrid. Because the Schwarz smoother operates on an extended domain, fdm executes on data that is extended to $N+2$ in each direction compared with its corresponding Ax operation. The advection operation is dealiased (i.e., integration is on a finer mesh than the underlying velocity representation), so that kernel also operates on a relatively large data set. We see that the work-intensive (high-$N$) and 32-bit kernels achieve impressive floating-point performance, well in excess of 1 TFLOPS (incidentally, the speed of ASCI Red, the world’s fastest computer just 25 years ago). NekRS also provides a conservative estimate of the overall FP64 floating point rate per rank—here, close to 1 TFLOPS—which includes the message-passing overhead. (For this overall rate, each 32-bit operation is counted as half a flop.)

Figure 5 shows CPU and GPU strong-scaling performance for each code on Summit. The upper figures show standard

| Platform  | Kernel      | $N$ | FP  | GB/s | GFLOPS | KV |
|----------|-------------|----|-----|------|--------|----|
| Summit   | advSub (3)  | 10 | 64  | 613  | 3775   | 7  |
| NVIDIA   | advSub (1)  | 10 | 64  | 1137 | 2446   | 8  |
| V100     | Ax          | 8  | 64  | 844  | 1622   | 5  |
|          | Ax          | 8  | 64  | 900  | 1731   | 4  |
|          | Ax          | 8  | 32  | 901  | 1732   | 4  |
|          | Ax          | 8  | 32  | 859  | 3303   | 4  |
|          | Ax          | 4  | 64  | 832  | 975    | 5  |
|          | Ax          | 4  | 32  | 711  | 1667   | 6  |
|          | fdm         | 10 | 32  | 611  | 6210   | 3  |
|          | fdm         | 6  | 32  | 713  | 4422   | 3  |
| Crusher  | advSub (3)  | 10 | 64  | 491  | 3018   | 11 |
| AMD      | advSub (1)  | 10 | 64  | 868  | 1867   | 8  |
| MI250X   | Ax          | 8  | 64  | 662  | 1272   | 2  |
|          | Ax          | 8  | 64  | 736  | 1416   | 2  |
|          | Ax          | 8  | 32  | 736  | 1415   | 2  |
|          | Ax          | 8  | 32  | 742  | 2854   | 2  |
|          | Ax          | 4  | 64  | 708  | 830    | 6  |
|          | Ax          | 4  | 32  | 658  | 1543   | 0  |
|          | fdm         | 10 | 32  | 546  | 5551   | 4  |
|          | fdm         | 6  | 32  | 521  | 3234   | 4  |
| Summit   | Sustained   | 64 |      | 833  |        |    |
| Crusher  | Sustained   | 64 |      | 937  |        |    |
time vs. node-count plots, which clearly indicate that it is
easier to strong-scale on the CPU. On Summit, however,
that point is moot given that one needs 128 nodes using a
CPU-only configuration in order to get to the same time-per-
step as using 4 nodes with 6 GPUs each (i.e., a factor of 32
difference in required node-hours to do the same work).

Strong- and Weak-Scaling Performance

We next consider GPU-only performance on Summit using a
single V100 per MPI rank. Figure 6, top, shows performance
in terms of $t_{\text{step}}$ for strong scaling as a function of the
number of GPUs, $P$, in the left column and as a function
of number of points per rank, $n/P$, in the center column.
Weak-scaling performance is presented in the right column.
The wall-time figure also shows the ideal speed-up curves
scaling as $P$. The lower plots show parallel efficiency,

$$P_{\text{eff}} := \frac{t_0 P_0}{t_{\text{step}} P},$$

where $P_0$ is the smallest value of $P$ that will hold the given
problem and $t_0$ is the $t_{\text{step}}$ value corresponding to $P_0$.

We see that at the lower resolution of $n = 512^3$, the
performance of the two codes is within a factor of 2 of
each other out to $P = 78$. From the efficiency figures we can see that both curves have dropped below 80% efficiency
by that point, so a more realistic point of comparison would
be at $P = 66$ which is a power of 2, as seen in Table 5 for the
higher-resolution $n = 512^3$ case. The weak-scale efficiency reaches 80% at around $P = 2000$
GPUs for all the cases save the AMR-Wind case with $n/P = 2.2M$, which crosses the 80% mark at $P \approx 1100$.

Tables 5 and 6 provide a detailed breakdown of several of
the key metrics for the code performance, including iteration
counts ($v_i$, $p_i$, $T_i$, for the respective velocity, pressure,
and temperature iterative solvers), $t_{\text{step}}$, parallel efficiency
($P_{\text{eff}}$), and the wall-time to physical-time ratio ($r_t$). This last
quantity is of particular interest since it must be smaller than
unity for weather modeling applications. We also note that
$P$ is denoted by gpu in the tables. We see from Table 5
that, for a fixed value of $n/P$, $r_t$ effectively doubles with
each doubling of (linear) resolution. The reason for this
increase is that the number of timesteps must also double
whenever the number of points in each direction is doubled
(for fixed domain size). Throughout the table, we see that
roughly two iterations are required per timestep for each of
the linear solvers, indicating that the preconditioners are
robust with respect to mesh size, although NekRS does show
some increase in iteration count in the weak-scale results.

We remark that AMR supports block-structured adaptive
mesh refinement, which means that static grids do not
leverage one of its main features. It is nonetheless highly
performant on this problem. Moreover, AMR-Wind has a
significant performance boost when the number of ranks is a
power of 2, as seen in Table 5 for the $n = 1024^3$ case for $P = 512$ and in the $n = 2048^3$ case for $P = 4096$. In the former
case, the parallel efficiency jumps from 49% to 67% as $P$
changes from 480 to 512. In the latter, it jumps from 40% for
$P = 3840$ to 51% for $P = 4096$. These performance gains
derive from the block decompositions used in AMR-Wind,
which favor block sizes (and thus, processor counts) that are
powers of 2.

We close with a scaling comparison of Summit and
Crusher performance for NekRS in Fig. 7. The upper
figures show standard strong scaling as a function of
the number of ranks on the left (one GPU or GCD per
rank) and as a function of $n/P$ on the right. The lower
plots show the timing for the makef kernel (left), which

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**Figure 5.** NekRS and AMR-Wind: CPU vs. GPU performance on Summit: 100 steps average from 200 step runs for $n = 512^3$.  
NekRS is only a factor of 1.6 faster than AMR-Wind for the $n = 512^3$ case. 
Figure 6, right, shows weak-scaling results for $n/P = 2.2M$ and 4.4M. For the heavily loaded cases, AMR-Wind is
within a factor of 1.6 of NekRS, but this figure increases
roughly a factor of 2 for the 2.2M points-per-GPU case.
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plots show the timing for the makef kernel (left), which

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evaluates the nonlinear advection term and does not require communication, and for the coarse-grid solve (right), which is communication dominated. The coarse-grid problem, which has roughly $E$ degrees of freedom (with $E = 262144$ in this case), is solved by using algebraic multigrid (hypre) on the host CPUs. The performance for these two platforms is remarkably similar.

**Conclusion**

We presented profiling and timing results for two CFD codes, NekRS and AMR-Wind, applied to the GABLS atmospheric boundary layer test problem, which is of direct relevance to wind farm modeling and weather forecasting. Strong and weak scaling were demonstrated on up to $P = 4800$ NVIDIA V100 GPUs on OLCF’s Summit. For NekRS, wall-clock times of 0.11 s were observed for $n/P = 2M$, which is the 80% efficiency point across a range of
### Table 5. NekRS GPU vs. AMR-Wind GPU strong-scaling performance study.

| Node | NekRS | AMR-Wind |
|------|-------|----------|
| P | T | \(t_{\text{step}}\) | \(P_{\text{eff}}\) | \(r_t\) | P | T | \(t_{\text{step}}\) | \(P_{\text{eff}}\) | \(r_t\) |
| 4 | 24 | 5.592e+06 | 2 | 1.81 | 2.44e-01 | 100 | 3.90 | 2 | 2 | 3.19e-01 | 100 | 5.10 |
| 8 | 48 | 2.796e+06 | 2 | 1.82 | 1.39e-01 | 87 | 2.22 | 2 | 2 | 2.37e-01 | 67 | 3.80 |
| 11 | 66 | 2.0336e+06 | 2 | 1.85 | 1.11e-01 | 79 | 1.78 | 2 | 2 | 1.79e-01 | 64 | 2.87 |
| 16 | 96 | 1.3981e+06 | 2 | 1.90 | 8.66e-02 | 70 | 1.38 | 2 | 2 | 1.75e-01 | 45 | 2.80 |
| 24 | 144 | 9.3207e+05 | 2 | 2.00 | 6.87e-02 | 59 | 1.09 | 2 | 2 | 1.60e-01 | 33 | 2.56 |
| 32 | 192 | 6.9905e+05 | 2 | 2.00 | 6.77e-02 | 45 | 1.08 | 2 | 2 | 1.46e-01 | 27 | 2.34 |
| 64 | 384 | 3.4953e+05 | 2 | 2.00 | 4.40e-02 | 34 | 0.70 | 2 | 2 | 1.43e-01 | 13 | 2.30 |
| 128 | 768 | 1.7476e+05 | 2 | 2.00 | 4.02e-02 | 18 | 0.64 | 2 | 2 | 1.28e-01 | 7.7 | 2.05 |
| 256 | 1536 | 8.7381e+04 | 2 | 2.00 | 3.60e-02 | 10 | 0.57 | 2 | 2 | 1.41e-01 | 3.5 | 2.26 |

### Table 6. NekRS GPU vs. AMR-Wind GPU weak-scaling performance study with fixed mesh density and resolution per GPU.

| Node | NekRS | AMR-Wind |
|------|-------|----------|
| P | T | \(t_{\text{step}}\) | \(P_{\text{eff}}\) | \(r_t\) | P | T | \(t_{\text{step}}\) | \(P_{\text{eff}}\) | \(r_t\) |
| 2 | 1 | 2.34e-01 | 100 | 7.50 | 2 | 2 | 0.369 | 100 | 11.82 |
| 4 | 2 | 2.04e-01 | 91 | 6.54 | 2 | 2 | 0.402 | 73 | 12.86 |
| 8 | 4 | 1.72e-01 | 87 | 5.50 | 2 | 2 | 0.288 | 82 | 9.21 |
| 16 | 8 | 1.27e-01 | 84 | 4.06 | 2 | 2 | 0.303 | 56 | 9.72 |
| 32 | 16 | 1.15e-01 | 81 | 3.68 | 2 | 2 | 0.301 | 49 | 9.65 |
| 64 | 32 | 1.08e-01 | 76 | 3.47 | 2 | 2 | 0.217 | 60 | 6.95 |
| 128 | 64 | 9.57e-02 | 78 | 3.06 | 2 | 2 | 0.219 | 54 | 7.01 |

### Acknowledgments

This material is based upon work supported by the U.S. Department of Energy, Office of Science, under contract DE-AC02-06CH11357 and by the Exascale Computing Project (17-SC-20-SC). The research used resources at the Oak Ridge Leadership Computing Facility at Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract DE-AC05-00OR22725.

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