



ECP Milestone Report
Engage second wave ECP/CEED applications
WBS 2.2.6.06, Milestone CEED-MS23

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Office of Advanced Scientific Computing Research
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National Nuclear Security Administration
US Department of Energy

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EXECUTIVE SUMMARY

The CEED co-design center aims to impact a wide range of ECP application teams through focused 1-to-1 and 1-to many interactions, facilitated by CEED application liaisons, ultimately targeted to provide easy-to-use discretization libraries for high-order FEM-based application simulations.

The goal of this milestone was to extend our reach by identifying a second wave of ECP applications that can benefit from the efficient discretization algorithms and software developed in CEED. These applications were added to the list of the CEED first wave ECP applications (ExaSMR and MARBL), which continue to be main targets for our work.

As part of the milestone, we also appointed liaisons on the CEED team that will be responsible for engaging each application, identifying its challenging discretization needs, and outlining a plan for interaction with CEED. Working with all CEED thrusts, the liaisons will be ultimately responsible for ensuring the adoption of CEED technologies in each application as well as for demonstrating their benefits.

The selected second wave applications and CEED liaisons are:

- Urban – liaison Aleks Obabko (ANL)
- ExaWind – liaison Paul Fischer (UIUC)
- ExaAM – liaison Tzanio Kolev (LLNL)

In addition to details and results from these efforts, in this document we report on other project-wide activities performed in Q1 of FY19, including: engagements with performing scaling on V100 GPUs, collaboration with ECP/MPICH, participation in ECP/ST's E4S release, the Laghos-2.0 release, papers, presentations, and other outreach efforts.

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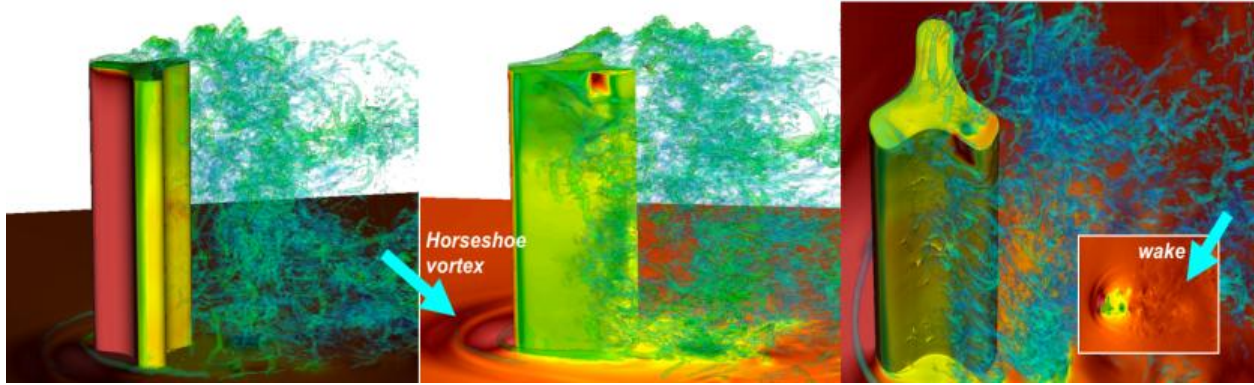


Figure 1: Urban lake point tower simulation with $Re = 8000$, $n = 160M$, $(N, E, P) = (15, 47920, 16384)$ with 6000 timesteps.

1. INTRODUCTION

The CEED co-design center aims to impact a wide range of ECP application teams through focused 1-to-1 interactions, facilitated by CEED application liaisons, as well as through 1-to-many interactions, ultimately targeting to provide easy-to-use discretization libraries for high-order finite element methods for those FEM-based application simulations.

In this milestone we expand our reach by identifying a second wave of ECP/CEED applications which may and may not use our current software but are still targeting high-order methods. For this, we focused on new applications including Urban, Exascale Predictive Wind Plant Flow Physics Project (ExaWind) and Exascale Additive Manufacturing Application Project (ExaAM).

As part of the milestone, we appointed application liaisons on the CEED team, responsible for engaging each application, identifying its challenging discretization needs, and outlining a plan for interaction between CEED and application team.

In addition, we continued the engagements with the previously selected first wave applications, Coupled Monte Carlo Neutronics and Fluid Flow Simulation of Small Modular Reactors (ExaSMR) and Next-gen Multi-physics Simulation Code (MARBL), and provide an update on our interactions with them.

2. SECOND WAVE ECP/CEED APPLICATIONS

2.1 Urban

In order to move forward to urban simulation capability at exascale, we expanded our focus in utilizing the highly scalable Nek5000 code [4], in collaboration with the ECP Urban team, for high-fidelity thermal-fluid calculations involving direct numerical simulations (DNS) and large-eddy simulations (LES), as well as low-fidelity Reynolds-Averaged Navier-Stokes (RANS) modelings. The collaboration materials, results and discussions between CEED and Urban teams are shared at <https://github.com/misunmin/ceed-urban>.

2.1.1 Lake Point Tower Capturing Turbulence at Fine Scale

Our recent simulations demonstrate wake turbulence in a model of Lake Point Tower (LPT) at Chicago's Navy Pier (see Figure 1). The simulation required about 10 hours of run time on 512 nodes (8192 cores) of ALCF's BG/Q, Cetus using the Nek5000 CFD package. The purpose of the study was to assess the feasibility of conducting high resolution turbulence simulations at scale. The LPT model was for an isolated building, but significant resolution of the turbulent flow field is required whether one has a single building or multiple ones, so addition of more buildings would not significantly alter the runtime costs if the overall domain size does not change. For these calculations, the costs scale as the size of the domain (measured in acres, say) and with the level of resolution of the turbulent structures. The present simulation used only one percent of Mira, meaning

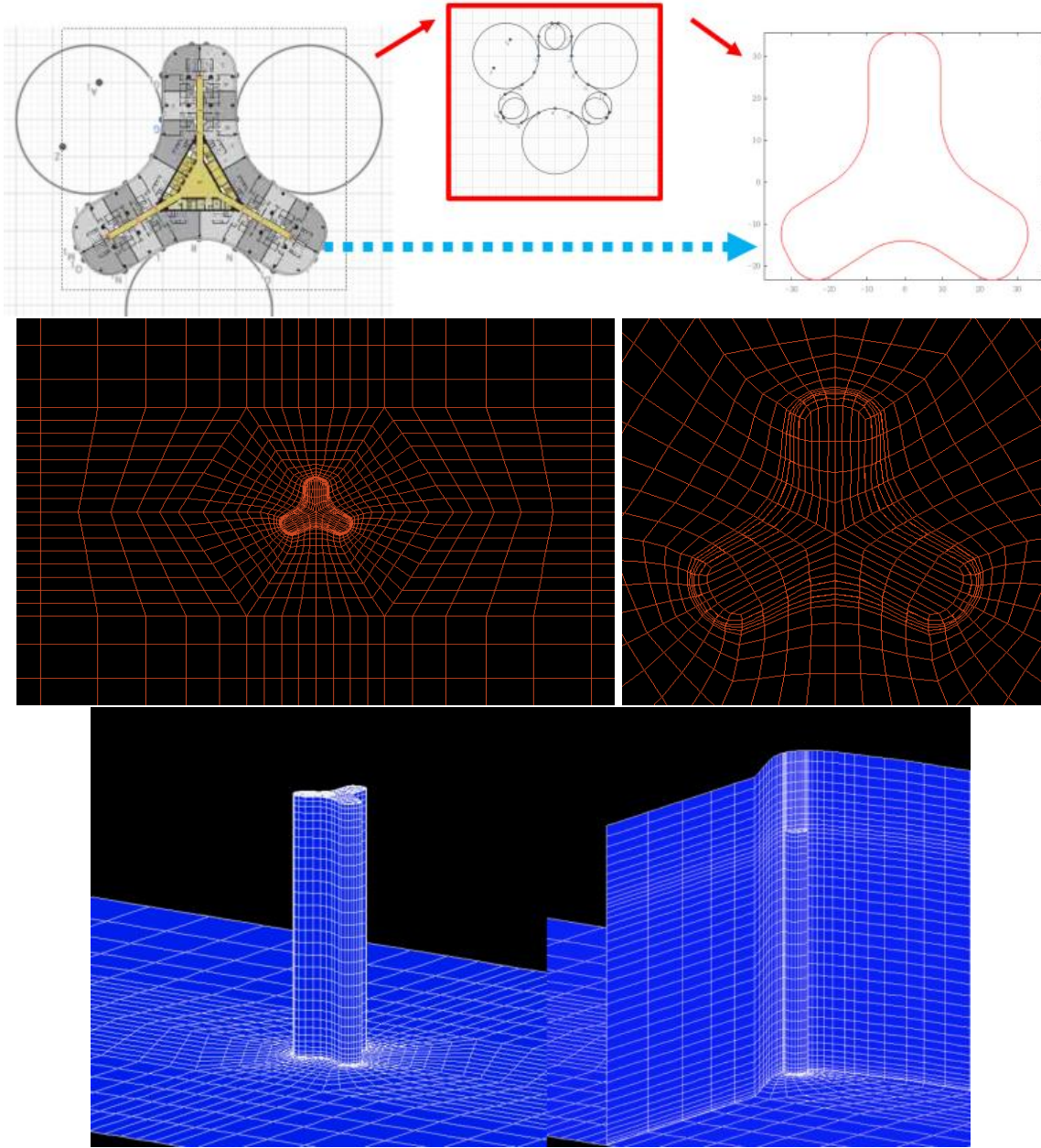


Figure 2: Lake point tower mesh with boundary layer refinement ($E = 47920$); The profile defining the top-roof (top); The boundary layer refinement for the top-roof: zoom-out (center left) and zoom-in (center right) and the vertical direction (bottom).

that one could simulate a 100-fold larger (approximately 10-block by 10-block) region using all 800,000 cores of Mira. An effective strategy for exascale simulations of this problem would be to run multiple large-scale simulations at different parameter (e.g., wind direction or thermal loading) conditions. The simulation data could then be averaged and correlated to provide estimated paths and recirculation regions for particulate transport in an Urban configuration such as Chicago. Possible model reduction strategies for condensing this data into a useful engineering tool include proper orthogonal decomposition and other data assimilation techniques as used in current weather and climate models.

The geometric complexity inherent in urban systems has complicated such studies by limiting them to

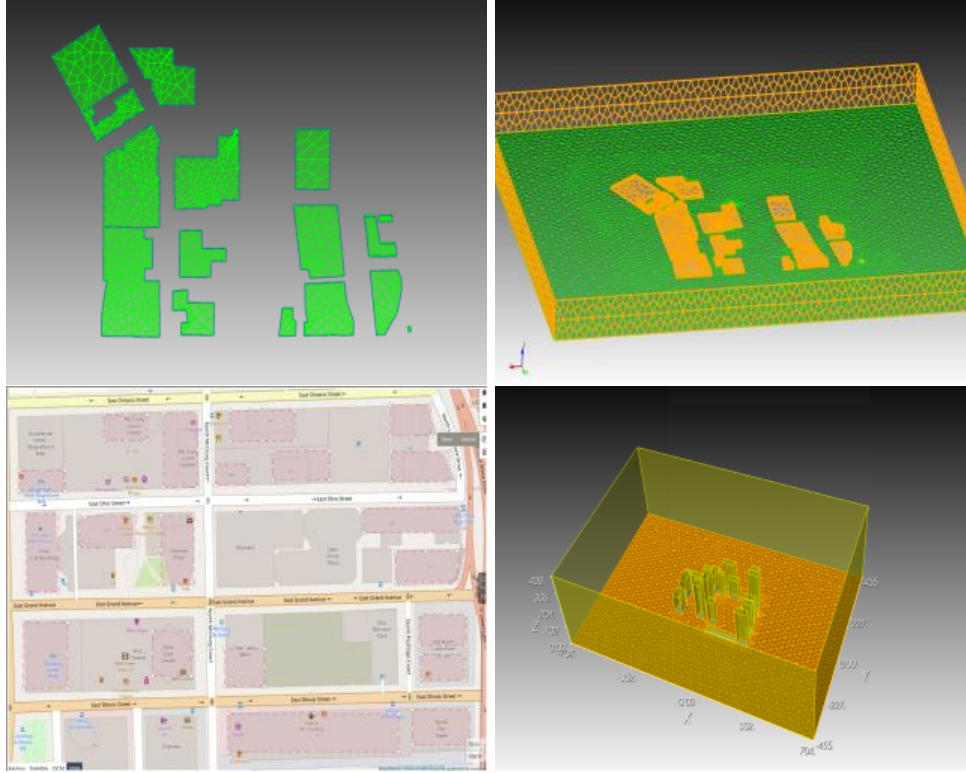


Figure 3: Urban meshes needing improvement for Goose Island in Chicago area (top) and Chicago downtown block including 20 buildings (bottom).

low Reynolds numbers and small numbers of buildings. In collaboration with Urban team, CEED researchers generated high-quality urban meshes as shown in Figure 2. Such meshes help in capturing fine-scale structures in urban simulations, which is an important task in understanding the physical behaviors of the flows in the urban environment.

2.1.2 *Goose Island Mesh with Boundary Layer Refinement*

We are currently performing the simulation of Goose Island which is a 160 acres (0.65 km^2) artificial island in Chicago, Illinois, formed by the North Branch of the Chicago River on the west and the North Branch Canal on the east. It is about 1.5 miles (2.4 km) long and 0.5 miles (0.80 km) across at its widest point. Figure 3 (left) shows a given coarse mesh that CEED researchers are currently working to improve. We also have a highly refined spectral-element mesh consisting of $E = 1,206,966$ elements (additional improvements are also possible) and currently running high-resolution runs on OLCF/Titan and ALCF/Mira, with $N = 15$ (a total number of grid points of more than $n = 4,9$ billions).

2.1.3 *Downtown Chicago Block with 20 Buildings*

We are currently working on improving the 20-building mesh for a downtown Chicago block that Urban team generated (see Figure 3 (bottom right)). The given mesh is not representing precisely the actual building shapes, orientation, and dimensions and the mesh is not well-refined near the surfaces of the building. CEED researchers are currently building an improved mesh for efficiently representing the flow profiles around the building structures.

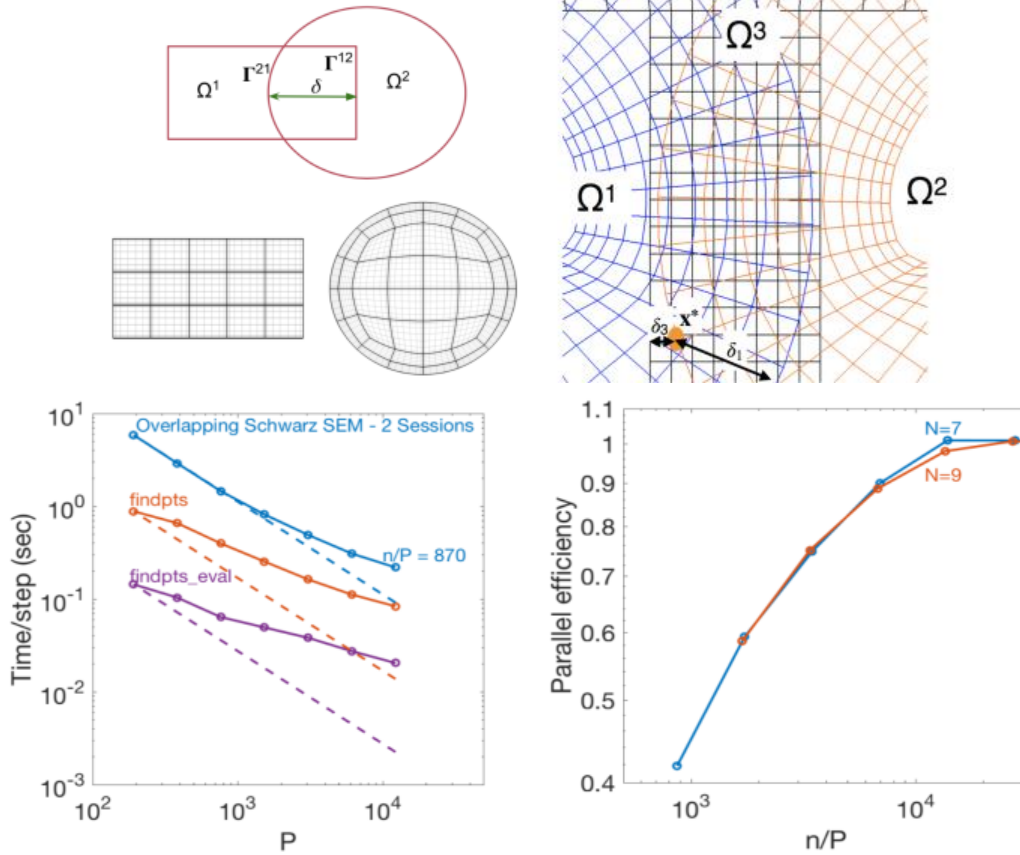


Figure 4: NekNek: multimesh configurations. Two-meshes coupling (top left); Three-meshes coupling (top right). Strong-scaling (bottom left) with efficiency (bottom right). P represents the number of processors, N is the polynomial order, and n is the total number of grid points.

2.1.4 NekNek Coupling Approach Toward 100~200 Multiblocks.

We are currently applying CEED team’s multimesh coupling strategy [6] to building geometries, which will allow more flexibility when boundary layer refinement is required. This non-conforming multi-mesh coupling through NekNek can be extended more feasibly to the full range of simulations of the urban area up to the computing limit with the demand of exascale computing resources.

The NekNek approach is based on the spectral-element-based Schwarz overlapping (overset) methods and has been implemented for Nek5000 incompressible Navier-Stokes solver. The SEM-based overset grid method is implemented at the level of the Navier-Stokes equations, which are advanced independently within separate subdomains using interdomain velocity and pressure boundary-data exchanges at each timestep or sub-timestep. Central to this implementation is a general, robust, and scalable interpolation routine, gslib [3]-findpts, that rapidly determines the computational coordinates for any arbitrary point. The communication kernels in gslib execute with at most $\log P$ complexity for the NekNek multimesh coupling. The original interpolation routine has been extended to account for multiple overlapping domains. The new implementation discriminates the possessing subdomain by distance to the domain boundary, such that the interface boundary data is taken from the inner-most interior points as shown in Figure 4 (top).

Figure 4 (bottom) shows scaling for overall time per step and time spent in findpts and findpts eval. Due to the inherent load imbalance in overlapping grids, owing to the fact that all interface elements might not be located on separate processors, the scaling for findpts and findpts eval is not ideal. However, findpts takes only 10% and findpts eval takes 1% of time compared to the total time to solution per timestep, and as a

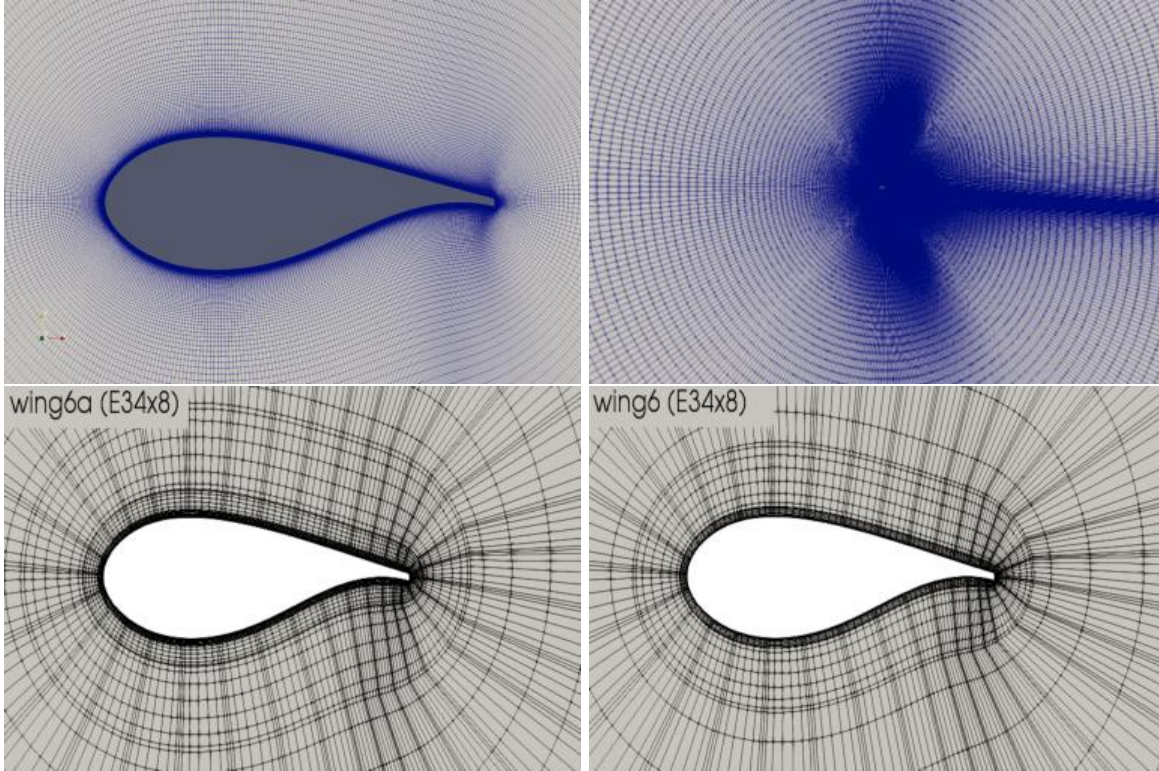


Figure 5: ExaWind mesh (DTU 10 MW reference wind turbine structure): point data with total of 131841 (513×257) (top), down-sampled SEM mesh with $E = 34 \times 8$ having coarser (bottom left) and denser (bottom right) boundary layers of the wing surface with 2 times lower resolution in parallel direction and 4 times lower resolution in the normal direction to the wing surface.

result the scaling of the overall method is maintained. The parallel efficiency of the calculation is more than 90% until the number of MPI ranks exceeds the number of interface elements. The parallel efficiency drops to 60% at $n/P = 1736$.

2.2 ExaWind

In collaboration with ExaWind team, we focused on performing RANS simulations to compute a steady solution for an FFA airfoil structure. Here we utilize a novel wall function approach (recently developed in Nek5000), to lower resolution requirements and deliver the drag and lift coefficient profiles for $Re = 10M$ that the ExaWind team is interested in. The collaboration materials, results and discussions between the CEED and ExaWind teams are shared at <https://github.com/misunmin/ceed-exawind>.

2.2.1 Novel RANS Wall-Functions Yield Reduced Boundary Layer Resolution

We investigated two different approaches for the boundary layer treatment in our Nek5000 RANS solver: (1) the wall resolved *regularized* approach [1] where we have to use adequate resolution inside the very thin log and viscous sub-layers and (2) the new *wall function* approach [2] where we do not need such high resolution as we move the boundary to a y^+ of about 50-100. The wall function approach does not need to resolve the very sharp profiles immediately adjacent to the wall. Because of that, the source terms in the omega equation, which are treated explicitly, are not as large in the wall function approach and create less of a stability problem. However, in both approaches the time step is still limited by the $CFL \sim 0.5$ which is a convective restriction while we are using the backward difference formula (BDF) for the diffusion and extrapolation

timestepping method	BDF + EXT	BDF + EXT	BDF + EXT	BDF + EXT
resolution	(E=544,N=7)	(E=544,N=7)	(E=272,N=7)	(E=272,N=7)
BC	wall	shl	shl	shl
boundary layer	very thin	very thin	thin	coarse
$Re = 10M$	$\Delta t=5E-7$	$\Delta t= 2E-5$	–	$\Delta t= 5E-5$
$Re = 1M$	$\Delta t=1E-5$	$\Delta t= 1E-4$	$\Delta t= 1E-4$	$\Delta t= 5E-4$
$Re = 100K$	$\Delta t=2E-5$	$\Delta t= 1E-4$	$\Delta t= 1E-4$	$\Delta t= 1E-3$

Table 1: Down-sampled spectral-element meshes for an FFA airfoil. “shl” represents the shear horizontal local boundary condition used in the wall function approach. BDF: backward difference formula and EXT: extrapolation. BDF and EXT both use the second order. Δt represents the maximum timestep size for each case of the simulations.

	drag coefficient (C_d)	lift coefficient (C_l)
Literature	0.013	0.2
NREL	0.013	0.3
CEED	0.3	0.2

Table 2: Reference drag (C_d and lift (C_l) coefficients from the literature, and the results from NREL and CEED.

(EXT) for the nonlinear convective term. There remains room for further improvement with characteristics [7] and Jacobian-free Newton-Krylov (JFNK) methods [5, 8] where the CEED team has expertise.

2.2.2 Drag and Lift Coefficients for Wind Turbine Airfoil up to $Re = 10M$

Here we demonstrate our results for the airfoil studies using the wall function approach with time-stepping based on 2nd-order BDF and EXT methods. Figure 5 (top) shows ExaWind team’s airfoil mesh consisting of 513×257 of grid points which is equivalent to 512×256 (131072) cells. Based on the given point data, CEED team added 32 more points in the direction parallel to the wing surface around the wing tail region where more resolution is required, and then generated several down-sampled spectral-element meshes, using $E = 68 \times 16$, $E = 34 \times 16$, and $E = 34 \times 8$ (cells or elements).

In particular we have created two different set of meshes with the coarsest mesh $E = 34 \times 8$, referred as **wing6a** and **wing6**, as shown in Figure 5 (down left and right). **wing6a** and **wing6** have the distances to the wall boundary of the first layer as $2.7E-3$ and $2.00E-5$, respectively. Table 1 demonstrates the maximum allowable timestep sizes for each mesh. CEED team performed simulations with Nek5000 RANS solver with all those meshes generated and found the mesh (**wing6a**) with ($N = 7$, $E = 272$) allows the largest Δt with reasonable solution profiles that we demonstrate here. consisting of the total number of grid points $n = EN^2 = 13328$ which is 10 times less resolution than the original data points 512×256 (131072). for each Re . The mesh with $E = 272$ having a coarser boundary layer allows for a $100\times$ larger timestep size when using the new wall function approach with “shl” boundary treatment, compared to the regularized standard boundary treatment with wall boundary conditions.

Figure 6 demonstrates a full set of steady solution profiles for varying Reynolds numbers of $Re = 100K$, $1M$ and $10M$. The solution profiles include velocity components, vorticity, k and ω , pressure on multiple sets of streamlines. Figure 7 shows magnified images of the solution profiles for the case of the largest Reynolds number ($Re = 10M$) to demonstrate the detailed behaviors of the profiles near the tail region.

In collaboration with the NREL team, the CEED team is analyzing the results. From our results based on high-order SEM, we observe a very small - separation bubble right behind the airfoil tail in our simulations. Moreover, when the Re goes over $6M$ or $8M$ this originally “steady” separation bubble starts to shed very small vortices, which is likely due to our low numerical viscosity which allows this kind of behavior. However we note that this recirculation/separation and even the weak shedding have almost no effect on the drag/lift or even on the rest of the flow field around the airfoil. Also, it is possible that this behavior may change

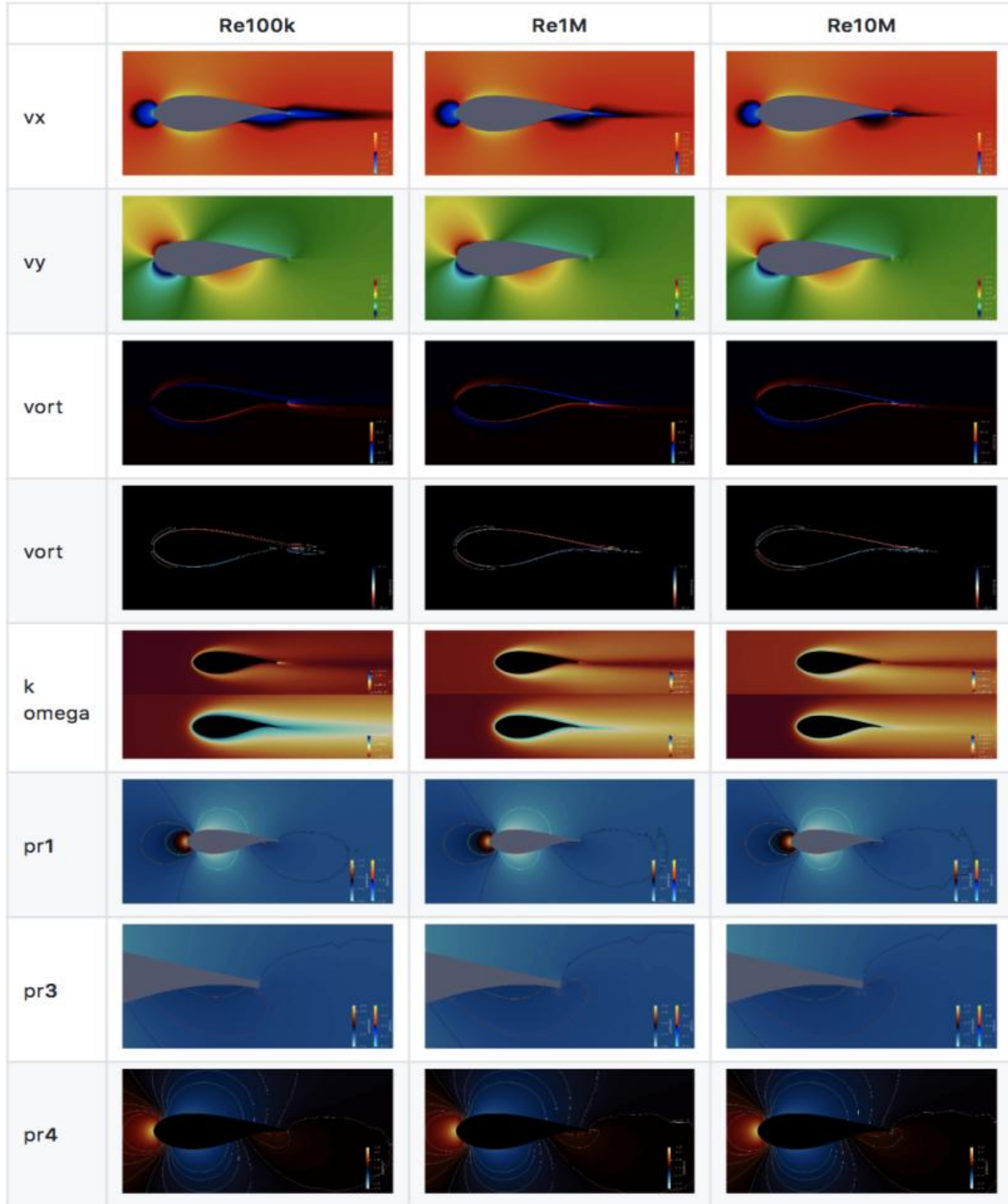


Figure 6: ExaWind RANS simulations for varying Reynolds numbers ($Re = 100K, 1M, 10M$), demonstrating profiles for steady solutions for the velocity, vorticity, k and ω , pressure, using a mesh with $E = 272(34 \times 8)$; Pressure is represented with three different set of stream lines referred as pr1, pr2, and pr3 (pr1: $[-0.2, -0.1, 0.0, 0.1, 0.2]$, pr2: $[-0.2, -0.1, -0.05, 0.0, 0.05, 0.1, 0.2]$, pr3: $[-0.2, -0.15, -0.1, -0.05, 0.0, 0.05, 0.1, 0.15, 0.2]$).

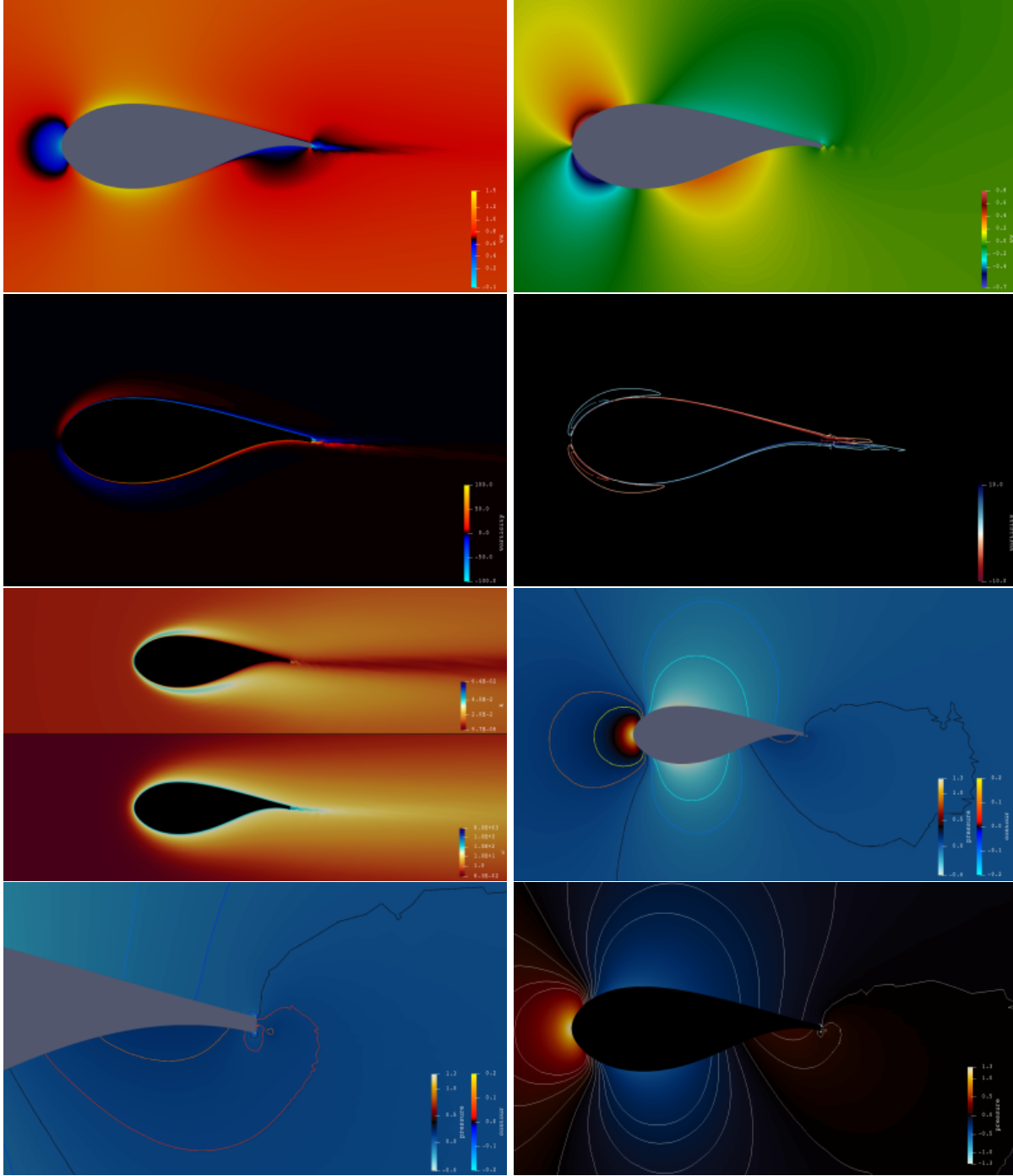


Figure 7: ExaWind RANS steady solution, magnified images for $Re = 10M$ for the velocity components (v_x , v_y : first row left and right), vorticity (second row left and right), k and ω (third row left up and down, respectively), pressure on different streamlines on $[-0.2, -0.1, 0.0, 0.1, 0.2]$ (third row right), $[-0.2, -0.1, -0.05, 0.0, 0.05, 0.1, 0.2]$ and $[-0.2, -0.15, -0.1, -0.05, 0.0, 0.05, 0.1, 0.15, 0.2]$ (fourth row left and right).

somewhat depending on the resolution.

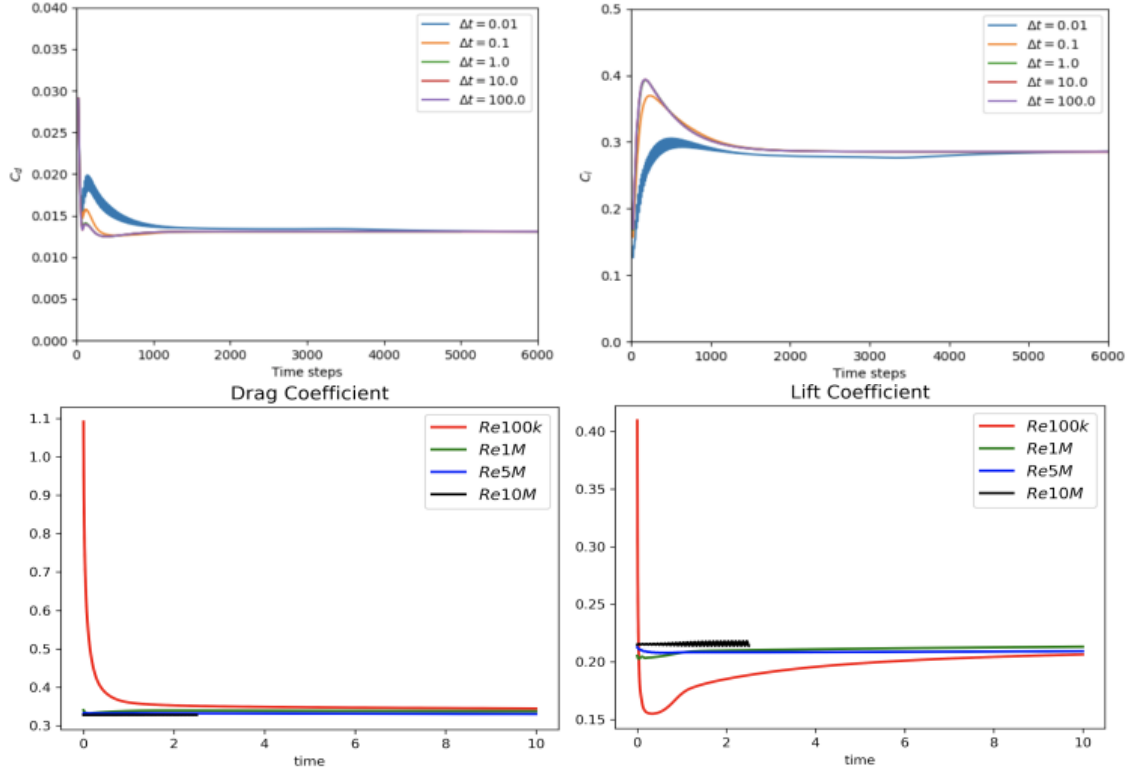


Figure 8: Drag coefficient (C_d) and lift coefficient (C_l) for FFA airfoil from NREL (top left and right) for $Re = 10M$ and from CEED (bottom left and right) for varying Reynolds numbers ($Re = 100K, 1M, 5M, 10M$).

Figure 8 demonstrates the profiles of the drag and lift coefficients for the airfoil from CEED team, indicating the shedding behaviors with dependency on resolution. The top figures show the results from NREL team, and the bottom shows the results from CEED team. Figure 9 demonstrates the oscillating behaviors of the drag and lift profiles when using different resolutions as we noted above in the analysis. Table 2 summarizes the current results compared to the reference. In the CEED team results, we have agreement on the lift coefficient to the value from the literature while there remains some discrepancy in the drag coefficient. While the predicted viscous drag is about 0.013, we obtain pressure drag of about 0.3 which causes the discrepancy. The CEED and NREL teams are currently looking into those results and discussing the differences and time step comparisons to develop better strategies and further improve accuracy and performance.

2.2.3 Wall Function Approach Extended to Characteristics and JFNK

We have extended the wall function approach combined with a characteristic-based (CHAR) timestepping and Jacobian-free Newton Krylov (JFNK) method. Table 3 shows preliminary results for RANS channel flow simulations in the case of $Re = 100K$, demonstrating that $100\times$ larger Δt can be taken when using the wall function approach (“shl”), compared to the regularized standard approach with wall boundary. Figure 10 shows the meshes for test cases including thin and coarse boundary layers. The wall function approach is not very sensitive to the mesh resolution near the boundary layers.

2.3 ExaAM

The ECP Exascale Additive Manufacturing Application Project (ExaAM) is using multiple codes to solve coupled multi-physics problems and facilitate the qualification of Additive Manufacturing (AM) built parts.

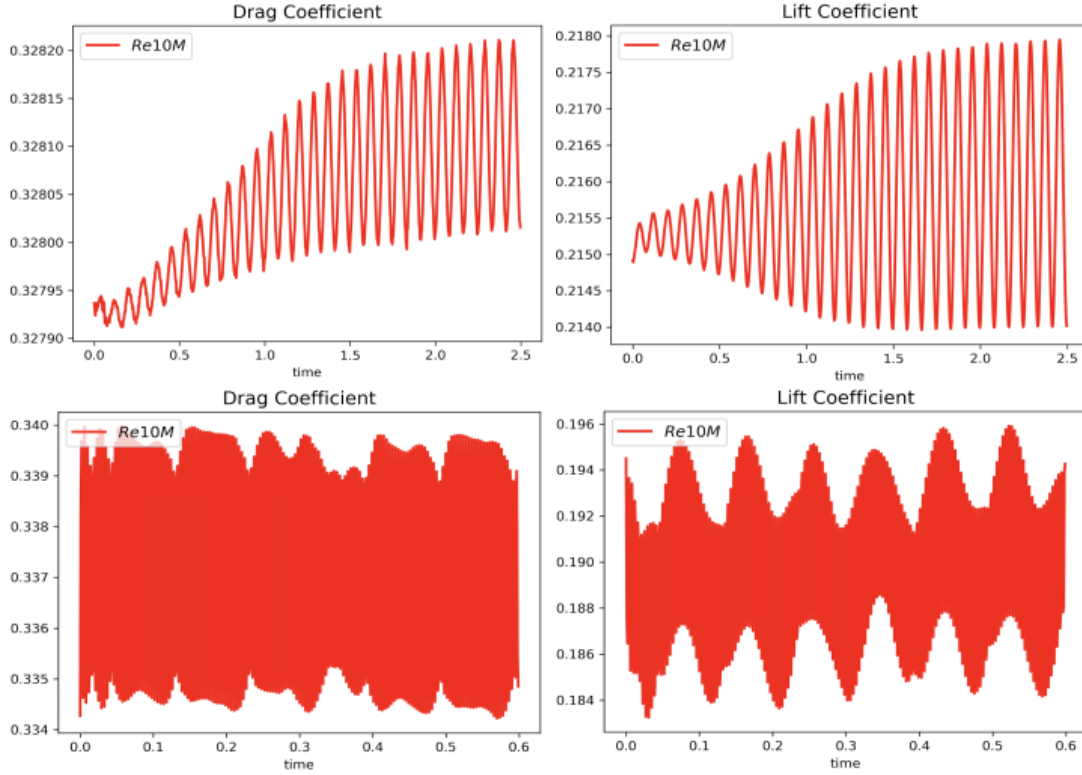


Figure 9: Zoom-in profiles for the drag (C_d) and lift (C_l) coefficients for the FFA airfoil simulation from CEED for $Re = 10M$, demonstrating oscillating behaviors for different resolutions with $E = 34 \times 16$ (top) and $E = 34 \times 8$ (bottom).

Robust solution drives toward exascale computing and exposes interesting computational workflows.

Fundamentally, this requires coupling of microstructure development and local property analysis with

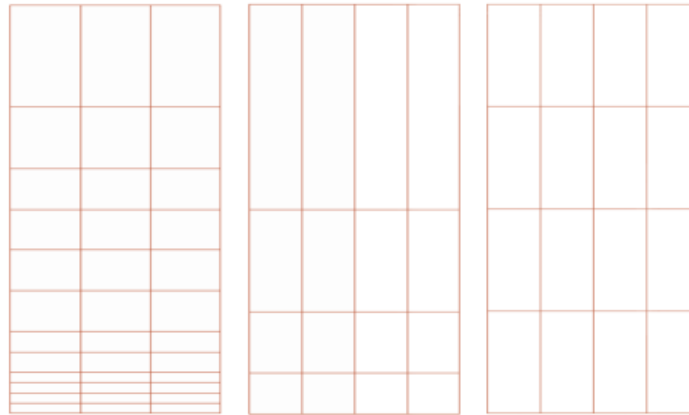


Figure 10: Validation of the new wall function approach for Nek5000 RANS solver for different meshes with varying boundary layer refinement. Minimum sizes of elements in the vertical direction are, 0.025, 0.1, and 0.25 from left to right on the domain $y \in [0, 1]$, allowing the coarser meshes to have Δt 50 ~ 100 \times larger.

timestepping method	CHAR + EXT	JFNK	CHAR + EXT	JFNK
resolution	(E=12×3,N=7)	(E=12×3,N=7)	(E=12×3,N=7)	(E=12×3,N=7)
BC	wall	wall	shl	shl
boundary layer	thin	thin	thin	thin
$Re = 100K$	$\Delta t = 2E-4$	$\Delta t = 2E-4$	$\Delta t = 1.8E-2$	$\Delta t = 1.3E-3$

Table 3: RANS channel flow simulations with characteristic (CHAR+EXT) and JFNK. Δt represents the maximum timestep size for each case of the simulations, demonstrating 100× larger Δt with the wall function approach with the shear horizontal local boundary (“shl”) compared to the regularized standard approach with wall boundary.

process simulation. Given the length scales, physical mechanisms, and response characteristics of interest, finite element codes employing crystal-mechanics-based constitutive models are the appropriate computational approach for part of the overall ExaAM problem. A survey of crystal-mechanics-based codes indicated that none of the existing codes are suited to ExaAM needs – due to limitations on distribution and a lack of suitability to exascale computing platforms.

2.3.1 The ExaConstit Miniapp

The ExaAM team is therefore creating a miniapp specifically for local property analysis, see Figure 11. This development is in collaboration with the CEED team. The initial release is planned to remain ExaAM’s miniapp for this application area and will become the foundation of a prototype application, **ExaConstit**, as required physics, inline results processing, and other features are added to meet wider ExaAM needs. Significant integration between the ExaAM and CEED ECP activities is planned during this process. The new miniapp is currently available at <https://github.com/mfem/mfem/tree/exaconstit-dev/miniapps/exaconstit> and, after approval, will be part of the MFEM release on GitHub.

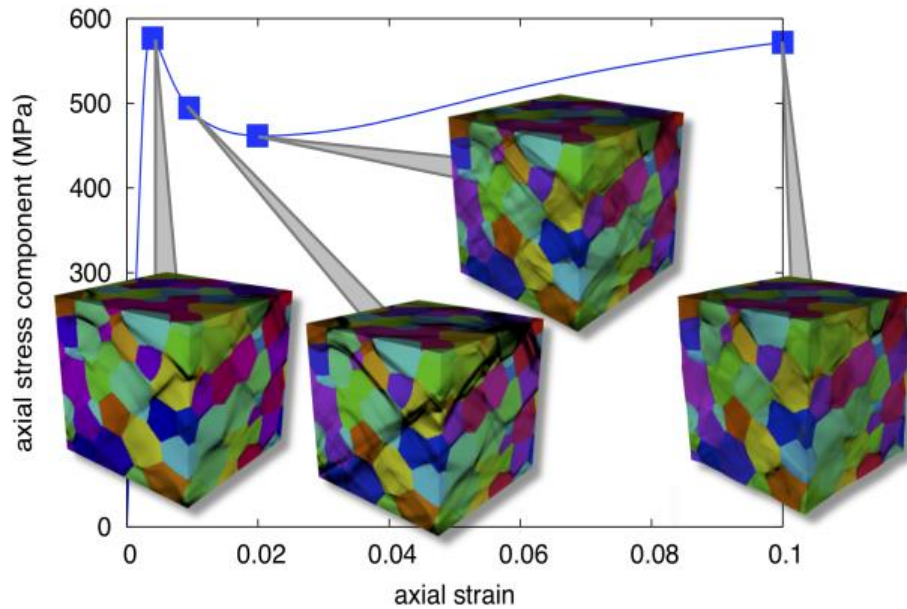


Figure 11: The ExaConstit miniapp aims to develop the capability to compute constitutive stress-strain curves given microstructural properties such as grain distribution and orientation. This will be accomplished by solving quasi-static solid mechanics with a polycrystal model on a representative material volume. (Source: Nathan Barton, LLNL).

Miniapp development to date has focused on the finite element formulation required to create a code that is well-suited to ExaAM needs. Specifically, it is attractive to formulate the constitutive models for use with a velocity-field-based updated-Lagrangian finite element method for solving the quasi-static version of the balance of linear momentum. Given this focus, we have employed a community-standard User-defined MATerial model (UMAT) constitutive model interface. Software design decisions for this interface have been informed by the exascale strategy in MFEM and by concurrent work on constitutive model developments for exascale platforms.

Testing of this formulation in the MFEM framework has initially made use of linear elastic and hyperelastic UMATs. Testing of the crystal-mechanics-based UMAT is in progress, with performance results from those runs serving as an important point of reference for relevant aspects of the ExaAM challenge problem. Over the course of the ExaAM activity, we plan to make use of the MFEM capabilities for higher-order finite elements to achieve unprecedented fidelity in the resolution of microstructure-level material response features that are important for modeling initiation events such as the nucleation and growth of porosity.

3. UPDATE ON FIRST WAVE ECP/CEED APPLICATIONS

3.1 ExaSMR

In collaboration with ExaSMR team, we focused on extending our steady-state thermal solver that we developed during FY18 Q4 to the mesh representing a long rod geometry that ExaSMR team provided. The studies include applying the steady thermal solver for heat transfer and also conjugate heat transfer problems. The collaboration materials, results and discussions between CEED and ExaSMR teams are shared at <https://github.com/misunmin/ceed-exasmr>.

3.1.1 Accelerating Heat Transfer Simulations.

Turbulent convective heat transfer often features a broad range of space and time scales that present significant challenges for direct numerical simulation (DNS) or even large eddy simulations (LES), particularly in conjugate heat transfer cases where conduction in solids can take a long time to equilibrate compared to typical eddy turnover times of turbulent flow. An everyday example of this phenomenon occurs when you turn on hot water in your house. The flow quickly becomes turbulent almost everywhere in the pipe, but it takes a long time for the hot water to reach the faucet. Clearly, increasing the length of the pipe is not going to change the time required for turbulence to develop in the pipe, but it is going to increase the time for hot water to reach the faucet. Adding more thermal mass by having thicker pipes, for example, would be expected to further increase the thermal equilibration time of the system.

Systems of the form we are interested—transport through rod bundles or heat exchangers with (local or hydraulic) diameter D and length $L \gg D$ —will feature this intrinsic timescale separation, which makes numerical simulation challenging. Capturing turbulent fluctuations in the velocity, pressure, and temperature fields requires significant spatial and temporal resolution implying both a large number of gridpoints and a large number of timesteps. Long time simulations, $T = O(L/U)$, where U is say the mean velocity, imply an overall high cost. Basically, the issue is that one must simulate an extraordinarily large number of turbulent fluctuations in the time that it takes to bring the entire system to thermal equilibrium (in a statistical, mean, sense).

Ideally, one would like to decouple the thermal and hydrodynamic timescales in order to decrease the overhead applied to the hydrodynamics computation, whose cost is elevated in particular by the global coupling induced by the pressure/divergence-free constraint. One approach to accelerating thermal convergence is to reduce the thermal inertia until the system reaches thermal equilibrium. The advection-diffusion equation,

$$\rho C_p \left[\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right] = \nabla \cdot k \nabla T + q''' \quad (1)$$

plus boundary and initial conditions, can be modified either in the solid (where the advecting velocity $\mathbf{u} \equiv 0$), or in both the solid and fluid to have a reduced value of ρC_p , which basically allows diffusive effects to propagate further on each timestep. Note that, under steady-state conditions, changing ρC_p in the solid (only)

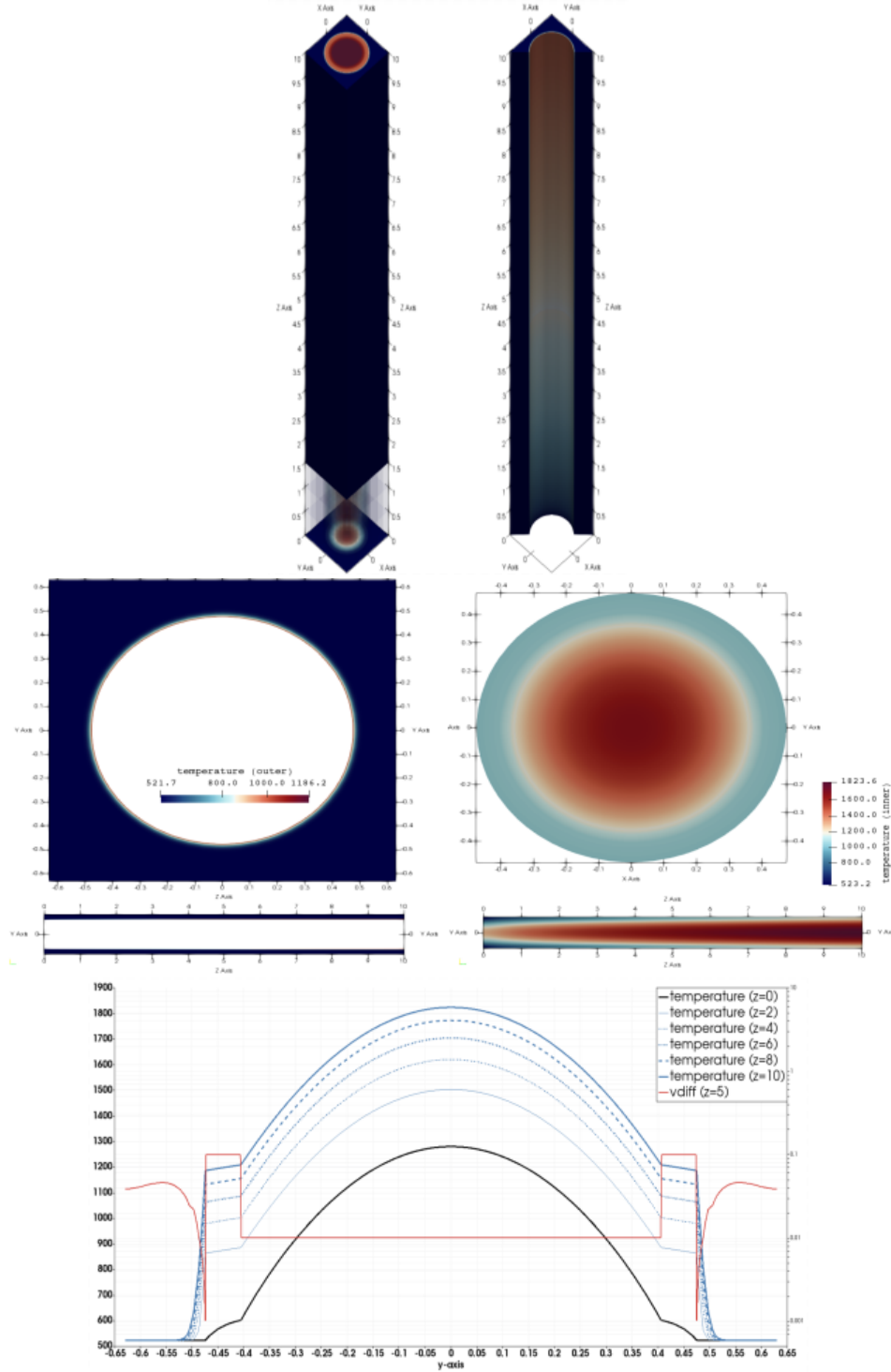


Figure 12: ExaSMR steady thermal solution from longrod conjugate heat simulations (top and center) using Schwarz preconditioner with local solver with tensor approximation for the linear advection diffusion operator, agreeing to the thermal solution from the standard Nek5000 using BDF/EXT (bottom), demonstrating $20\times$ speedup in total simulation time.

results no change to the steady-state solution because ρC_p in the solid has no influence once the temperature equilibrates since $\frac{\partial T}{\partial t}$ and \mathbf{u} are both zero there.

A drawback of the preceding approach is that it does not accelerate the convergence of the thermal advection, which is critical for long domains such as flow of hot water in a house or flow in reactors with long rod bundles. An approach that addresses this problem directly is to periodically “freeze” the turbulent velocity field, $\mathbf{u}(\mathbf{x}, t)$, and to advect over times $\tau \gg \Delta t$, where Δt is the step size for the Navier-Stokes/advection-diffusion (NS/AD) solver. One can even take $\tau = L/U$, which is the mean flow-through time, or $\tau = \infty$. The savings with this approach is two-fold. First, solution of the advection-diffusion equation is much cheaper than solving the Navier-Stokes equations at each step. Second, for $\tau = \infty$, one can use a steady-state solver, which can result in considerable savings over time marching to a steady-state solution.

Note that in the case of a steady-state solver, there is no real point to “periodically” performing the cycle,

- freeze the velocity,
- solve the steady-state temperature equation,
- advance NS/AD,
- repeat,

because the steady-state thermal solution has no history and will reach a new (spurious) equilibrium in the middle of each cycle. One might use this approach, however, to generate a sequence of plausible states over which statistics could be collected. Moreover, a single pass through the preceding sequence could provide a very good initial condition for DNS or LES of the NS/AD problem.

Still another viable acceleration technique is to replace $\mathbf{u}(\mathbf{x}, t)$ with a surrogate, $\tilde{\mathbf{u}}(\mathbf{x}, t)$, coming from a reduced-order model based on, say, proper-orthogonal decomposition (POD). This is the approach currently being pursued at UIUC in the spectral element analysis lab (SEAL).

3.1.2 Accelerating Conjugate Heat Transfer Simulations.

In collaboration with ExaSMR team, we further extended testing of our steady thermal solver for the conjugate heat transfer problem. The CEED team was given pre-defined velocity and varying viscosity data that the ExaSMR team obtained from Nek5000 RANS simulations using the long rod geometry shown in Figure 12 (top) and we applied our steady-state thermal solver with the data and mesh given. Figure 12 demonstrates validation of our thermal solution which agrees with the temperature profiles obtained by the NS and thermal simulation over time with the standard timestepping based on the BDF/EXT approach. Our preliminary measurement in timings shows $20\times$ of speedup in getting steady thermal solution, compared to the standard approach. Our next steps are to perform performance tests and extend the simulation capability for much larger problem with 17×17 rod bundles.

3.2 MARBL

The MARBL multi-physics code at LLNL has been working together with CEED researchers on getting the Lagrangian (moving-mesh) phase of its multi-material ALE hydrodynamics capability running on GPUs. This effort has been utilizing the kernels and abstractions developed under CEED in both the MFEM library and the Laghos miniapp.

As described in previous reports, the MARBL code utilizes high-order continuous and discontinuous Galerkin methods from MFEM for solving the conservation laws described by the multi-material Euler equations on a moving, high-order mesh. The Laghos miniapp, developed in CEED, is a simplified version of the Lagrange phase for the case of a single material and a simplified material stress (a scalar pressure derived from a simple ideal gas equation of state). The MARBL code in contrast, is multi-material and has many options for the material stress (including elastic-plastic stress, magnetic stress, radiations stress, etc.).

Nevertheless, the compute intensive, finite element operations for partial assembly of the mass and force matrices are identical which allows the MARBL code to directly benefit from developments in optimizing / porting these kernels in the Laghos miniapp. Last year, a major effort was completed to refactor the Lagrange phase of MARBL to be based on partial assembly as in Laghos.

3.2.1 *Laghos 2.0*

In the past period the CEED team released version 2.0 of Laghos. The major advance in this release is the introduction of GPU-based versions of the miniapp, namely, its pure CUDA, OCCA, and RAJA versions. The release also includes a version that demonstrates the AMR capabilities of MFEM in the context of Laghos. In addition, several minor improvements were made in the baseline MPI-based version, along with a synchronization of its serial variant.

The pure CUDA version rewrites the major computation kernels of Laghos without utilizing any intermediate abstraction layers. This version can be used as a performance baseline for abstraction-based GPU implementations. The OCCA and RAJA versions, as their names suggest, correspond to implementations of Laghos based on Virginia Tech's OCCA and LLNL's RAJA abstraction layers.

The AMR version of Laghos provides a demonstration of dynamic adaptive mesh refinement for a moving mesh that has arbitrary order. Although the refinement and derefinement decisions are specifically chosen for the Sedov problem, as shown in Figure 13, the code can serve as a starting point for various high-order applications that utilize MFEM.

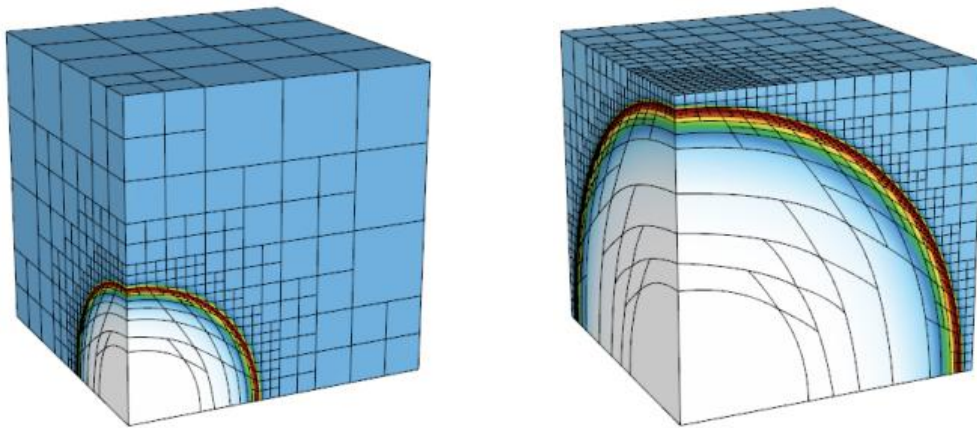


Figure 13: Dynamic AMR at different simulation times for the 3D Sedov explosion test in Laghos 2.0.

3.2.2 *High-order Kernels in MARBL*

This year, the MARBL team has been focused on taking the kernels / abstractions from Laghos in conjunction with a prototype MFEM abstraction layer and getting these running on Sierra based GPU hardware at LLNL. Specifically, the force operator kernel from Laghos was ported recently into MARBL and it was demonstrated that it can run on both CPUs and GPUs.

The GPU port uses an initial GPU device abstraction layer in MFEM, the so called MFEM-engines API, which was also used to port Laghos and is available in the latest Laghos-2.0 release described above. We'd like to emphasize again that our miniapp-based approach to performance improvement allowed us to develop and optimize the GPU algorithms needed in MARBL while working in the simplified settings of Laghos.

Since only one of the Lagrangian phase kernels have been transferred from Laghos to MARBL, the current performance is limited by data transfers between the host and the device. Porting of the other Lagrangian kernels, as well as other components of the overall ALE algorithms is in progress. This work has highlighted the need for a flexible set of abstractions in MFEM to enable incremental adoption of GPU kernels into a bigger code like MARBL, which includes its own GPU kernels, and needs to utilize LLNL libraries such as Umpire for pooled memory management and RAJA for loop parallel abstraction in portions of the code.

We have also started work in porting the advection-based ALE remap algorithm in MARBL to GPUs. Unlike the Lagrange phase, this algorithm is not readily adaptable to a matrix free implementation due to its use of algebraic, matrix-based operations for the Flux Corrected Transport (FCT) algorithm it utilizes. However, there are several aspects of the algorithm which will directly benefit from low-level, element-wise operator abstractions/kernels being developed under CEED which we hope to incorporate later in FY19.

4. OTHER PROJECT ACTIVITIES

4.1 libParanumal: BP5 Strong-Scaling on 8 V100 GPUs

We have performed extensive strong-scaling studies using CEED’s libParanumal [9] experimental set of finite element flow solvers focusing on our BP5 benchmark (diagonally-preconditioned conjugate gradient iteration of the Poisson operator using GLL quadrature) on the 8 V100 GPUs of JLSE at Argonne. The study compared a variety of polynomial orders, N or p , and element counts, E (total number of degrees of freedom is $n = EN^3$). Figure 14 demonstrates initial performance results of libParanumal for $P=1, 2, 4$, and 8 V100 GPUs on the BP5 test case for $p = 7, 11, 15$ (where $lx1=p+1=N+1$). For $n = 20$ million points, there is reasonable strong scaling, with a 4-fold speed up being realized on 8 GPUs. Below one million points, there is no speedup. We further note that the processing rate for a single V100 at for $n=20$ million is 2.5 GDOFS, which is about 20 times that realized on a single node of ANL’s BG/Q, Cetus.

We also demonstrate the performance on 6 GPU nodes ($2 \times$ Nvidia K40), ANL/LCRC systems (see Figure 15).

4.2 MPICH Collaboration: BP5 Heterogeneous Memory Utilization Test

We have been collaborating with the MPICH team, providing the BP5 CEED benchmark for HET-ERO-MEM-APP-ANALYSIS for heterogeneous memory utilization in MPICH on the Theta cluster, a KNL-based machine in the Argonne Leadership Computing Facility, using on-package Multi-Channel DRAM (MCDRAM). With the BP5 CEED benchmark, the MPICH team needed different memory placement configurations for MPICH intranode shared memory objects (using both DRAM and HBM), involving communication intensive configurations and compute intensive configurations of the experiment, with the resulting improvement on a tiny fraction of the overall runtime.

4.3 NAHOMCon19

CEED’s Paul Fischer and Tim Warburton will serve on the Scientific Committee of the inaugural North American High Order Methods Conference (NAHOMCon). With the next International Conference on Spectral and High-Order Methods (ICOSAHOM) meetings scheduled for 2020 in Vienna and 2022 in Seoul, it will be at least 10 years between US-based settings of the principal high-order methods conference, ICOSAHOM. Because of the growing importance of high-order methods, several institutions have joined together to organize NAHOMCon19, to be held in San Diego in summer of 2019, that will focus on the many developments in high-order discretizations and applications that are taking place in North America. Two of the CEED team members are on the Scientific Committee, which as a whole also voted to invite two CEED members to give plenary presentations.

4.4 MFEM Part of E4S Release

MFEM was part of the first release of the Extreme-Scale Scientific Software Stack (E4S) software collection put together by ECP/ST. According to <http://e4s.io/>, the primary purpose of this initial 0.1 release was to demonstrate the release approach based on Spack package maturity. Future release will include additional software products, with the ultimate goal of including all ECP ST software products.

4.5 Outreach

CEED researchers were involved in a number of outreach activities, including preparing a breakout session on high-order methods and applications at the ECP annual meeting, four papers (“Scalable low-order finite element preconditioners for high-order spectral element Poisson solvers”, “A Characteristic-Based Spectral Element Method for Moving-Domain Problems”, “The Target-Matrix Optimization Paradigm for High-Order Meshes” and “Low-Order Preconditioning of High-Order Triangular Finite Elements”), participation in SC18 and the AGU Fall meeting, initial work on defining new high-order benchmark problems, involvement in LLNLs CORAL-2 procurement activities and more. Nek5000 and NekCEM were also presented at the ANL booth and Nvidia Panel, respectively, at SC18. A number of presentations given by CEED researchers at the Argonne Training Program on Extreme-Scale Computing (ATPESC18) are now available online.

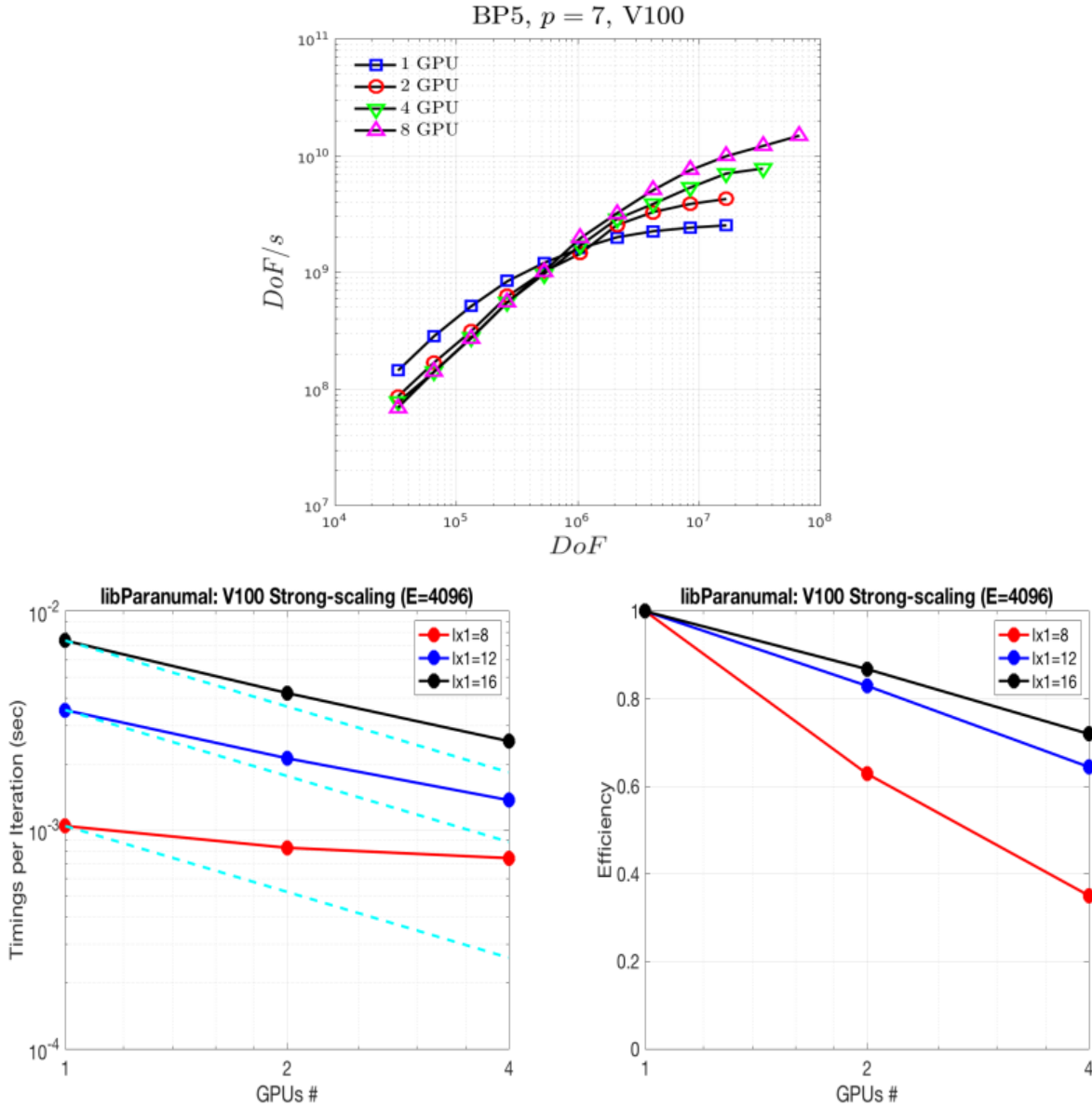


Figure 14: BP5 Strong-scaling on 8 V100 GPUs. p is the polynomial order, $lx1=p+1$, and E is the number of elements.

5. CONCLUSION

In this milestone we identified a second wave of ECP applications (Urban, ExaWind, and ExaAM) that can benefit from the efficient discretization algorithms and software developed in the CEED co-design center. These applications were added to the list of the CEED first wave ECP applications (ExaSMR and MARBL), which continue to be main targets for our work.

As part of the milestone, we also appointed application liaisons on the CEED team (Aleks Obabko, Paul Fischer and Tzanio Kolev), that will be responsible for engaging each application, identifying its challenging discretization needs, and outlining a plan for interaction with CEED.

In addition to details and results from these efforts, in this document we report on other project-wide activities performed in Q1 of FY19, including: engagements with performing scaling on V100 GPUs,

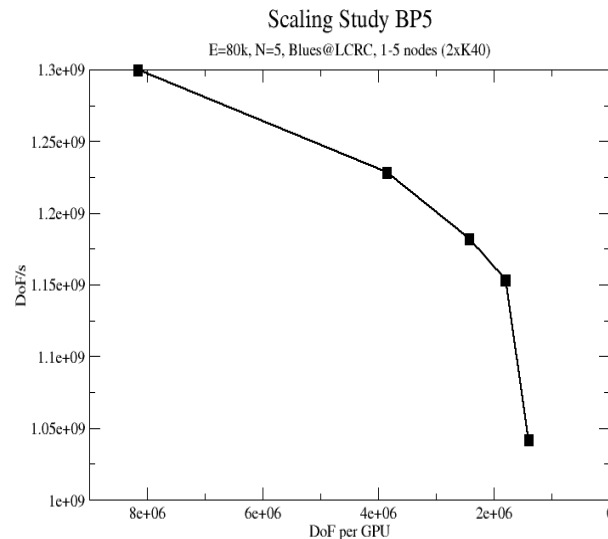


Figure 15: BP5 Strong-scaling: 6 GPU nodes (2×K40), ANL/LCRC Blues.

collaboration with ECP/MPICH, participation in ECP/ST’s E4S release, the Laghos-2.0 release, papers, presentations, and other outreach efforts.

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