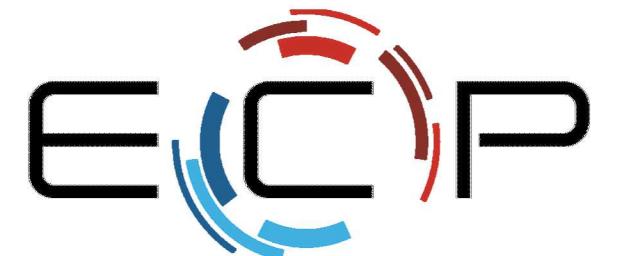


High order in Exawind

SAND2019-9280PE

Robert Knaus, Sandia National Laboratories

6 August 2019



EXASCALE COMPUTING PROJECT



U.S. DEPARTMENT OF
ENERGY

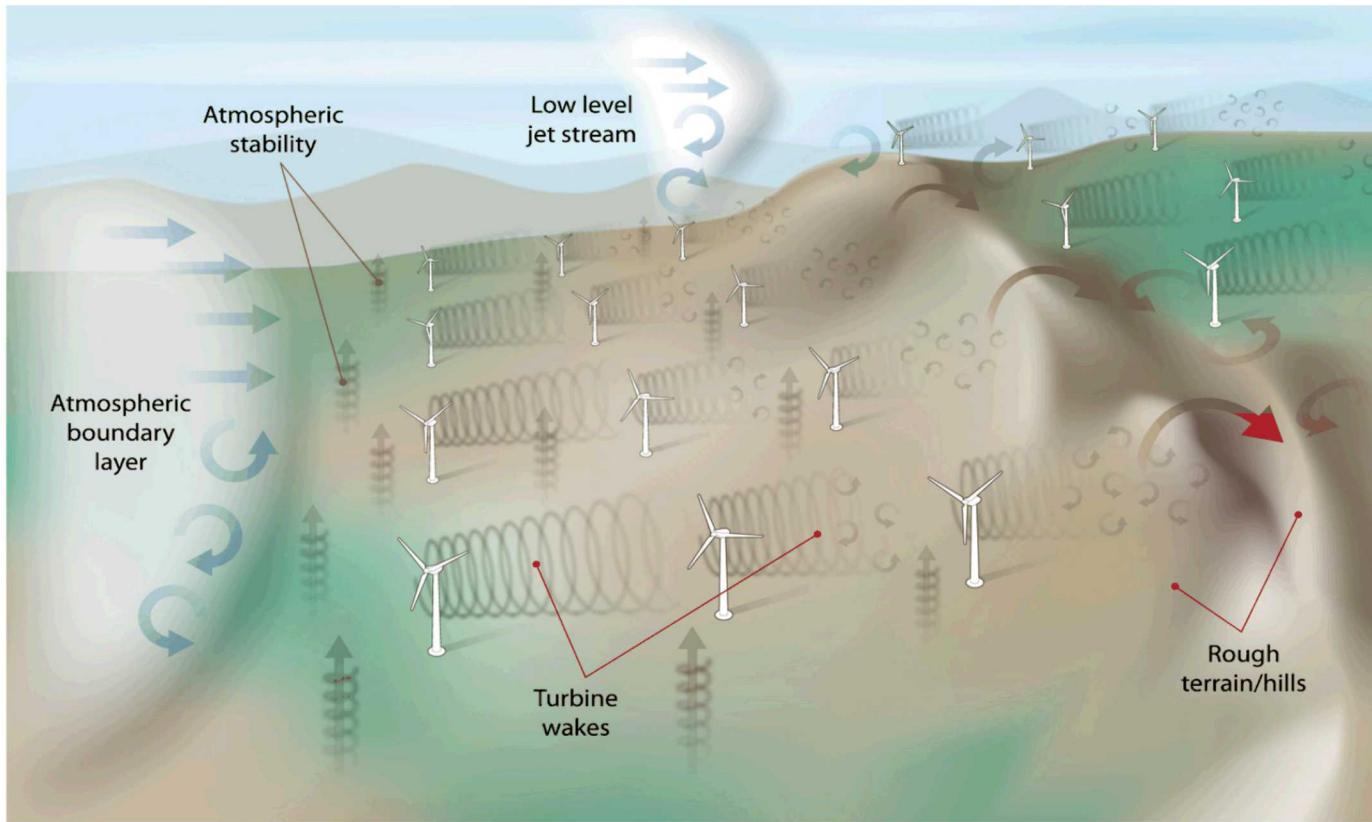
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Exawind project overview

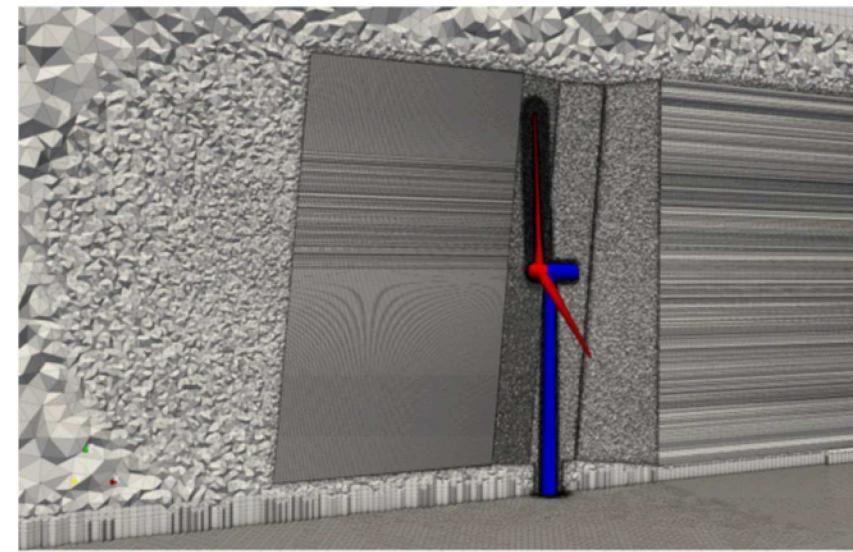
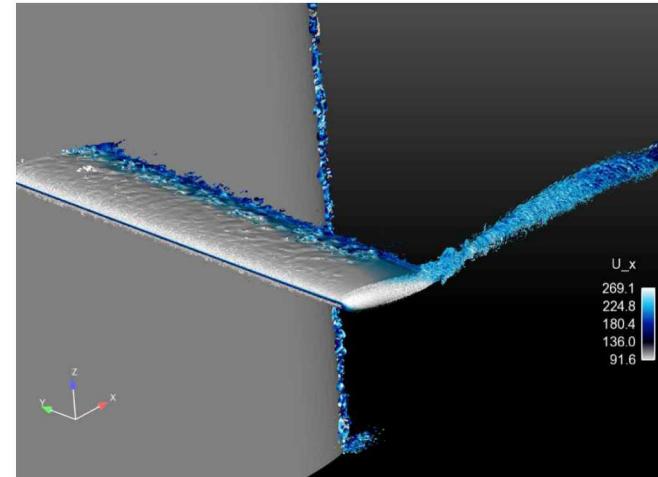
Goals/motivation for predictive simulations

- Advance our fundamental understanding of the flow physics governing whole wind plants
- Predict the response of wind farms to a wide range of atmospheric conditions



Nalu-Wind

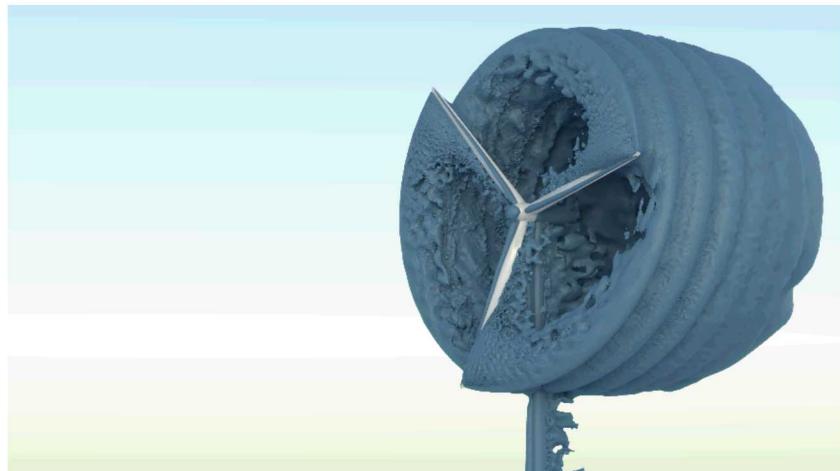
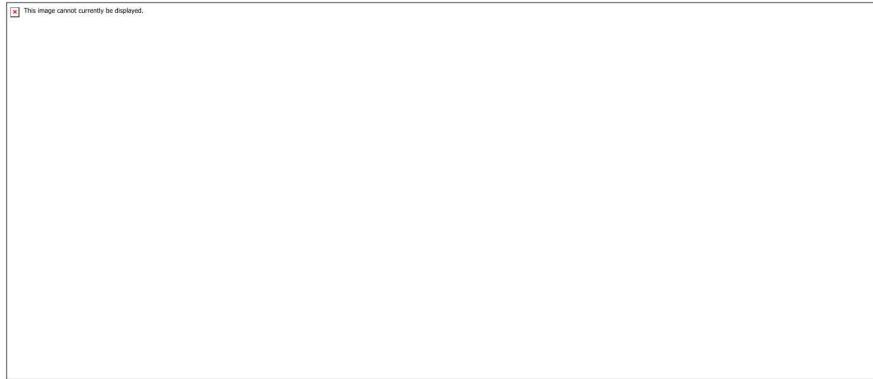
- Open source: <https://github.com/Exawind/nalu-wind>
 - Builds with Spack
- Unstructured finite volume, low-Mach flow solver
 - 2nd-order node-centered, low-dissipation FV scheme
 - **Arbitrary order accurate element-based continuous finite volume scheme**
 - Fully implicit
 - Mixed-order interfaces
- C++. Built on “Trilinos”
 - Kokkos for performance portability
 - Tpetra, MueLu, ShyLU, Ifpack2, Belos packages
 - Also support hypre
 - STK package
 - IOSS for IO



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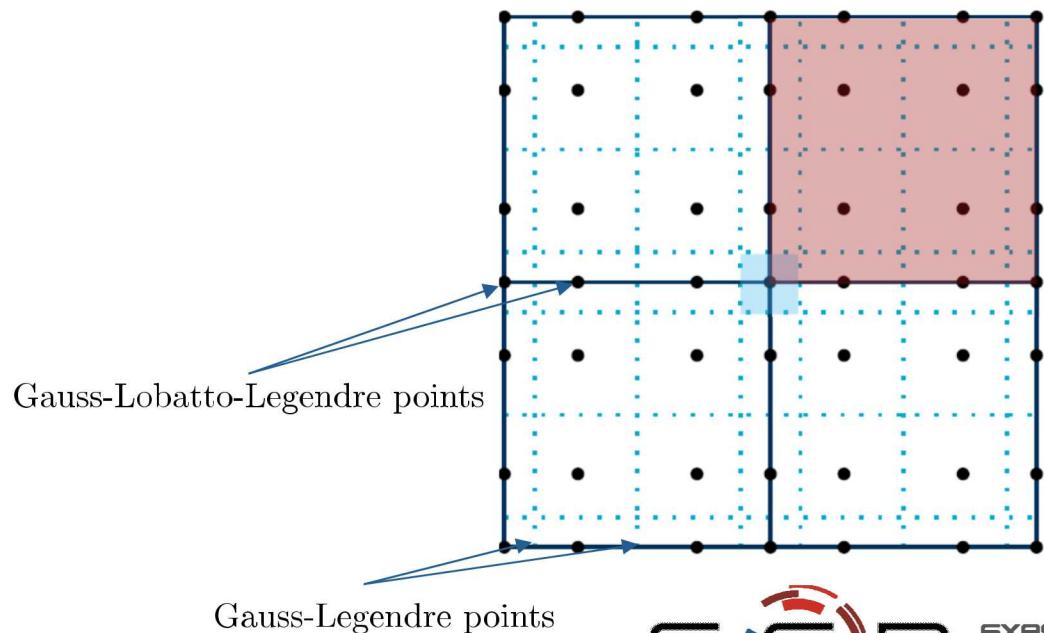
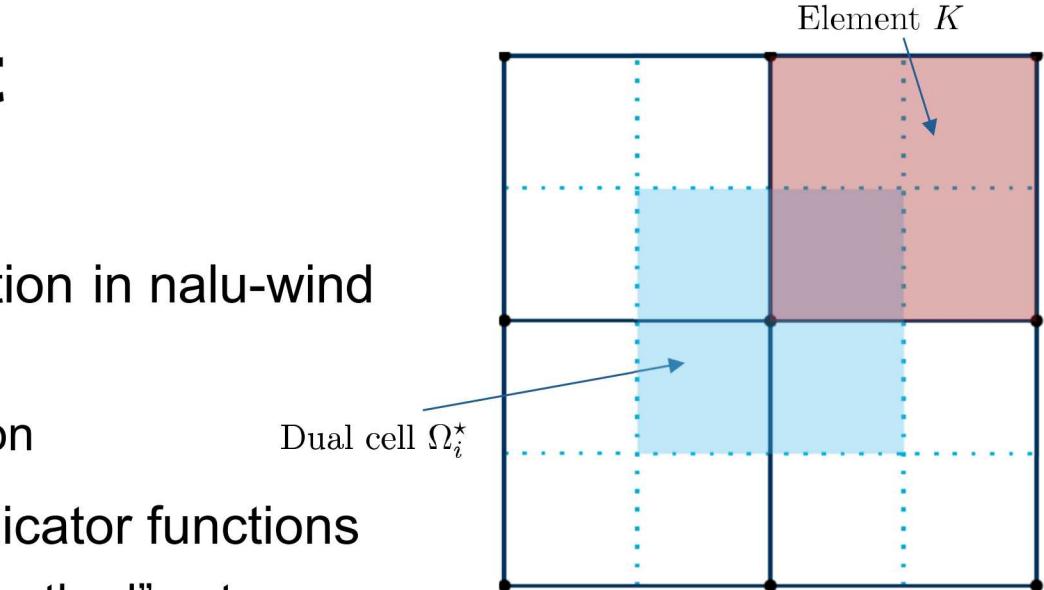
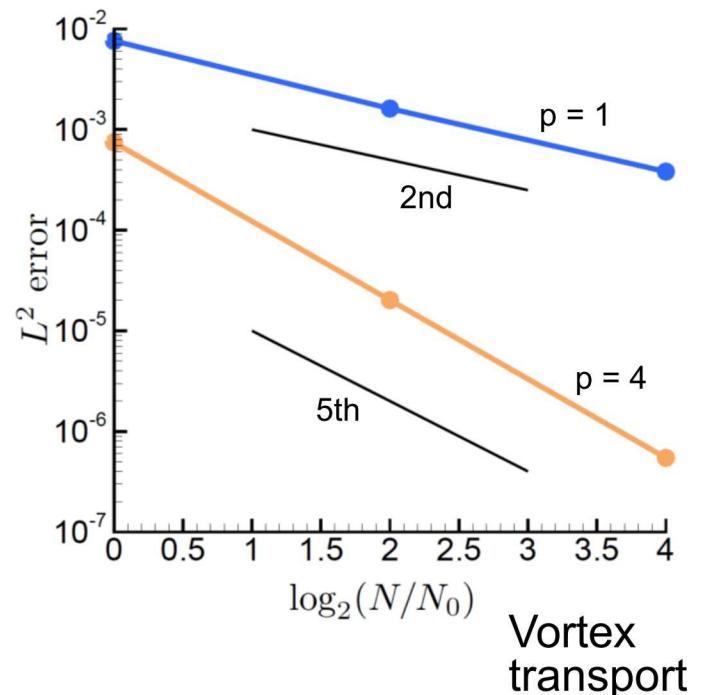
Nalu-Wind physics capabilities

- Atmospheric boundary layer modeling
 - Monin-Obukhov wall models
 - Boussinesq, Coriolis forcing
- Full turbine modeling
 - Sliding mesh, overset technologies
 - Hybrid RANS-LES models
 - "TAMS" model being developed at UT Austin
- Actuator line modeling
 - Coupling with the OpenFAST code



Control volume finite element

- Node-centered FV (EBVC) production discretization in `navi-wind`
 - Design is semi-flexible in terms of discretization
 - Linear CVFEM traditionally the “main” discretization
- Basic idea for CVFEM: define a test space of indicator functions
 - Other names “finite volume element”, “covolume method”, etc.



CVFEM Operators

- In one-dimension:



- Operators:

$$\begin{aligned}\tilde{I}_{ij} &= \ell_j(\hat{x}_i^{\text{GL}}), & \tilde{D}_{ij} &= \ell'_j(\hat{x}_i^{\text{GL}}) & \tilde{\Delta} &= \begin{cases} -1 & i = j \\ +1 & i = j + 1 \\ 0 & \text{otherwise} \end{cases} \\ W_{ij}^{-1} &= h_j(\hat{x}_i^{\text{GLL}}), & D_{ij} &= \ell'_j(\hat{x}_i^{\text{GLL}})\end{aligned}$$

where $h_j(\hat{x}) = -\sum_{k=1}^j d'_k(\hat{x})$ and d_k is the k -th Lagrange interpolant between $\{-1, \hat{x}_1^{\text{GL}}, \dots, \hat{x}_p^{\text{GL}}, +1\}$
This construction is done so $\int_{-1}^1 dx 1_{\Omega_i^*}(x)h_j(x) = \delta_{ij}$. ℓ_k is the k -th interpolant between $\{\hat{x}_j^{\text{GLL}}\}_{j=1}^{p+1}$

- For a tensor-product element in 3D, we have

$$\begin{array}{lll} S^{\hat{x}} = \tilde{\Delta} \otimes W \otimes W & \tilde{I}^{\hat{x}} = \tilde{I} \otimes I \otimes I & \mathbf{D}^{\hat{x}} = (\tilde{D} \otimes I \otimes I \quad \tilde{I} \otimes D \otimes I \quad \tilde{I} \otimes I \otimes D) \\ S^{\hat{y}} = W \otimes \tilde{\Delta} \otimes W & \tilde{I}^{\hat{y}} = I \otimes \tilde{I} \otimes I & \mathbf{D}^{\hat{y}} = (D \otimes \tilde{I} \otimes I \quad I \otimes \tilde{D} \otimes I \quad I \otimes \tilde{I} \otimes D) \\ S^{\hat{z}} = W \otimes W \otimes \tilde{\Delta} & \tilde{I}^{\hat{z}} = I \otimes I \otimes \tilde{I} & \mathbf{D}^{\hat{z}} = (D \otimes I \otimes \tilde{I} \quad I \otimes D \otimes \tilde{I} \quad I \otimes I \otimes \tilde{D}) \end{array}$$

Poisson Equation

- Over a dual cell:

$$\Delta u = f \Rightarrow \int_{\partial\Omega_i^*} \nabla u \cdot n \, dS = \int_{\Omega_i^*} f \, dx$$

- This becomes on an element,

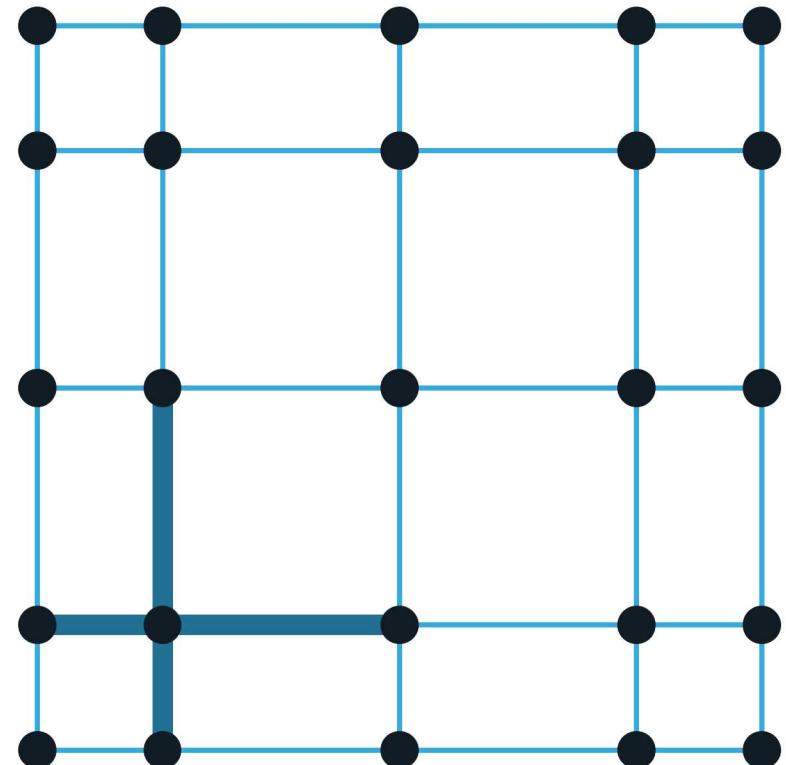
$$\sum_i S^{\hat{x}_i} [\mathbf{G}^{\hat{x}_i} \circ \mathbf{D}^{\hat{x}_i} u_e] = (W \otimes W \otimes W) [\det \mathbf{J} \circ f_e]$$

$$\mathbf{G}_{mjk}^{\hat{x}} = \det \mathbf{J}_{mjk} \left(\mathbf{J}^T \mathbf{J} \right)_{mjk}^{-1} \mathbf{e}_{\hat{x}} \\ 1 \leq m \leq p \quad 1 \leq j, k \leq p+1$$

- Use explicit SIMD types and sum factorization for apply
- Uses Trilinos-Belos package for the Krylov solver implementation
 - No matrix required

Matrix-free Preconditioning

- Just Jacobi for momentum
 - Does OK at low (~ 1) Courant numbers
- Continuity uses AMG with a sparsified “edge” Laplacian
 - Sparse system is passed to “MueLu”, which creates the preconditioner



Case (144 ³ dofs)	Avg Continuity GMRES iterations
Order 1 full system	5
Order 8 no preconditioner	129
Order 8 full sparsified system	15
Order 8 edge sparsified system	9

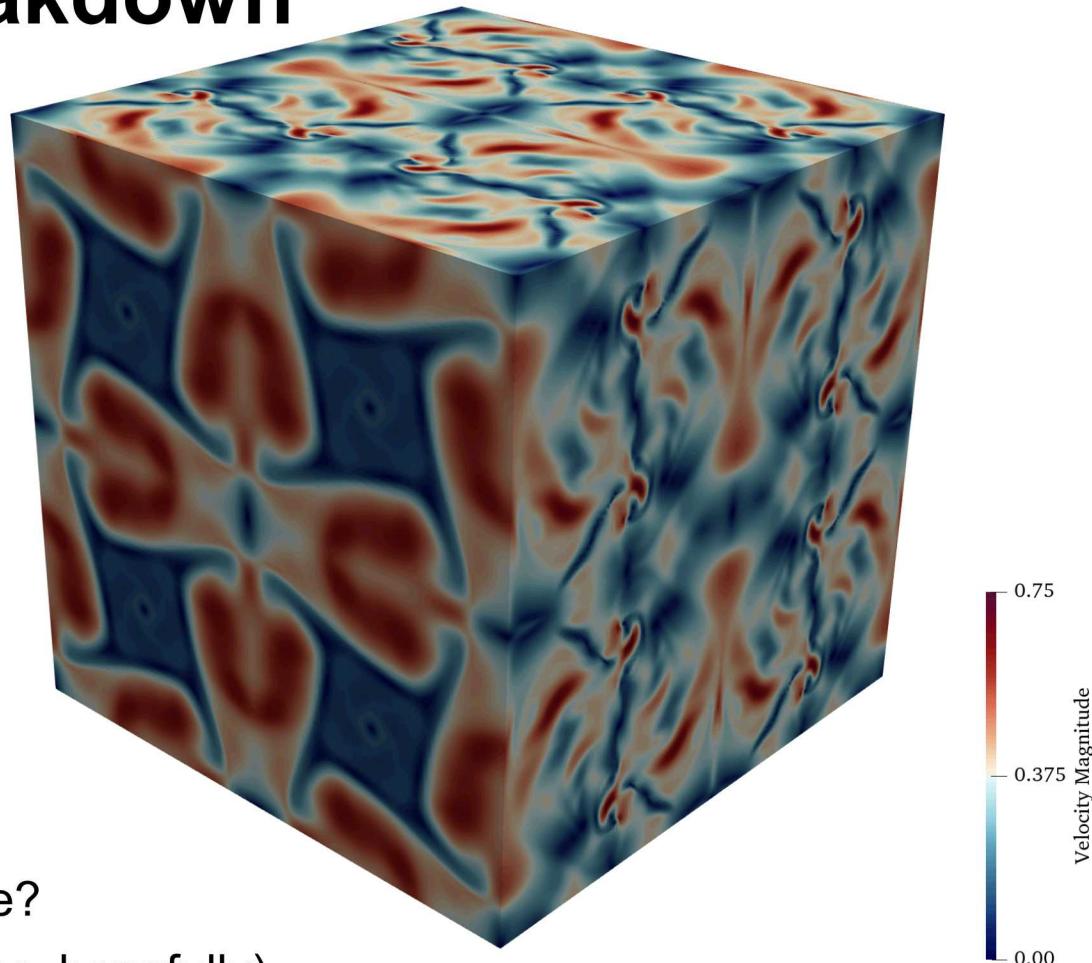
Re=1600 Taylor Green Vortex Breakdown

$$u(t = 0, x, y, z) = +u_0 \sin(x) \cos(y) \cos(z)$$

$$v(t = 0, x, y, z) = -u_0 \cos(x) \sin(y) \cos(z)$$

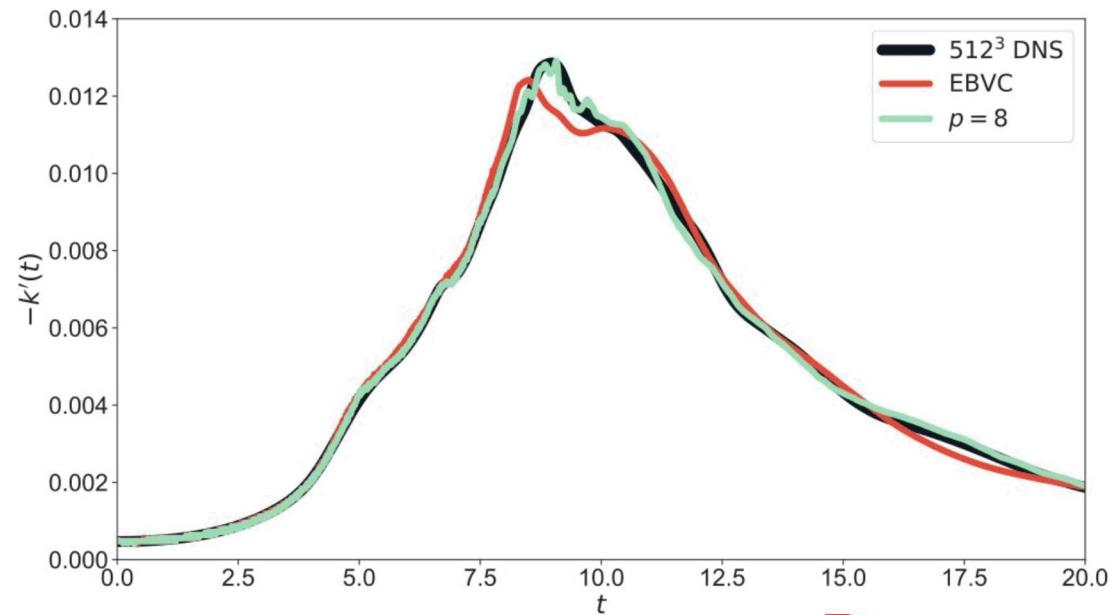
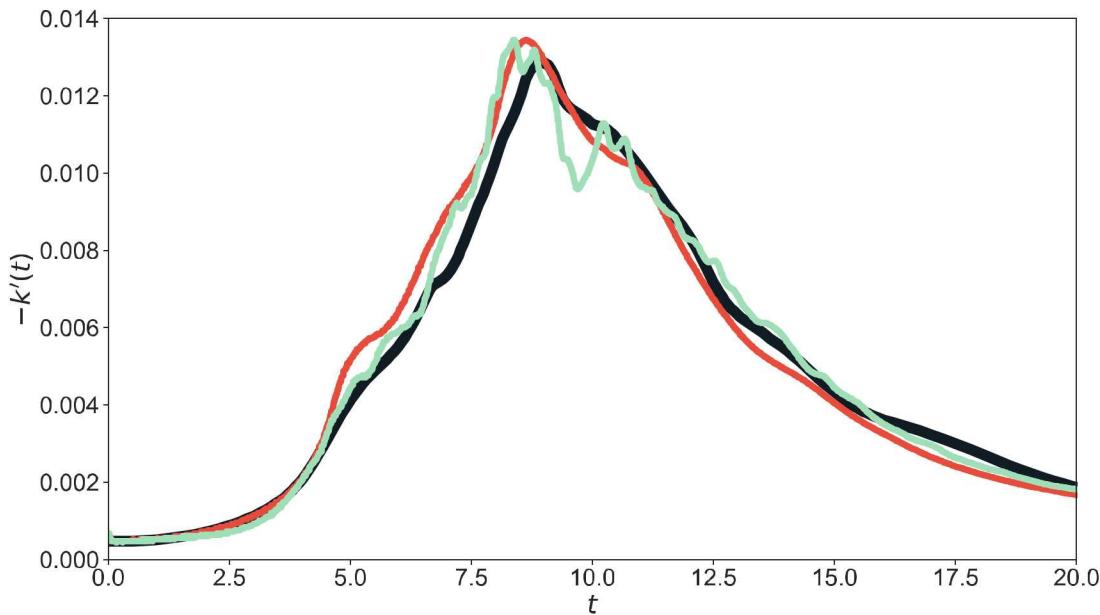
$$w(t = 0, x, y, z) = 0$$

- Standard, turbulent-like test case
 - Just trigonometric functions to set up
 - Three resolutions $(96/p)^3$, $(144/p)^3$, and $(192/p)^3$
- Cases are run underresolved (256^3 for DNS)
 - How does the scheme behave outside the asymptotic range?
 - LES will be underresolved (in localized spatiotemporal zones, hopefully)

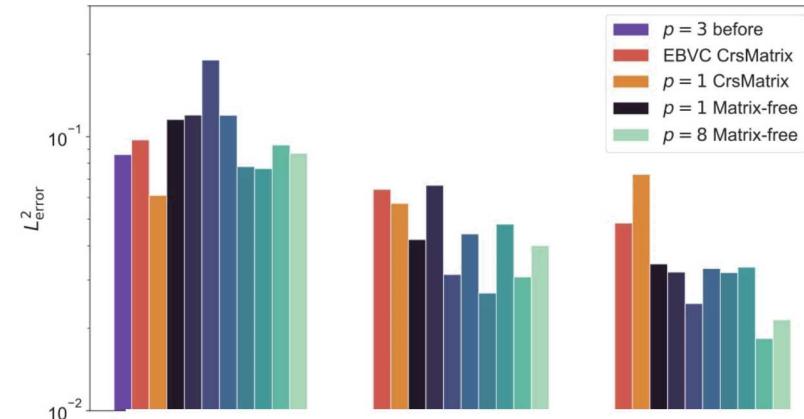
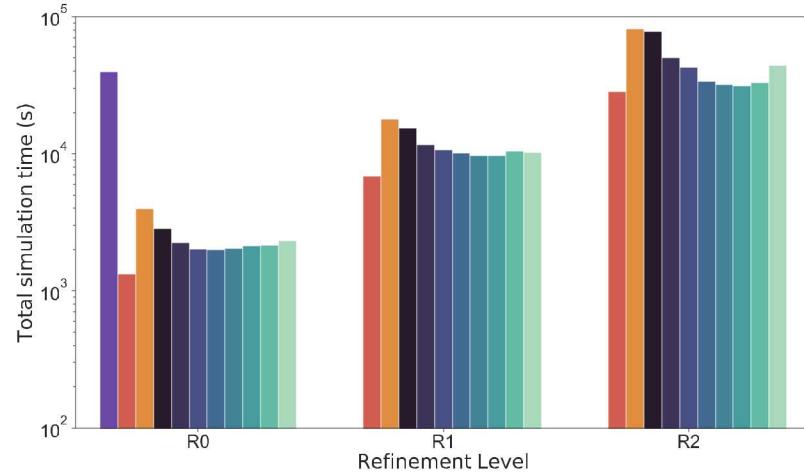


Results

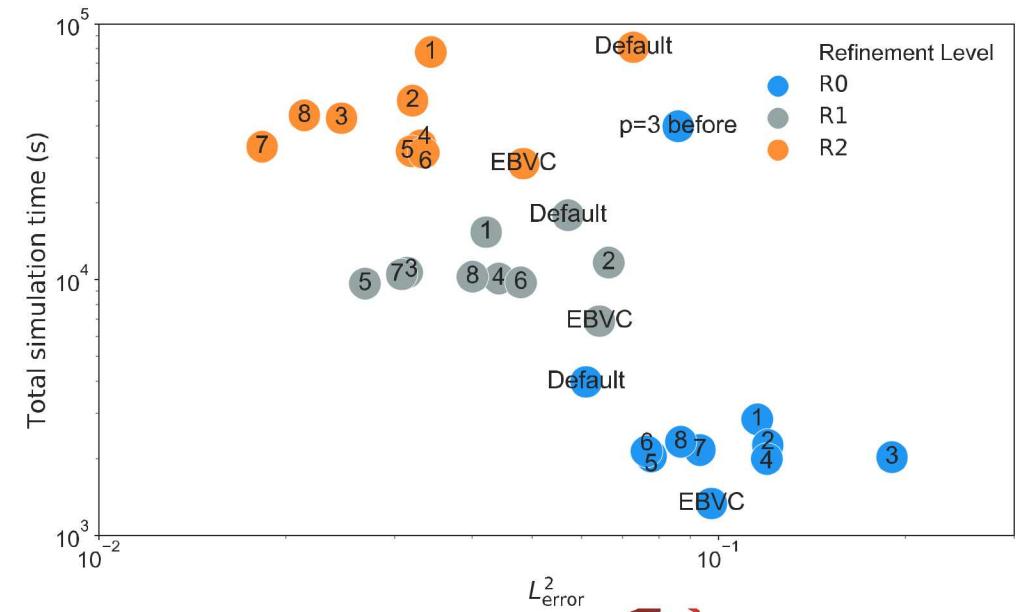
- High order scheme captures initial laminar breakdown and scale generation and behaves “OK” when resolution insufficient
 - Need some stabilization beyond the pressure stabilization



Overall

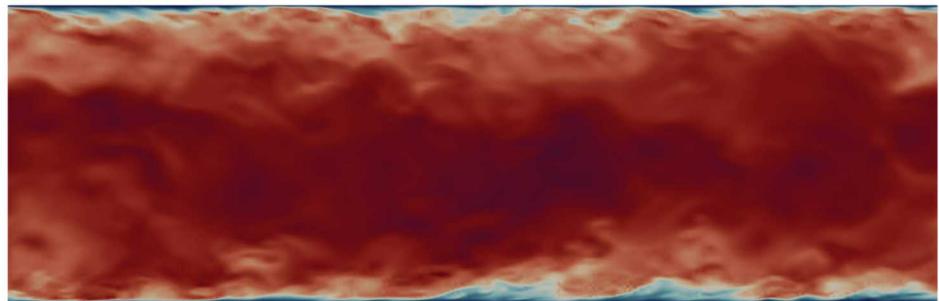
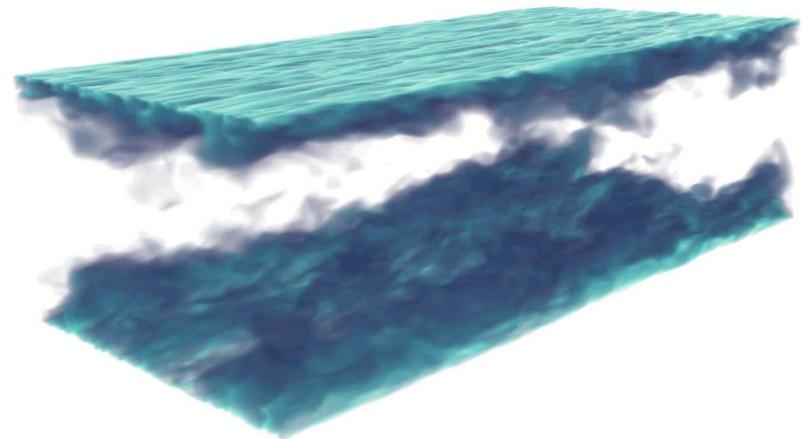


- Computational cost is roughly independent of polynomial order for polynomial orders 4-7
 - Slower than the edge-based finite volume
 - Slow down is due to extra equation essentially
 - Still faster than the default element scheme
- Maybe some benefit in marginally underresolved case
 - Resolved region performs very well, affecting rest of result

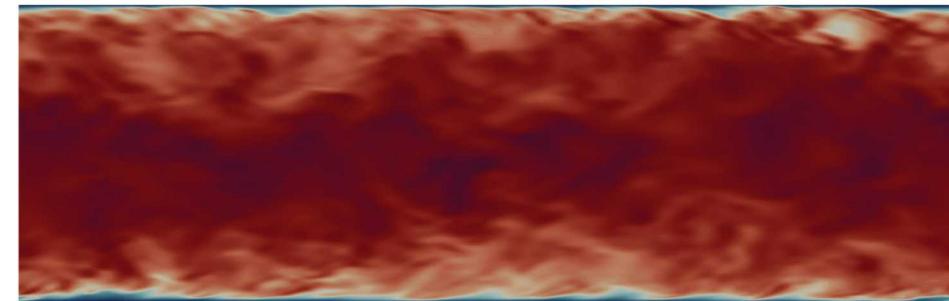
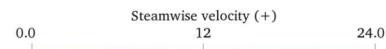


Wall-resolved channel flow LES

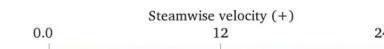
- Kim, Moser, Mansour (1999) $Re_\tau = 590$ case
- “Wall adapting local eddy-viscosity” model of Nicoud and Ducros (1999)
- Run 64x64x48 nodes up to 192x192x128 in 3/2 increments
 - DNS: 384x257x384
 - Constant pressure gradient



$p = 7$

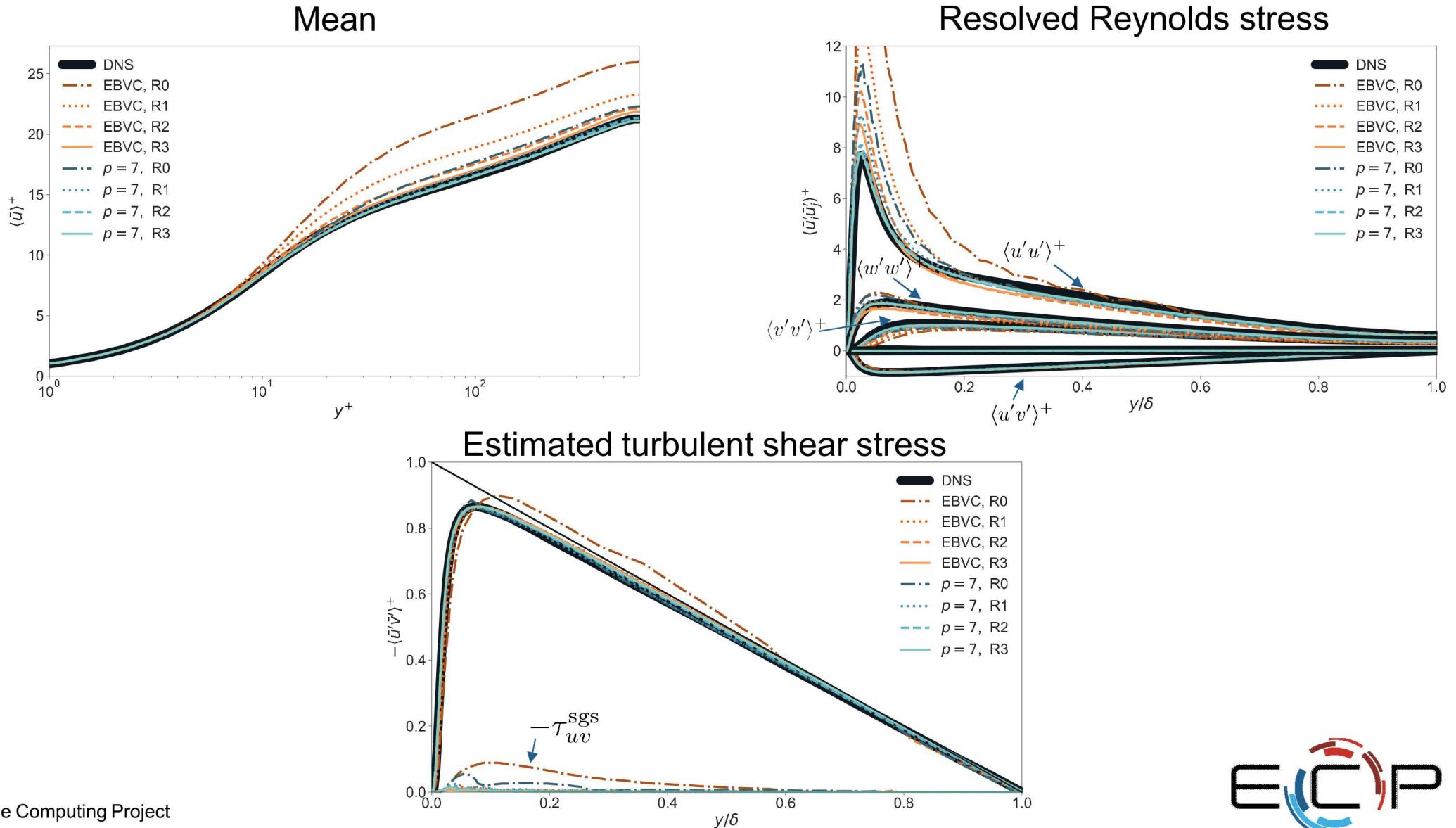


$EBVC$

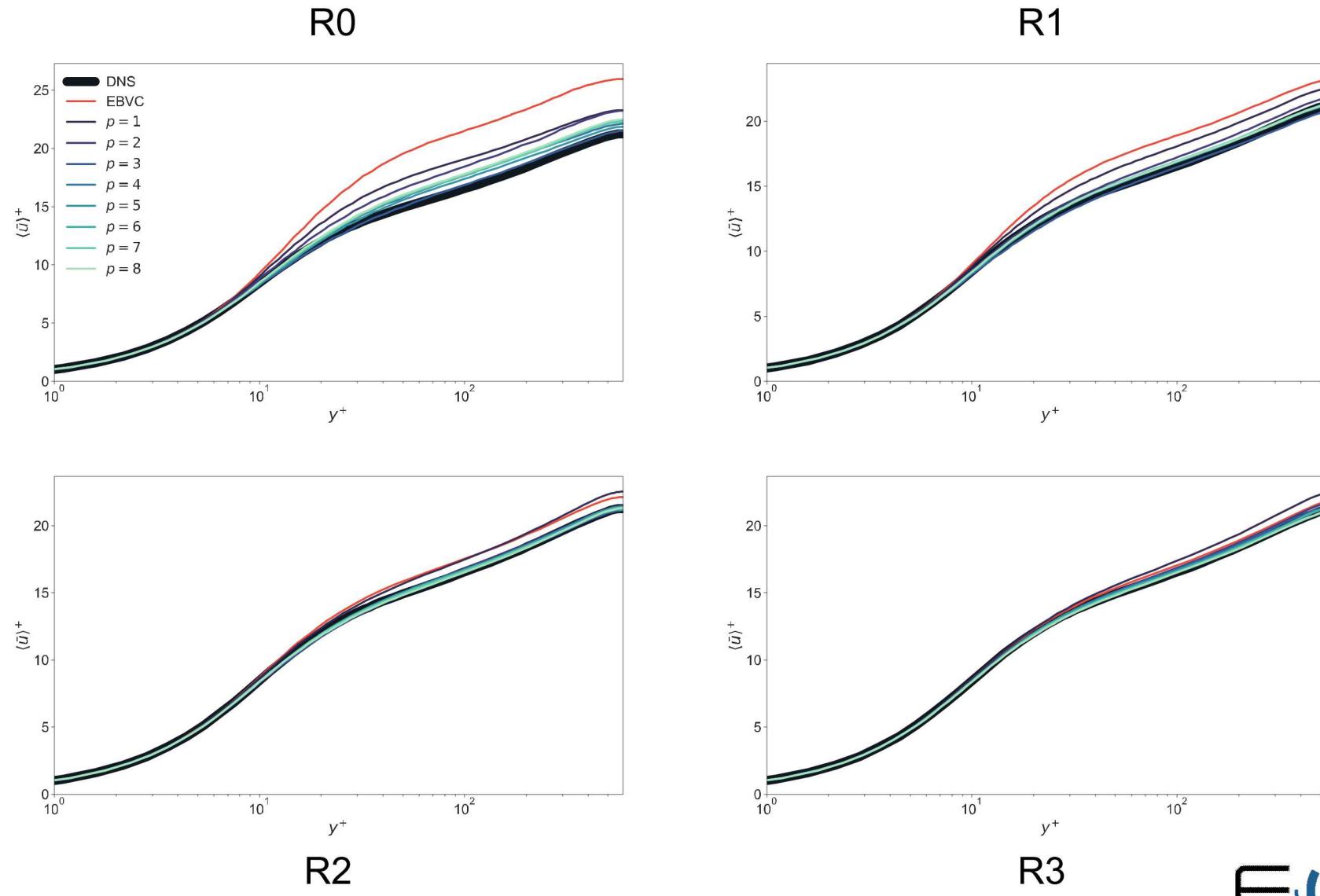


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Effect of resolution on predictions

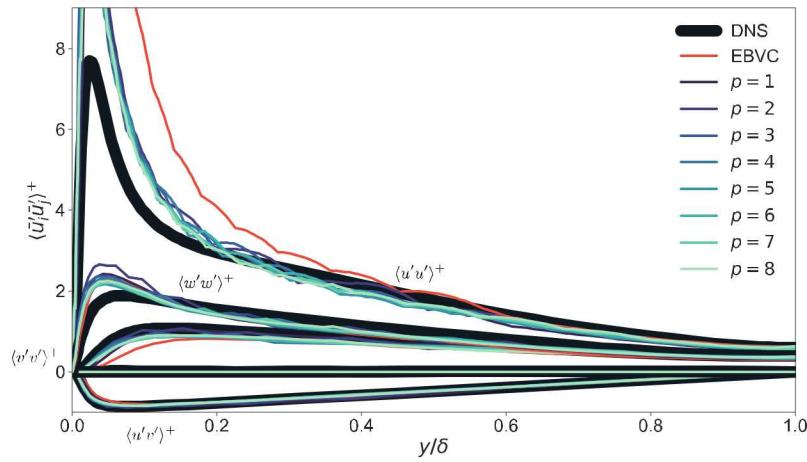


Effect of polynomial order on mean velocity prediction

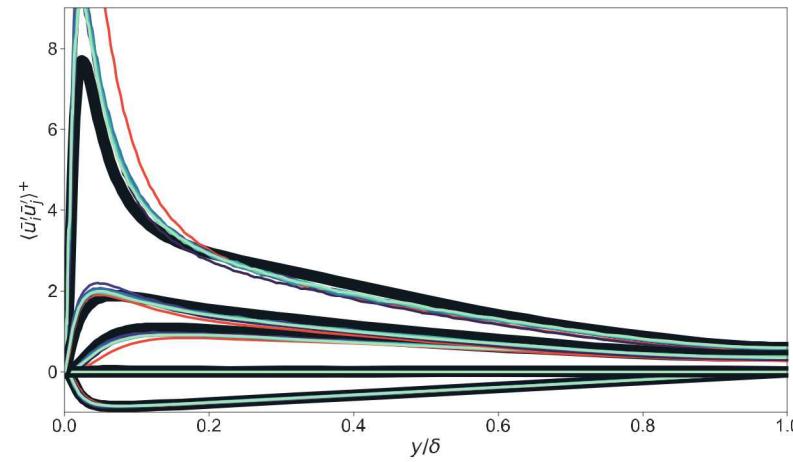


Effect of order on the resolved Reynolds stress

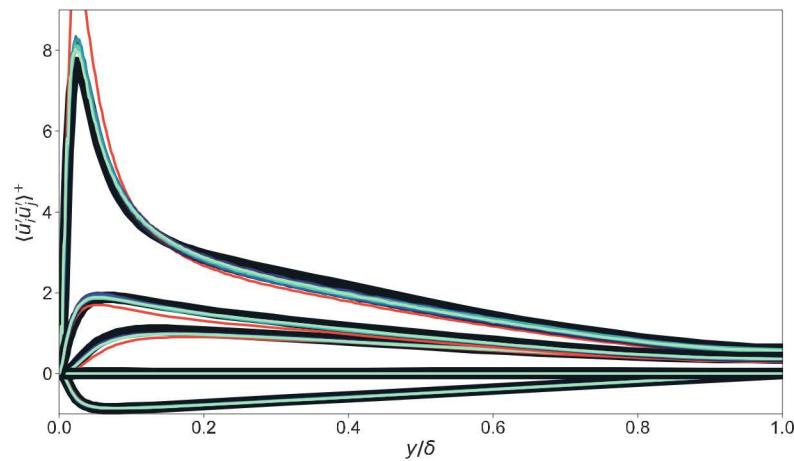
R0



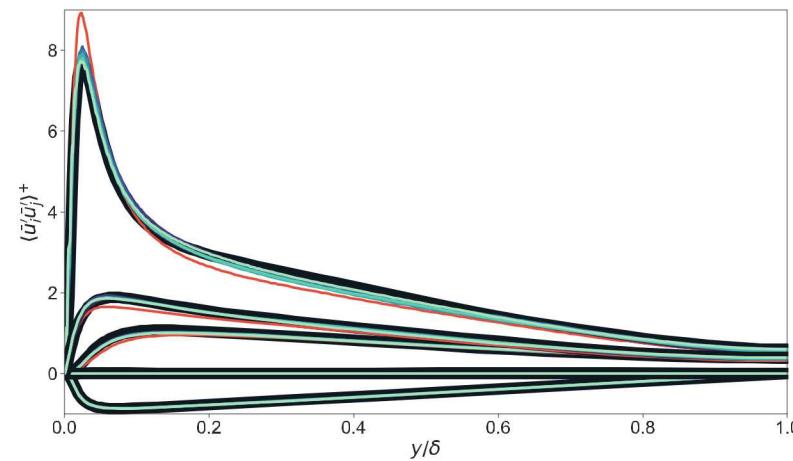
R1



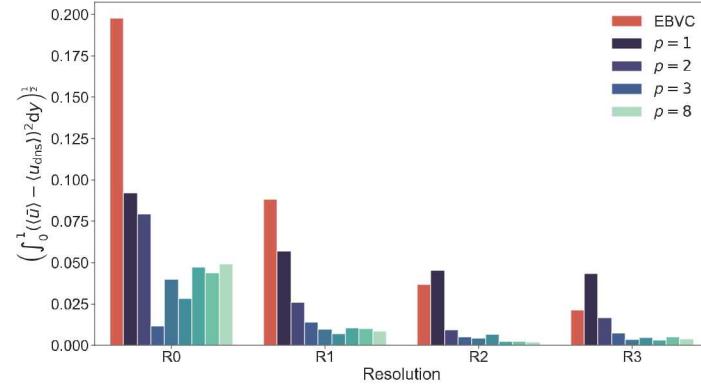
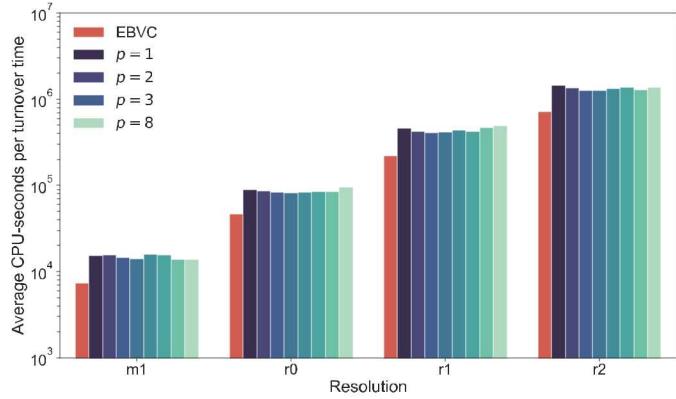
R2



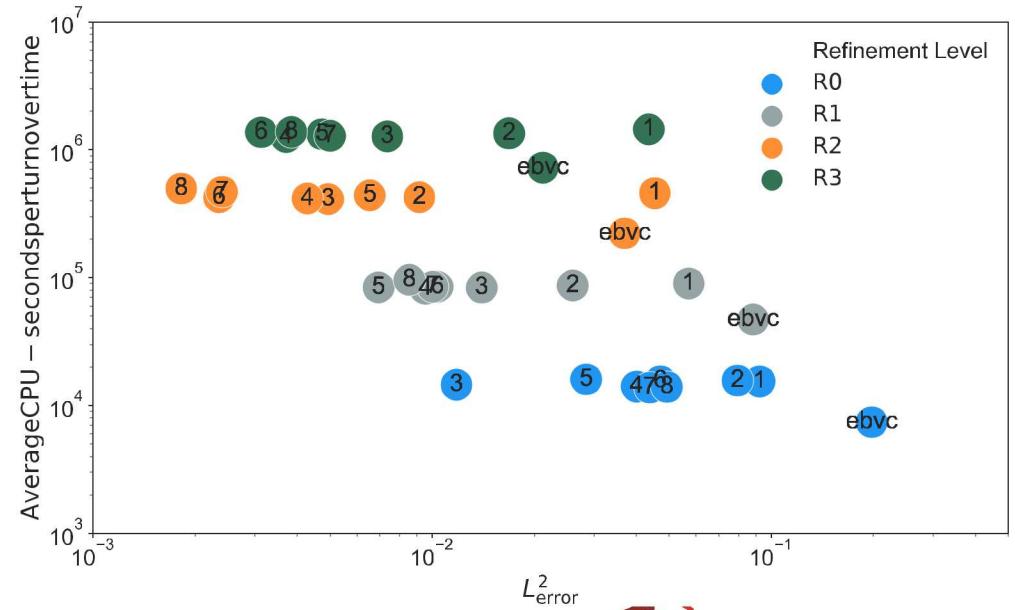
R3



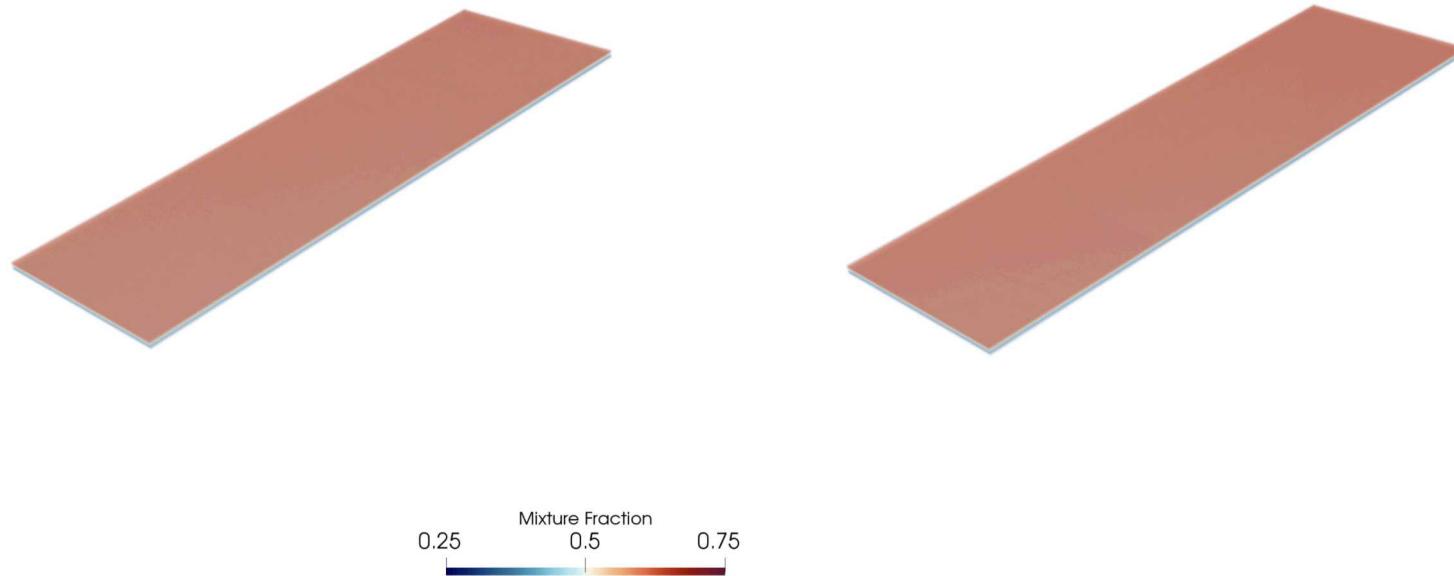
Overall



- High order performs better
 - Some variation for lower-high order
 - Turbulence model does well but could be adapted
- EBVC is relatively faster than the Taylor-Green
 - Preconditioner somewhat worse, momentum particularly
 - Partially due to switch to Haswell

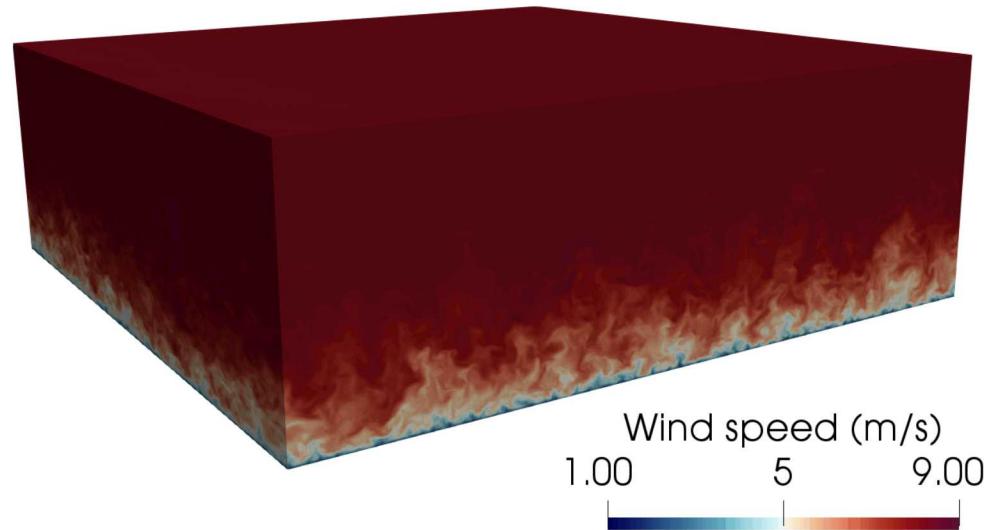


Mixing layer



Closing

- Accuracy vs time looks good for LES flows
 - Still places for improvement
- Not working on the GPU
 - Written using Kokkos heavily but still work to do
- Looking at a flow more directly relevant to wind
 - Looking at mixed discretization for near-turbine and off-turbine regions



Acknowledgement

- This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering, and early testbed platforms, in support of the nation's exascale computing imperative.

Citations

- Nicoud, Franck, and Frédéric Ducros. "Subgrid-scale stress modelling based on the square of the velocity gradient tensor." *Flow, turbulence and Combustion* 62.3 (1999): 183-200.
- Moser, Robert D., John Kim, and Nagi N. Mansour. "Direct numerical simulation of turbulent channel flow up to $Re \tau = 590$." *Physics of fluids* 11.4 (1999): 943-945.