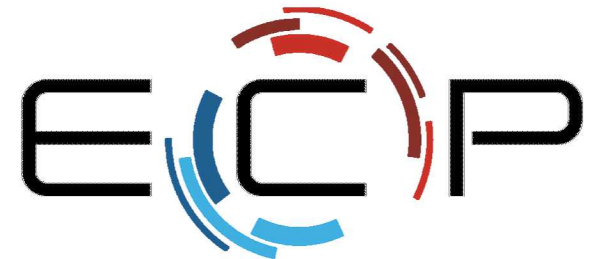


# High order in Exawind

SAND2019-9280PE

Robert Knaus, Sandia National Laboratories

6 August 2019

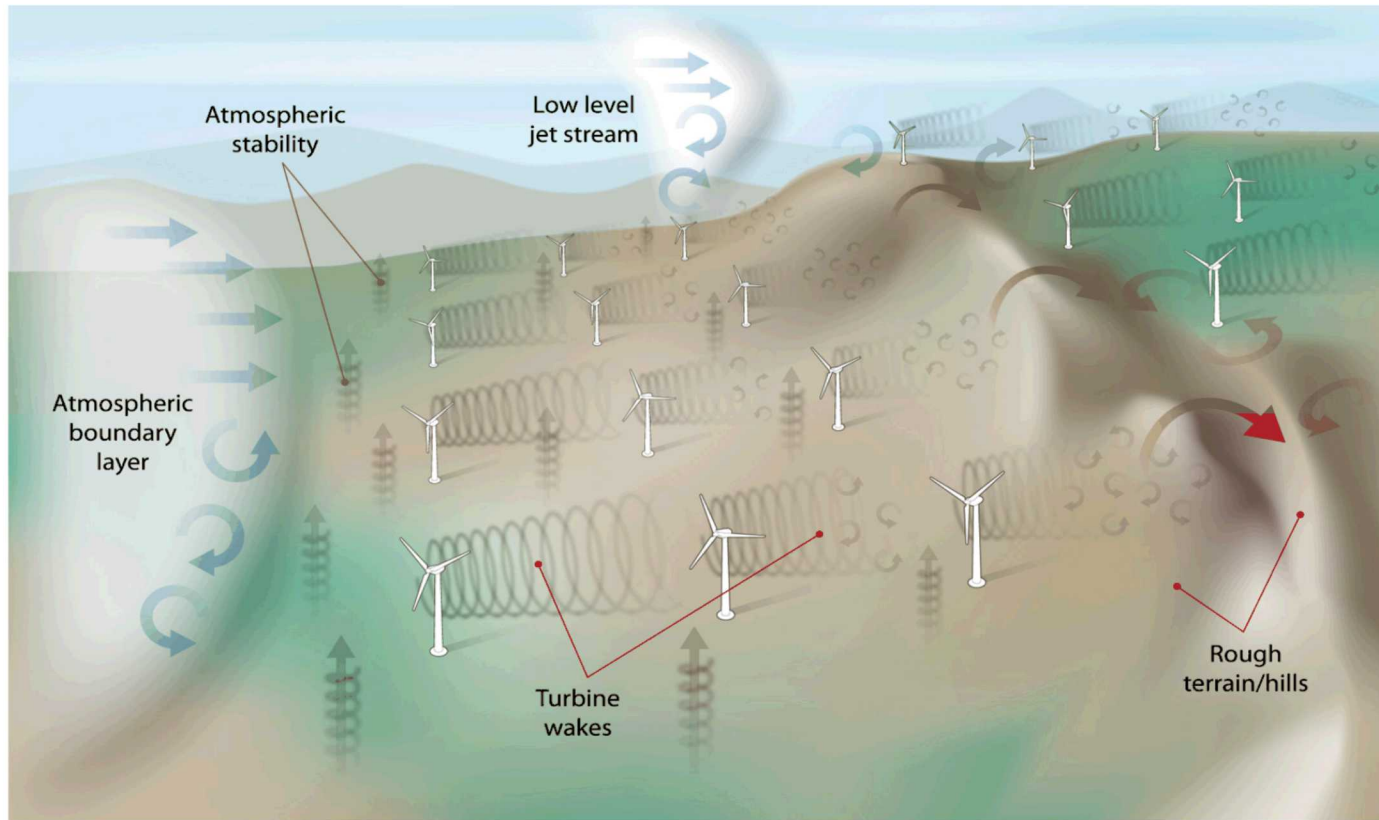


EXASCALE COMPUTING PROJECT

# Exawind project overview

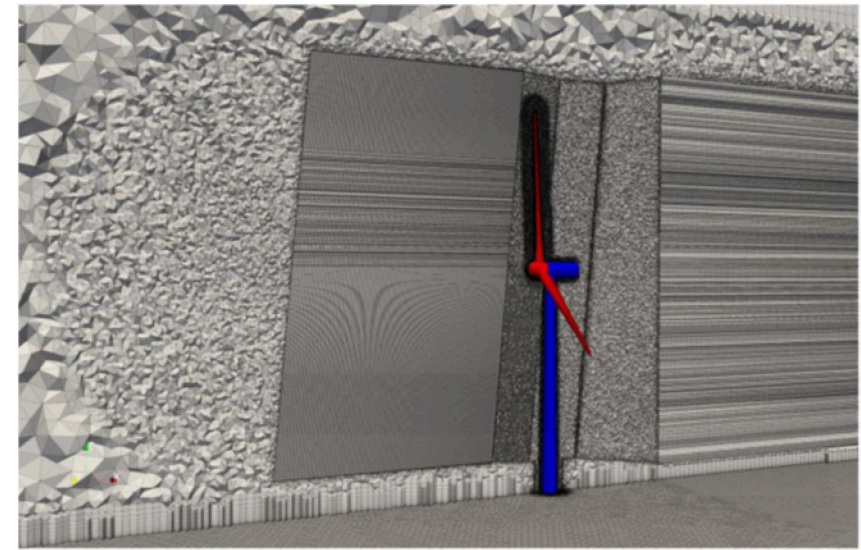
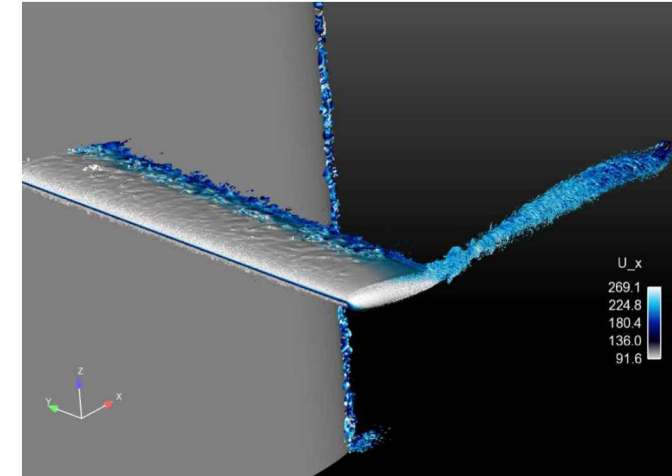
## Goals/motivation for predictive simulations

- 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



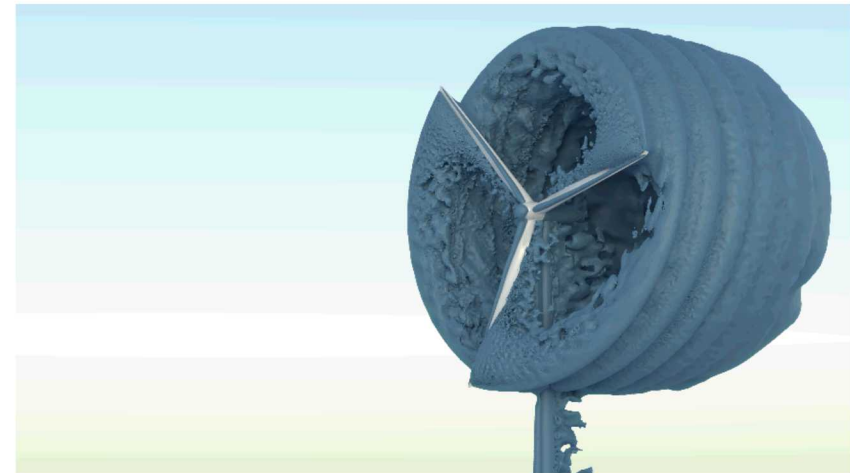
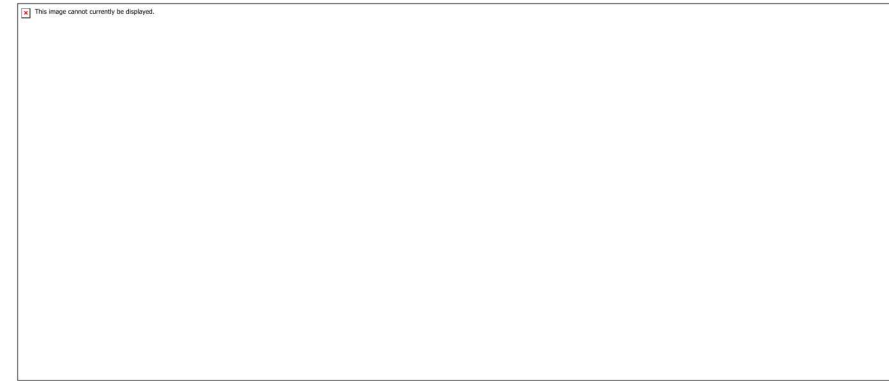
# Nalu-Wind

- Open source: <https://github.com/Exawind/nalu-wind>
  - Builds with Spack
- Unstructured finite volume, low-Mach flow solver
  - 2<sup>nd</sup>-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



# Nalu-Wind physics capabilities

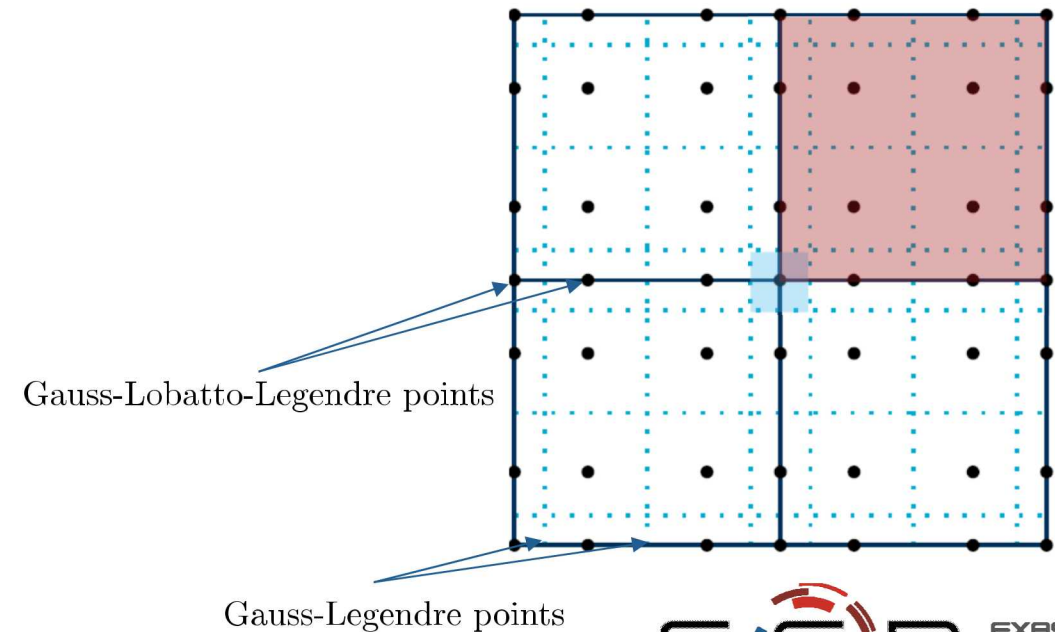
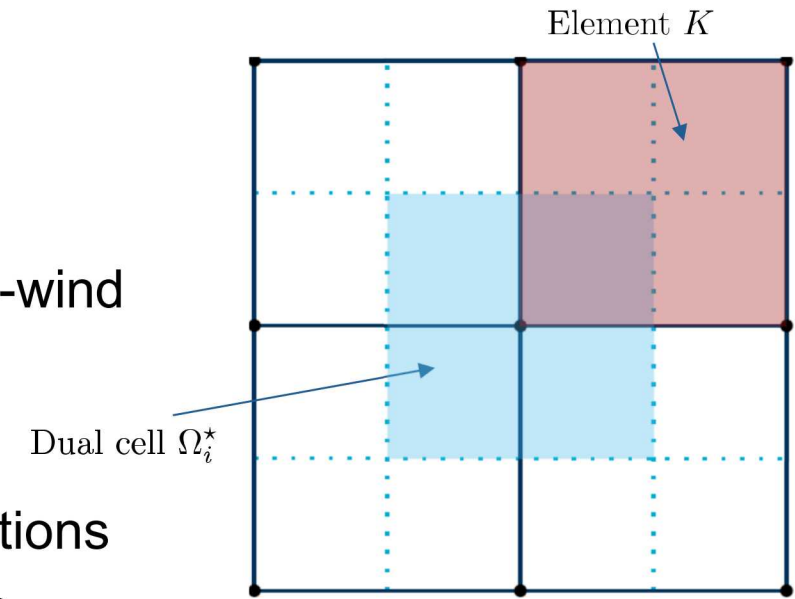
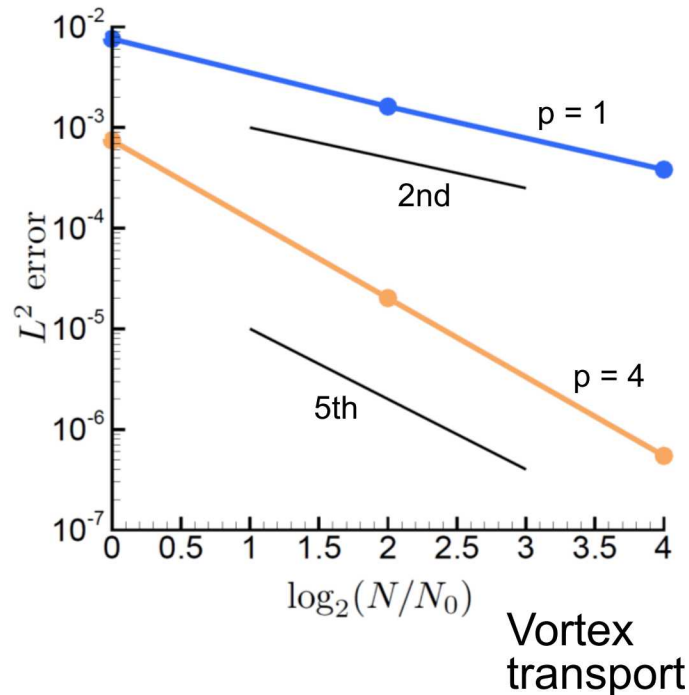
- Atmospheric boundary layer modeling
  - Monin-Obukhov wall models
  - Boussinesq, Coriolis forcing
- Full turbine modeling
  - Sliding mesh, overset technologies
  - Hybrid RANS-LES models
    - "TAMS" model being developed at UT Austin
- Actuator line modeling
  - Coupling with the OpenFAST code





# Control volume finite element

- Node-centered FV (EBVC) production discretization in nalu-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:

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

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  $\int_{-1}^1 dx \, 1_{\Omega_i^*}(x) h_j(x) = \delta_{ij}$ .  $\ell_k$  is the  $k$ -th interpolant between  $\{\hat{x}_j^{\text{GLL}}\}_{j=1}^{p+1}$ .

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

$$\begin{aligned} S^{\hat{x}} &= \tilde{\Delta} \otimes W \otimes W & \tilde{I}^{\hat{x}} &= \tilde{I} \otimes I \otimes I & \mathbf{D}^{\hat{x}} &= \begin{pmatrix} \tilde{D} \otimes I \otimes I & \tilde{I} \otimes D \otimes I & \tilde{I} \otimes I \otimes D \end{pmatrix} \\ S^{\hat{y}} &= W \otimes \tilde{\Delta} \otimes W & \tilde{I}^{\hat{y}} &= I \otimes \tilde{I} \otimes I & \mathbf{D}^{\hat{y}} &= \begin{pmatrix} D \otimes \tilde{I} \otimes I & I \otimes \tilde{D} \otimes I & I \otimes \tilde{I} \otimes D \end{pmatrix} \\ S^{\hat{z}} &= W \otimes W \otimes \tilde{\Delta} & \tilde{I}^{\hat{z}} &= I \otimes I \otimes \tilde{I} & \mathbf{D}^{\hat{z}} &= \begin{pmatrix} D \otimes I \otimes \tilde{I} & I \otimes D \otimes \tilde{I} & I \otimes I \otimes \tilde{D} \end{pmatrix} \end{aligned}$$

# 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,

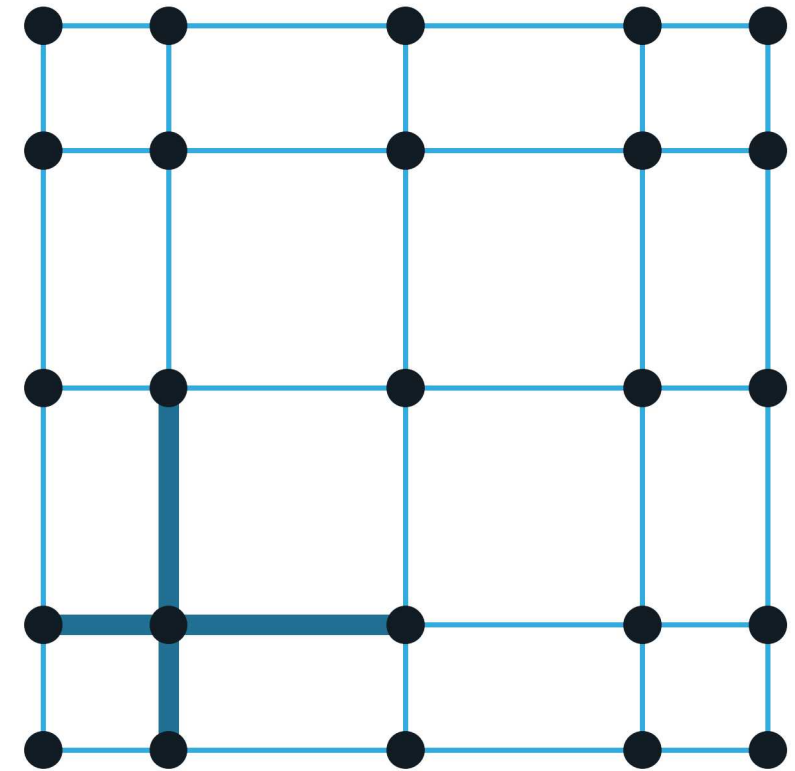
$$\sum_i S^{\hat{x}_i} [\mathbf{G}^{\hat{x}_i} \circ \mathbf{D}^{\hat{x}_i} u_e] = (W \otimes W \otimes W) [\det \mathbf{J} \circ f_e]$$

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

- 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 ( $\sim 1$ ) Courant numbers
- Continuity uses AMG with a sparsified “edge” Laplacian
  - Sparse system is passed to “MueLu”, which creates the preconditioner



Case (144 <sup>3</sup> 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



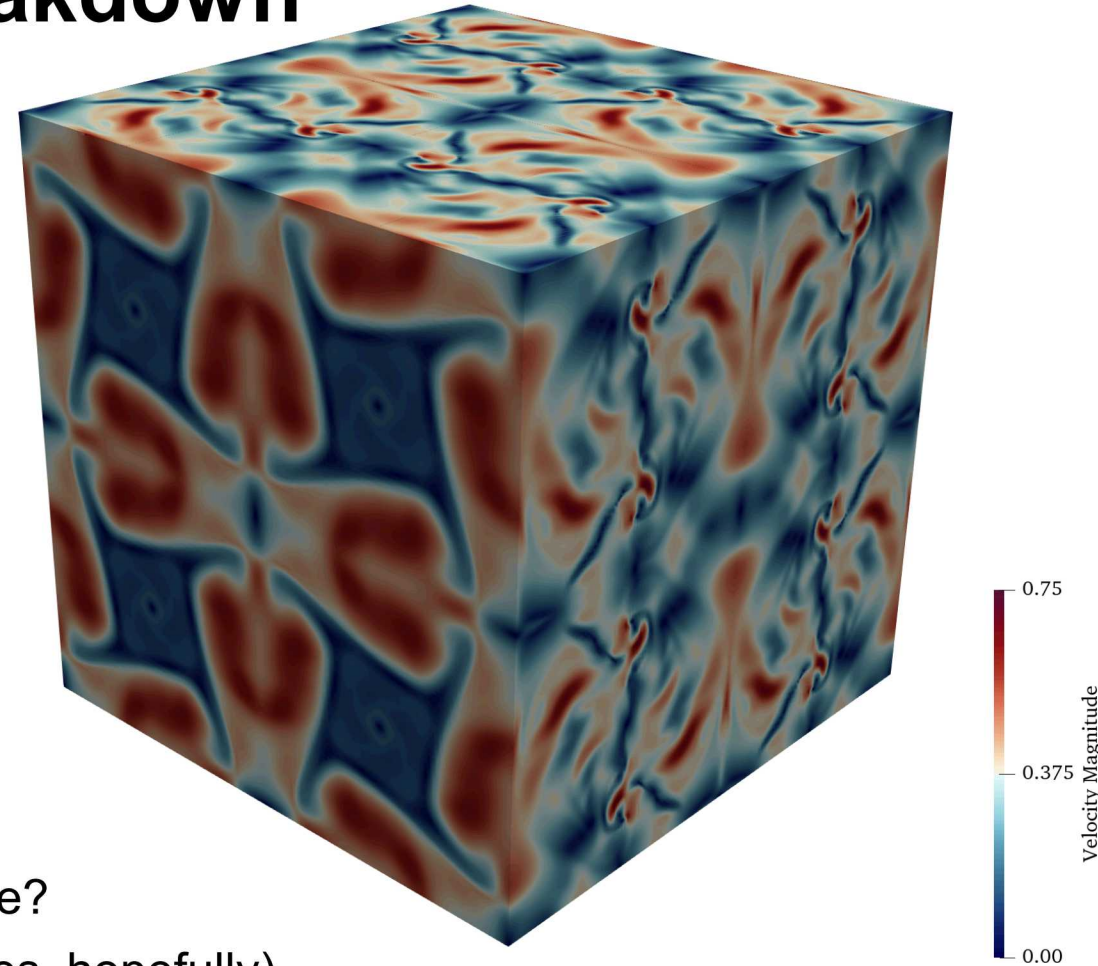
# Re=1600 Taylor Green Vortex Breakdown

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

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

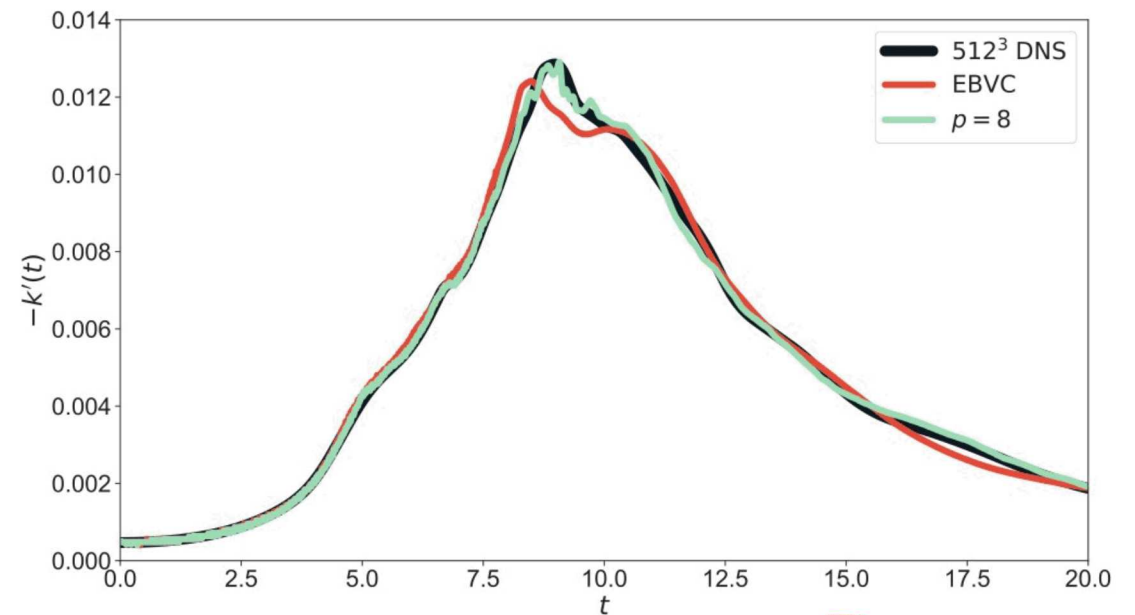
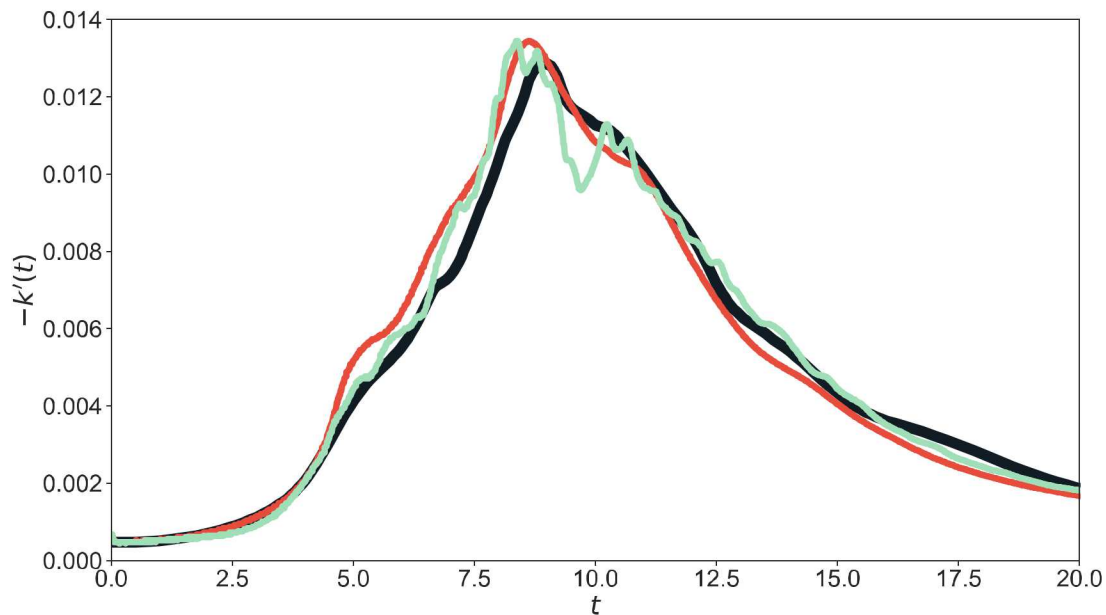
$$w(t = 0, x, y, z) = 0$$

- 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)

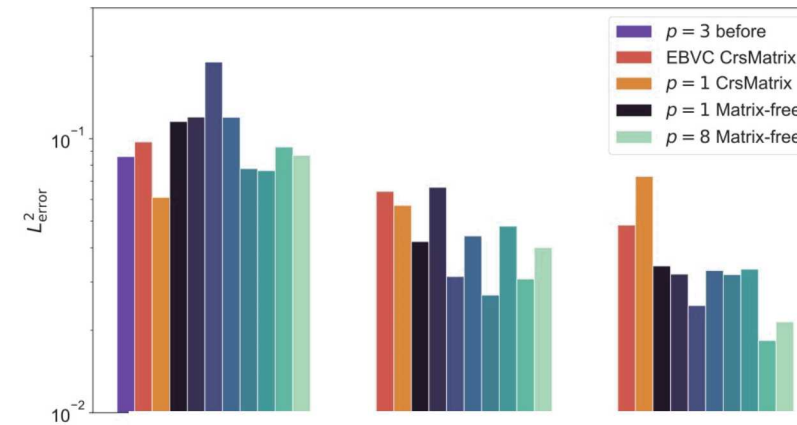
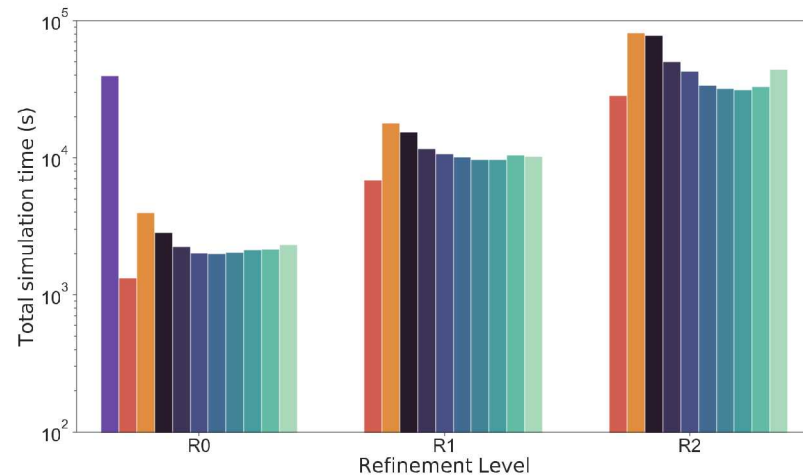


# Results

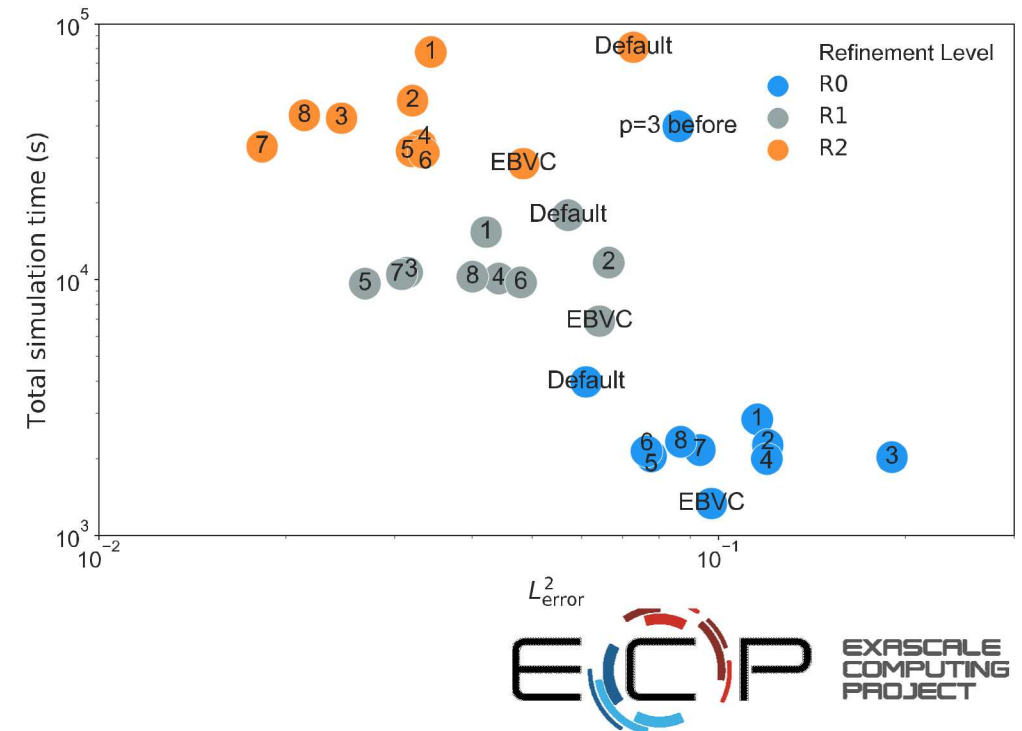
- High order scheme captures initial laminar breakdown and scale generation and behaves “OK” when resolution insufficient
  - Need some stabilization beyond the pressure stabilization



# Overall

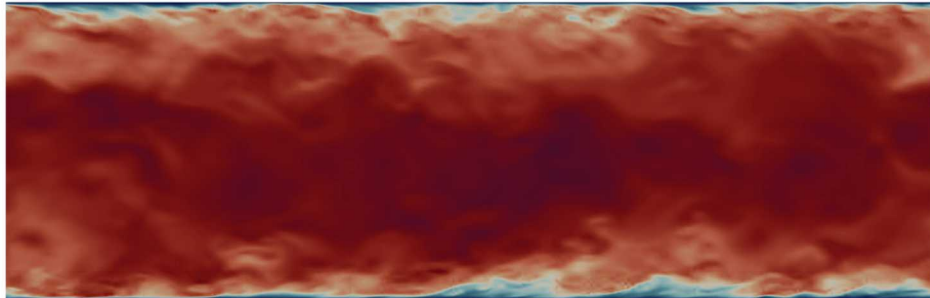
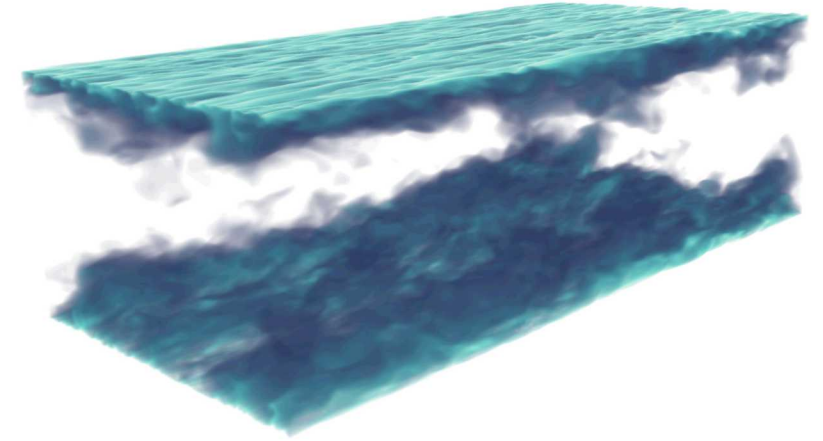


- Computational cost is roughly independent of polynomial order for polynomial orders 4-7
  - Slower than the edge-based finite volume
  - Slow down is due to extra equation essentially
  - Still faster than the default element scheme
- Maybe some benefit in marginally underresolved case
  - Resolved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

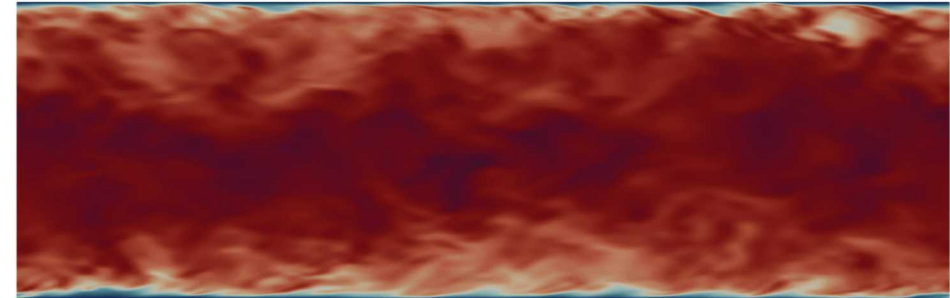
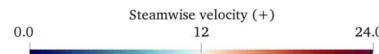


# Wall-resolved channel flow LES

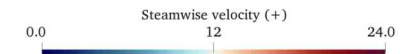
- Kim, Moser, Mansour (1999)  $Re_\tau = 590$  case
- “Wall adapting local eddy-viscosity” model of Nicoud and Ducros (1999)
- Run 64x64x48 nodes up to 192x192x128 in 3/2 increments
  - DNS: 384x257x384
  - Constant pressure gradient



$p = 7$



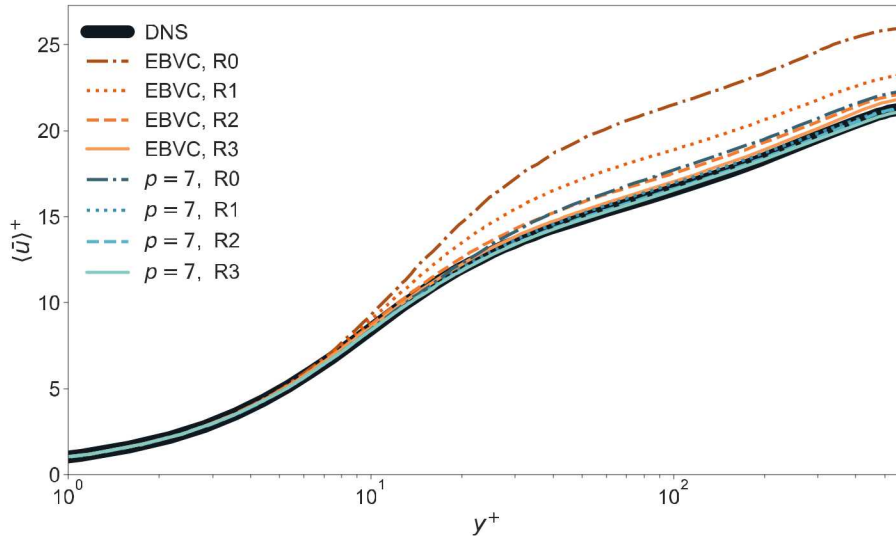
*EBVC*



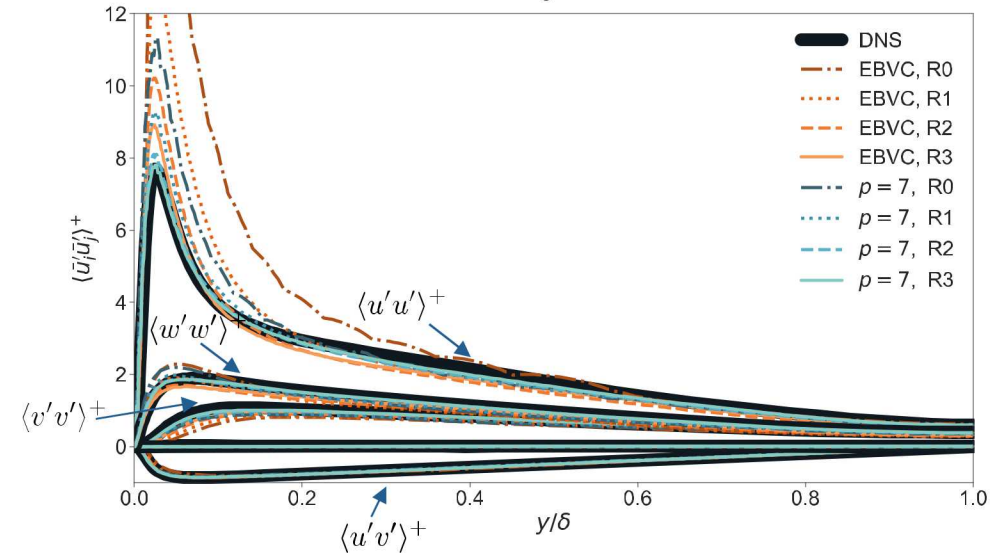


# Effect of resolution on predictions

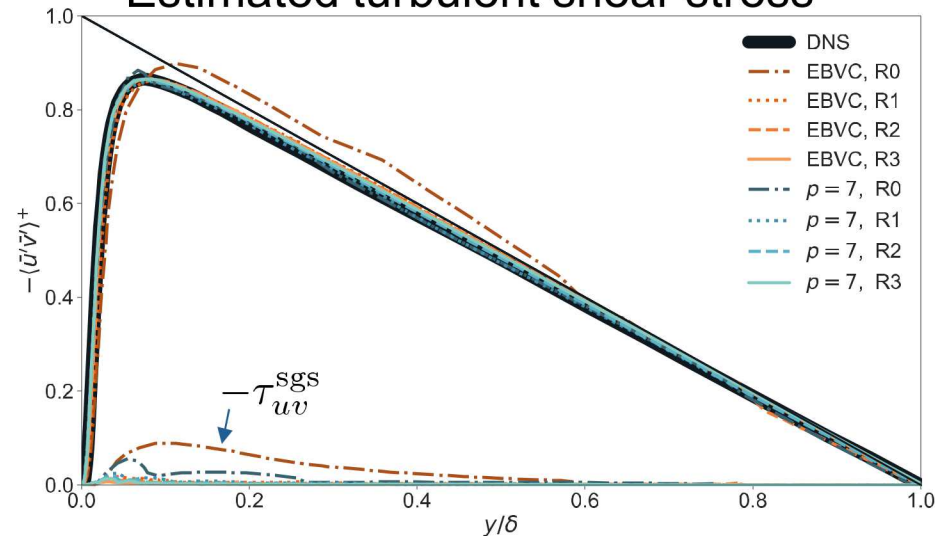
Mean



Resolved Reynolds stress

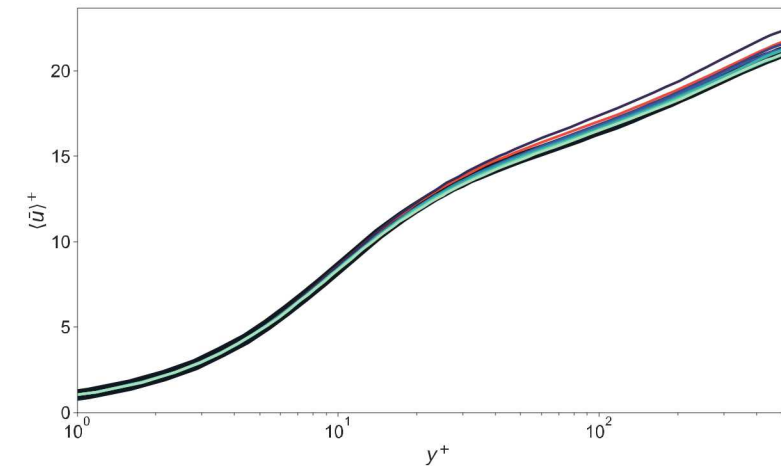
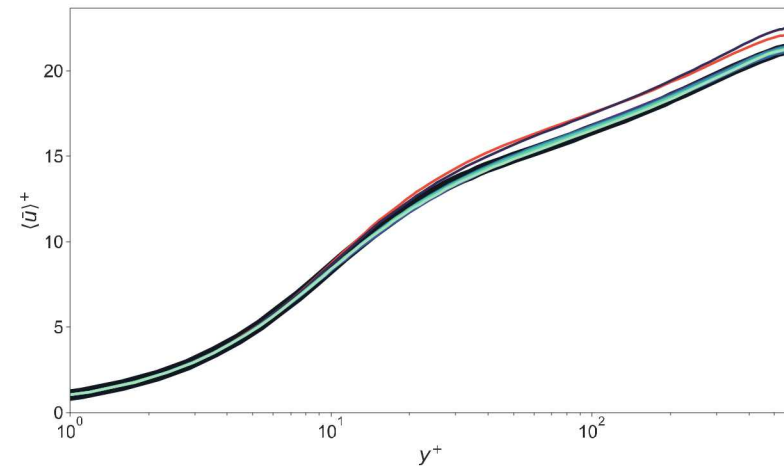
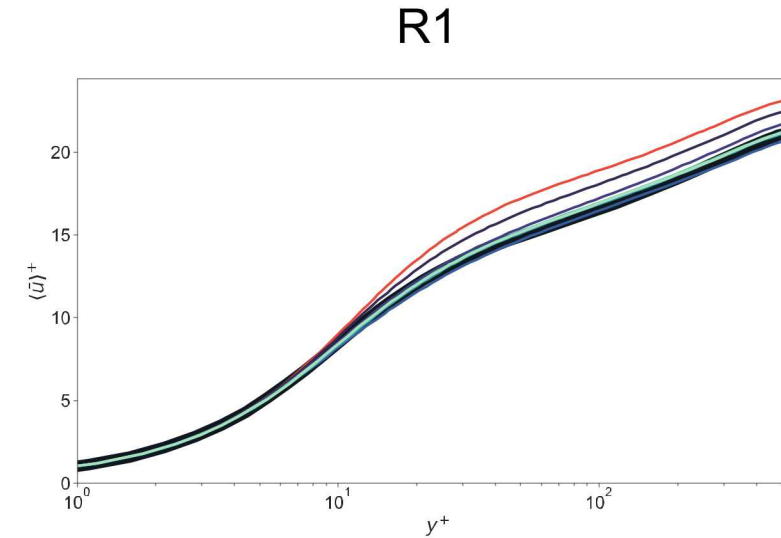
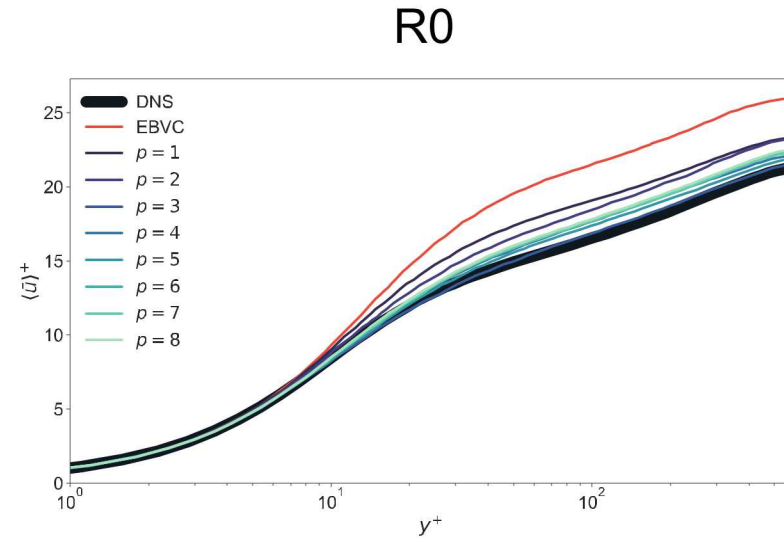


Estimated turbulent shear stress



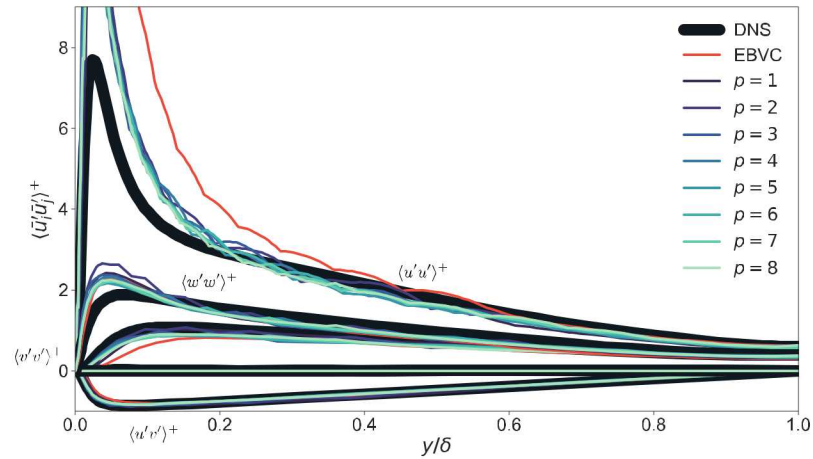


# Effect of polynomial order on mean velocity prediction

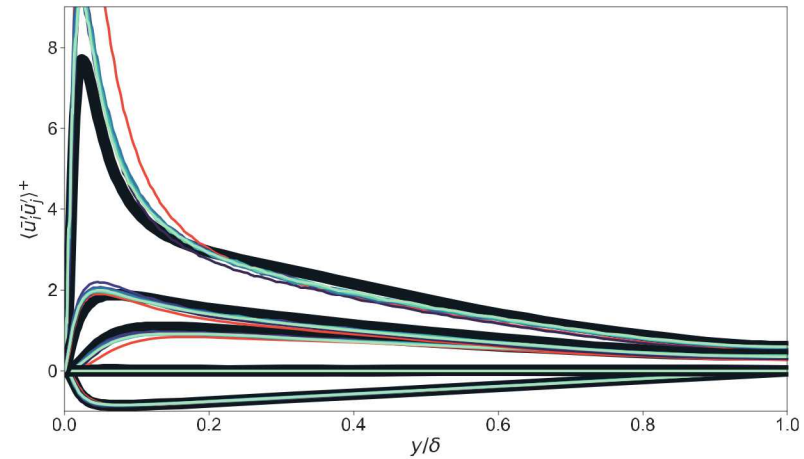


# Effect of order on the resolved Reynolds stress

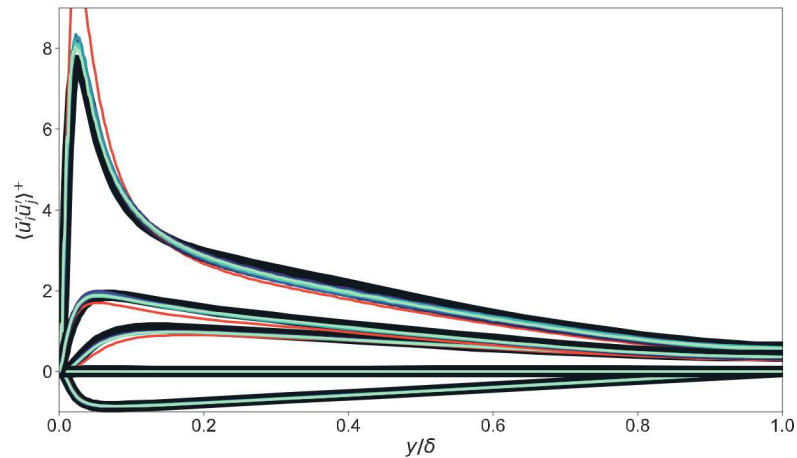
R0



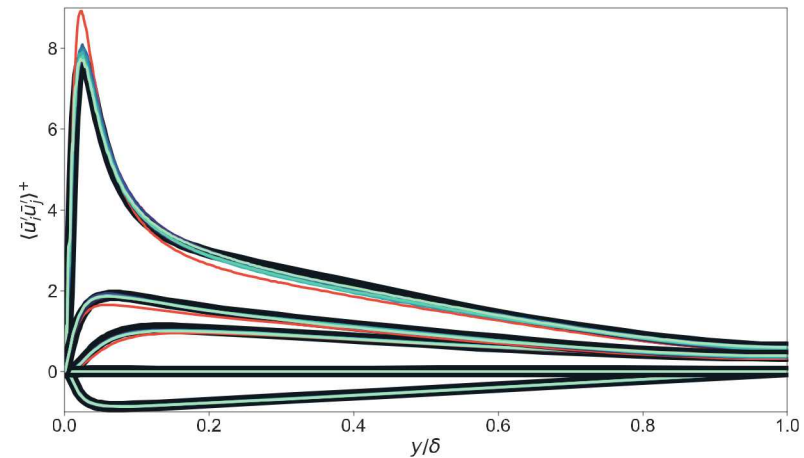
R1



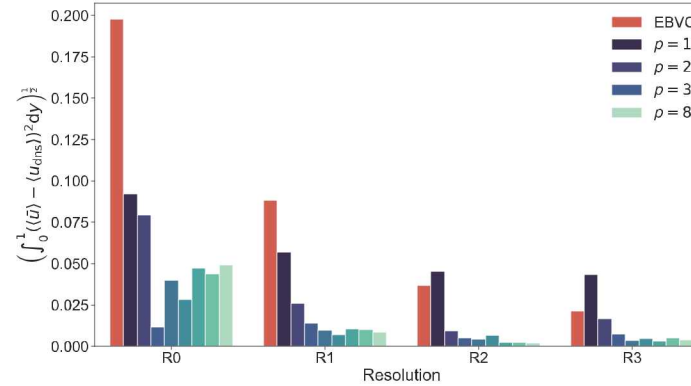
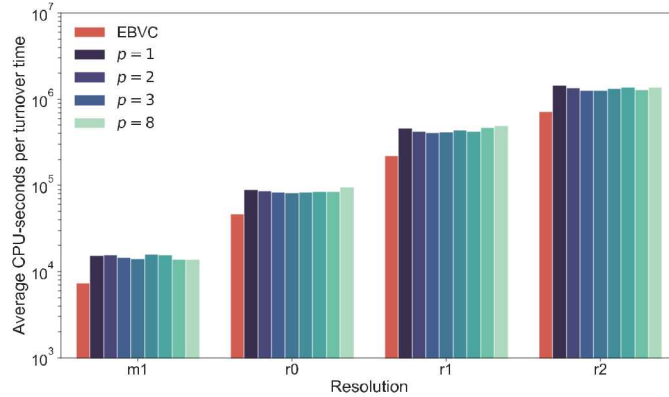
R2



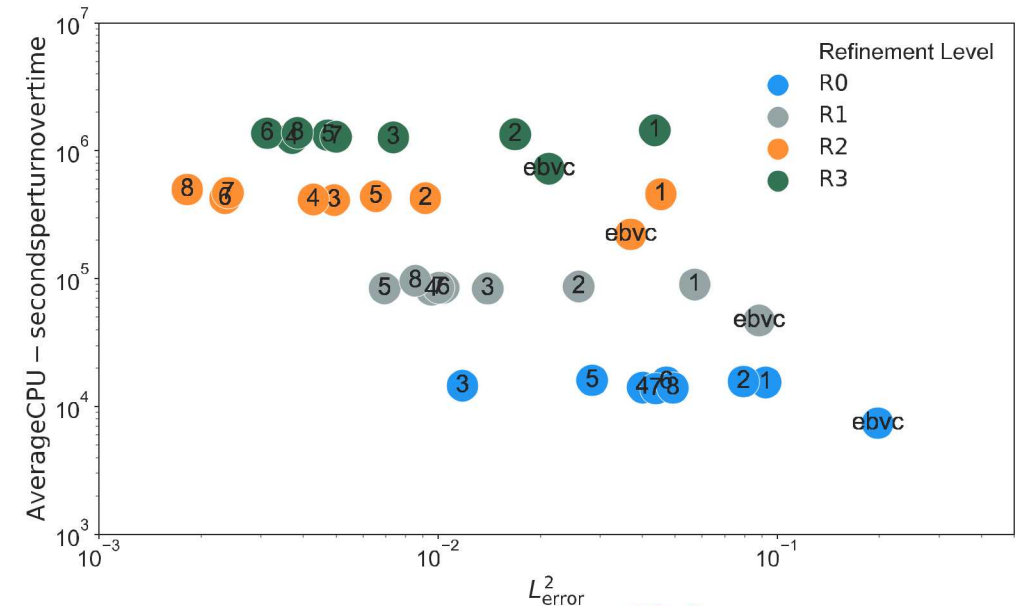
R3



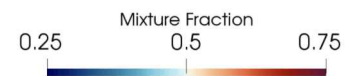
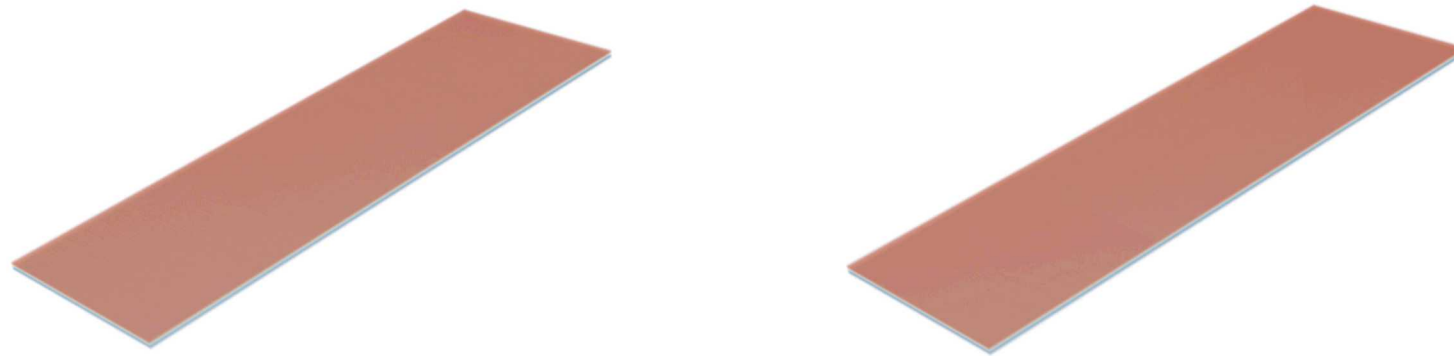
# Overall



- 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

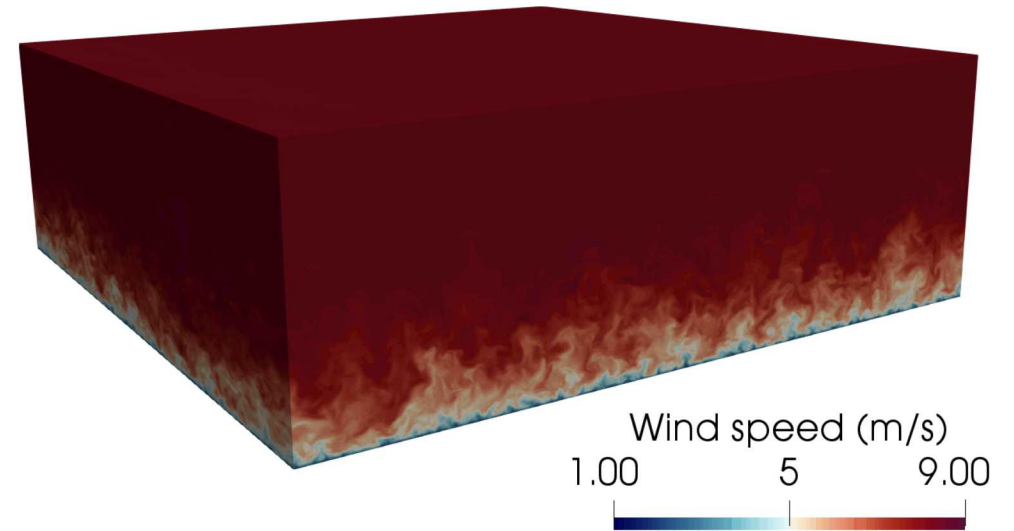


# Mixing layer



# 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.