SAND2017-10598PE

A2e High-Fidelity Modeling (HFM) Project

Overview of FY17 Q4 milestone: *Comparison of high-order and lower-order numerical discretization methods*

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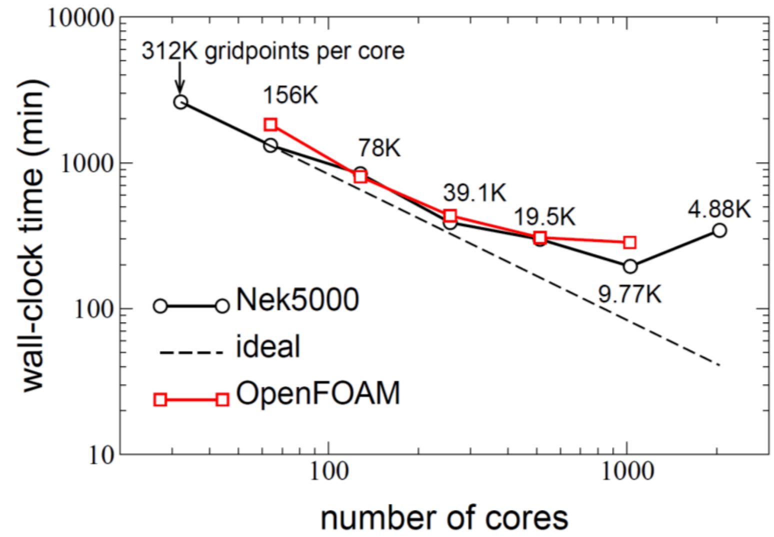
FY17 Q4 Milestone and background

- **Milestone:** Complete analysis on accuracy/compute-time comparison of high-order and low-order discretization approaches for a wind farm simulation using the team's ALCC computer-time allocation.
- **Background:**
  - Looking towards next-generation computer platforms, we will be moving into a "FLOPS are free" paradigm, where calculations are essentially free, and data movement will be the most significant barrier to fast code evaluation.
  - Typical CFD codes (like SOWFA) use low-order elements (e.g., finite volumes), but high-order methods are of great interest because
    - Can be much more accurate for a given model size, e.g., will propagate wake with much more fidelity;
    - Require much more "computation" for a given model size (which fits "FLOPS are free).
  - However, the accuracy vs. computational wall-clock time needs more investigation
  - The project needs evidence to decide early if future investments in high-order methods are appropriate.

Why are we interested in high-order methods?

- More work per datum communicated
  - Implications for next gen. platforms and exascale computing
- Is that added work really useful for wind applications?
  - Need to establish evidence
  - Does high-order provide better answers at a fixed model size?

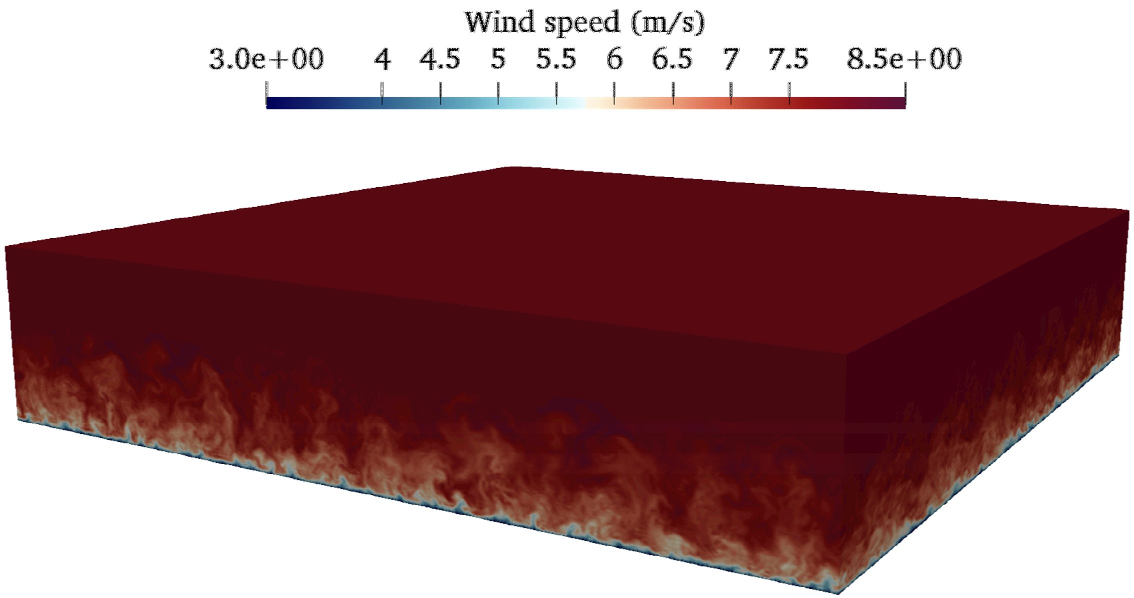


High-order code (Nek5000) run at polynomial order 7 is similar in cost to a traditional cell-centered finite volume code (OpenFOAM) run at the same number of degree of freedom (dof). "A comparison of Nek5000 and OpenFOAM for DNS of turbulent channel flow" MA Sprague, 2010

- "Nalu" is an unstructured, low-Mach fluids solver
  - C++, built on top of Sandia's "Trilinos" software stack (Muelu, Belos, STK, etc.)
  - Control Volume Finite Element Method provides path to polynomial higher order discretization
- A2e-HFM team believes HO may be useful for capturing persistent vortical structures like those in wind turbine wakes.

Objective

- Look at trade-off between mesh resolution and accuracy in wind-relevant applications
- Informs decision to invest in reducing compute-time for high-order (HO) methods



Example simulation target: 5km x 5km x 1km neutral atmospheric boundary layer; polynomial-order 2 (“P2”), 25 million nodes

Challenges in evaluating high order for LES

- Higher-order methods can show benefit, but does that benefit apply to wind relevant large-eddy simulation (LES)?

- Picture is more clear for higher-order in direct simulation vs LES
  - In typical LES calculations, no clear distinction between model error and discretization error is possible

$$\left|\nabla \cdot \left(\tau_{\text{sgs,model}} - \tau_{\text{sgs,true}}\right)\right| \lesssim h^p$$

  - Inertial range estimates for the Smagorinsky model show

$$\left|\tau_{\text{sgs,model}}\right| \lesssim h^{4/3}$$

- What benefits would there be to HO in LES?
  - Better capture resolved structures—e.g. vortices
  - Higher quality estimates of the model terms
  - Pure algorithmic benefits (computation v. communication)

Algorithm verification through comparison with analytical vortex solution

- Benefit for higher order is clear in verification of vortex transport

$$u = u_0 - \frac{\beta}{r_0 + \tau^2} \exp\left(\frac{1}{2}\left(1 - r^2/\tau\right)\right) C_y$$

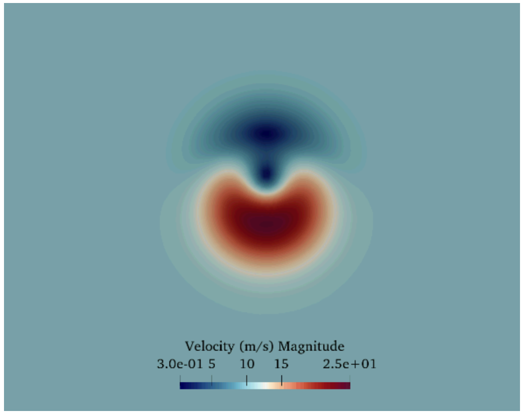
$$v = \frac{\beta}{r_0 + \tau^2} \exp\left(\frac{1}{2}\left(1 - r^2/\tau\right)\right) C_x$$

$$\tau = 1 + \frac{2\beta}{r_0 Re} t$$

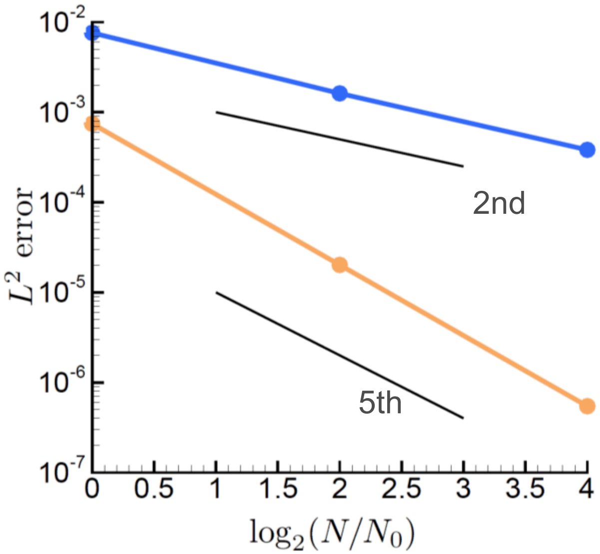
- Tests run on an unstructured, non-orthogonal mesh

- Higher accuracy with polynomial order and better convergence
  - Orders-of-magnitude error reduction at a particular resolution

Vortex verification problem



Error vs model size
P1 (blue); P4 (orange)



High order for atmospheric boundary layer simulation

- Atmospheric boundary layer (ABL) is canonical case that introduces issues related to model error in LES
- Significant body of literature on this type of flow
  - Nieuwstadt et. al. 1992 – Comparison of 4 codes, pseudo-spectral to 2^{nd} order finite difference – convective boundary layer – No control over model similarity – Very coarse by modern standards – good match between codes in mean profiles, not higher degree moments
  - Beare et. al. 2006 – Comparison of 12 codes, pseudo-spectral to 2^{nd} order finite difference – stable boundary layer requires higher resolution - No control over model similarity – no match between codes or within code with mesh refinement even for mean profile.
  - Sullivan and Patton 2011 – Effect of mesh resolution on convective boundary layer statistics and structure – Suggest criteria for grid convergence of mean profiles and variances, but observe no grid convergence for higher-degree moments.
- Choose a neutral boundary layer for this study
  - Wall model error is critical, but does HO still provide benefit?

Atmospheric boundary layer simulations

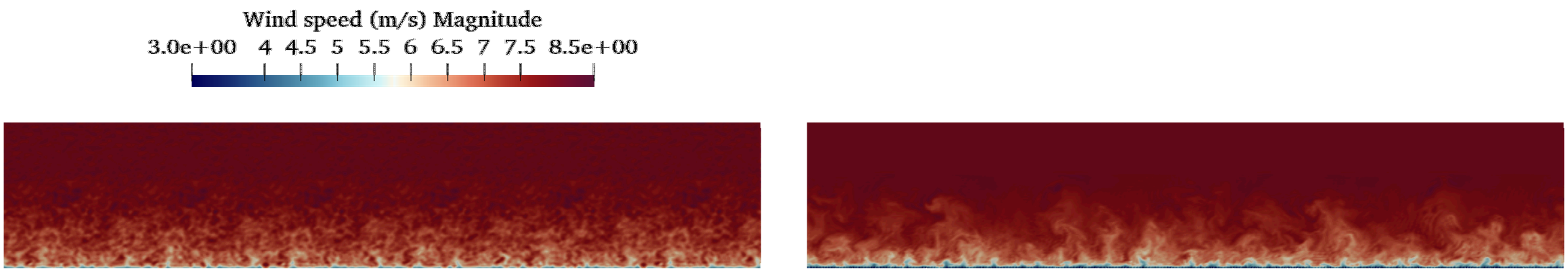
- Total of 5 simulations
  - 3.125 x 10^6 to 200 x 10^6 degrees of freedom (dof) with cubical cells
  - Simulations with polynomial-order 1 (P1) elements and polynomial-order 2 (P2) elements.
  - Expect the biggest difference to be between P1 and P2 for polynomial enrichment

Mesh refinement	
[redacted]	
3.125M	3.125M
[redacted]	
200M (gold)	

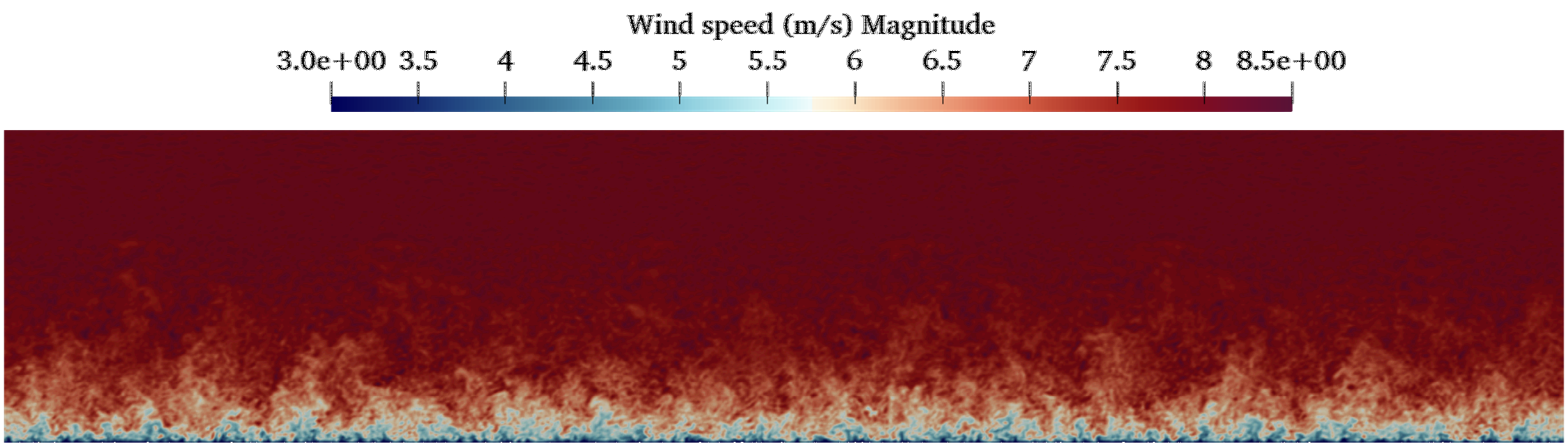
- Case description: the Nalu ABL test case
  - A 5x5x1 km^3 neutrally stable boundary layer with a capping inversion
  - Constant-coefficient Smagorinsky model for subgrid stress
  - Moeng ABL wall model
  - Unstabilized, no forcing function: results taken at the same time (1 hour), same initial condition
- Look at predictions of P1 and P2 simulations for various quantities
  - Planar averaged profiles and friction velocity

Side-to-side velocity fields

- P1 (left) v P2 (right) 10m: same number (25×10^6) of dofs
  - Higher order resolves some larger structures in the boundary layer
  - More dispersive-type error visible in the P1 solution



P1, 5m resolution (200×10^6 dofs)

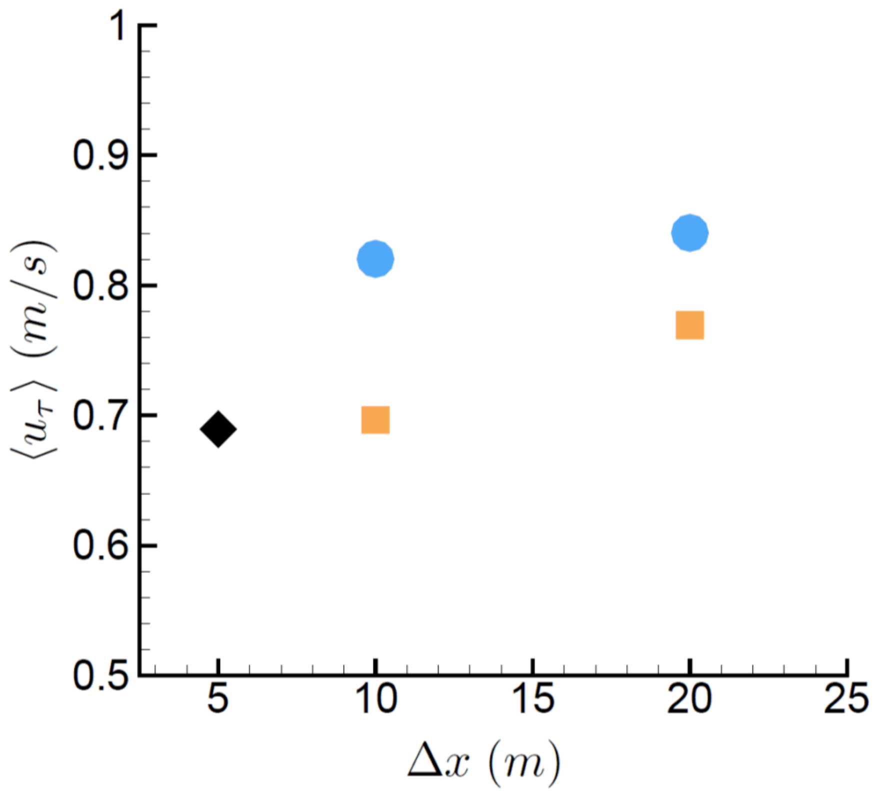


Friction velocity

- Higher order more similar to the most benchmark
  - P2 - 25 million case within 2% of gold

- Results are not grid convergent
  - Comparing under-resolved cases
  - Take highest resolution P1 case as the “gold” solution

- Working on improving the “gold”
  - Use a pseudo-spectral, 6th-order compact code specifically designed for ABL calculations in a box



High order (orange squares) vs. low order (blue circles) against the P1 gold (black diamond)

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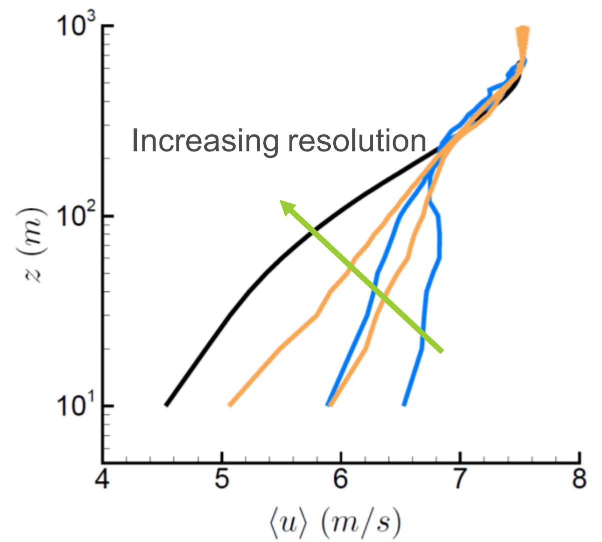
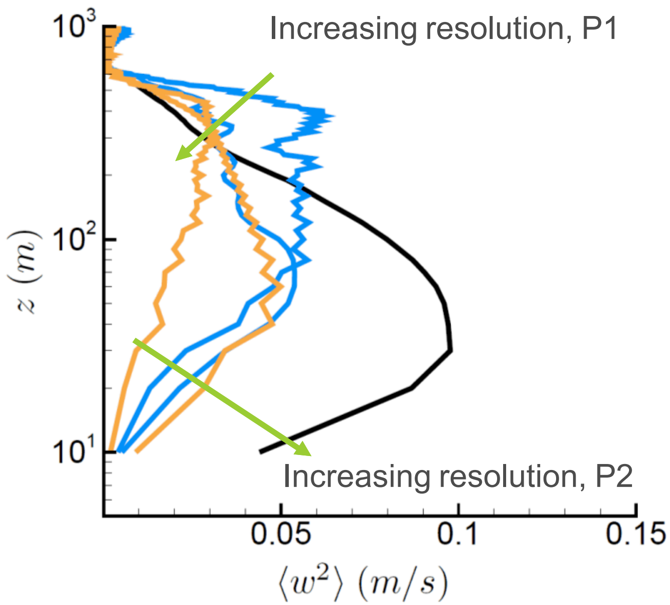
Effect of HO on mean velocity and variance profiles

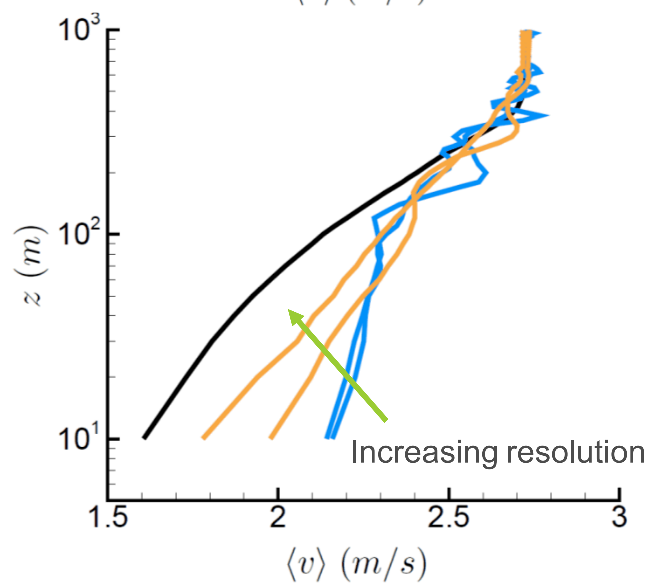
- Less clear for velocity profiles
  - Velocity means are closer to the gold for HO
  - Vertical velocity variance is not improved

- P2 provides an answer closer to the gold standard at the same model size





P2 (orange) v.
P1 (blue) v.
P1 gold (black)



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Higher-order discretization in Nalu is currently slow

- High-order implementation uses same framing as low order
  - Some algorithmic decisions for low order are sub-optimal for high-order efficiency
  - P2 is 4-5 times more expensive than P1 currently. Worse for higher P.
- ECP ExaWind project is pursuing algorithmic improvements
  - Initial hope is that residual evaluation time can be competitive per-dof for moderate polynomial order (< 8)
- Threaded, explicitly vectorized execution shows better speed up for high order on Knights Landing platform
  - P2 is about 30% slower than P1 in assembly on the KNL
  - See the ECP Q4 milestone report

	Speed up due to vectorization, threading	
Mesh (# elements)	**Haswell**	**KNL**
Coarse P=1 (17.5M)	**2.28**	**1.96**
Fine P=1 (140M)	**2.35**	**1.90**
Coarse P=2 (17.5M)	**2.47**	**4.60**

Conclusion

- Higher order methods show promise for wind LES simulations
  - Not clear cut with significant model uncertainty
  - Some gains with high order at a fixed model size
  - May benefit more from improved turbulence models

- Higher order time-to-solution needs to be competitive per degree-of-freedom with lower order
  - Not necessarily the same speed, but not many times slower
  - Need work on improving compute-time, memory efficiency of high order

Next steps

- A lot more work is necessary to truly answer the core questions about higher-order discretization in LES for wind applications
  – This is an ongoing effort that will be supported under the Exascale Computing Project ExaWind (PI: M.A. Sprague)

- Need to improve the gold-standard solution for testing
  – Looking to a specialized code to provide a high-quality gold standard

- Need to run more orders of accuracy (e.g., P3) and more quantities of interest
  – Look at higher-degree moments, spectra, etc.

- Look at problems with persistent vortices
  – Tip vortices, turbine wakes may benefit more from high order than the ABL

Thank You!