SAND2019-2149C

Efficient Implementation of a High Order Control Volume Finite Element Scheme for Low-Mach Flow

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EXASCALE COMPUTING PROJECT

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY | Office of

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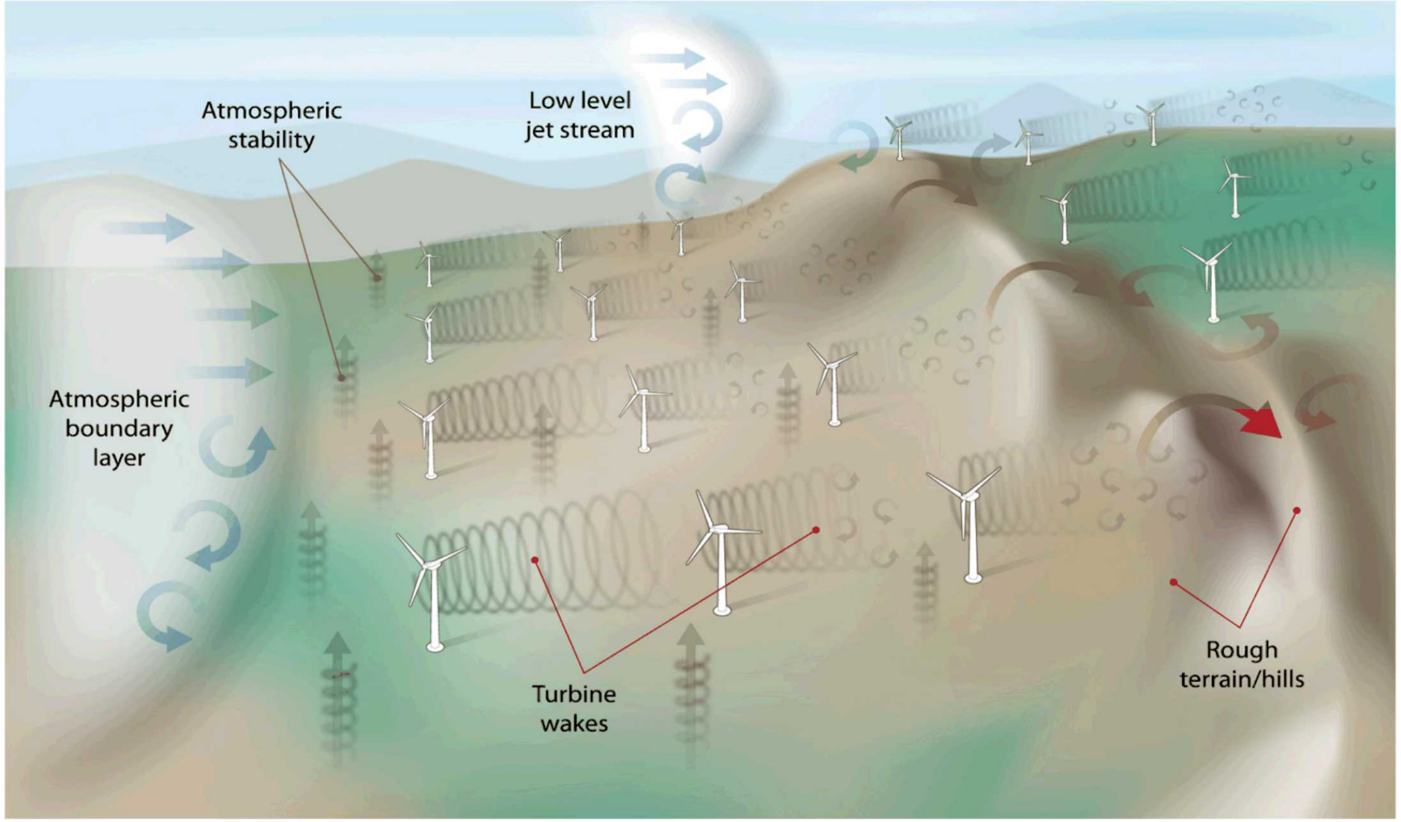
Exawind project overview

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



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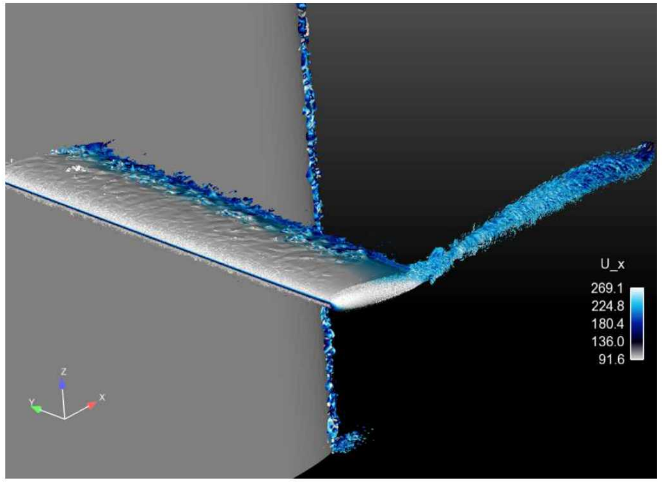
Nalu-Wind

- Open source: https://github.com/Exawind/nalu-wind
  - Builds with Spack
  - See tensor_tg_mms test for example of today's work
- Incompressible, unstructured finite volume
  - 2^{nd}-order node-centered edge FV scheme
  - **Arbitrary order accurate element-based continuous finite volume scheme**
  - Fully implicit
  - Mixed-order interfaces
- Demonstrated scaling up to 500k cores, 9 billion node simulation
- C++. Built on "Trilinos"



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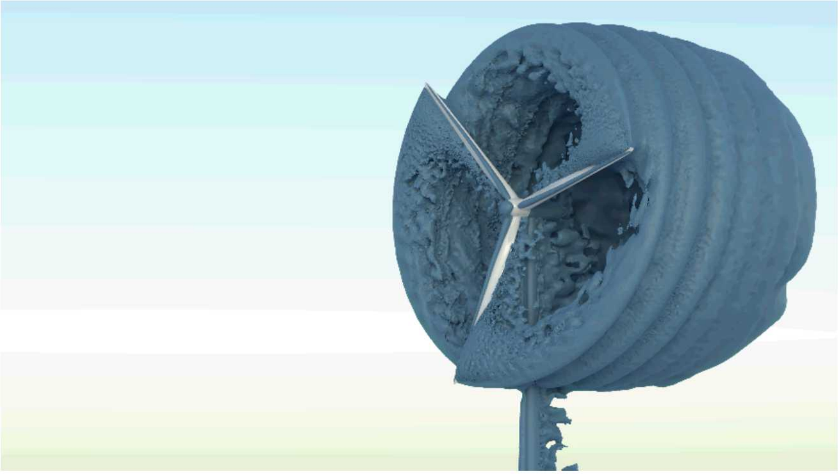
Nalu-Wind physics capabilities

- Atmospheric boundary layer modeling
  - Monin-Obukhov wall models
  - Boussinesq, Coriolis forcing

- Full turbine modeling
  - Sliding mesh, overset technologies
  - Hybrid RANS-LES models



- Actuator line modeling
  - Coupling with the OpenFAST code
  - Isotropic Gaussian spreading

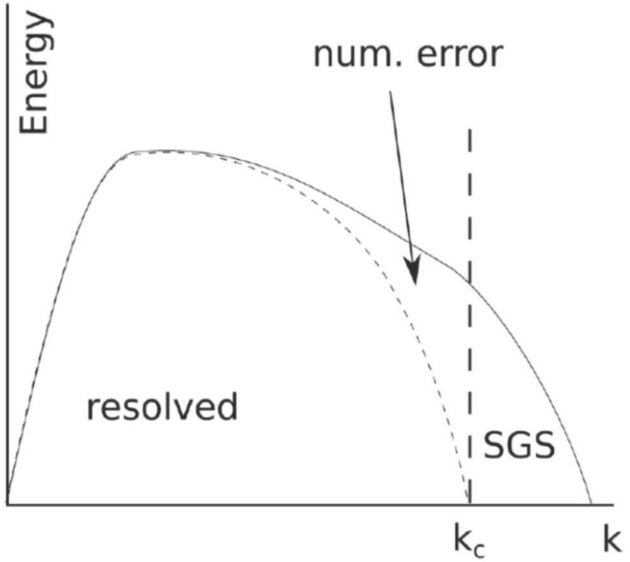
Why high order?

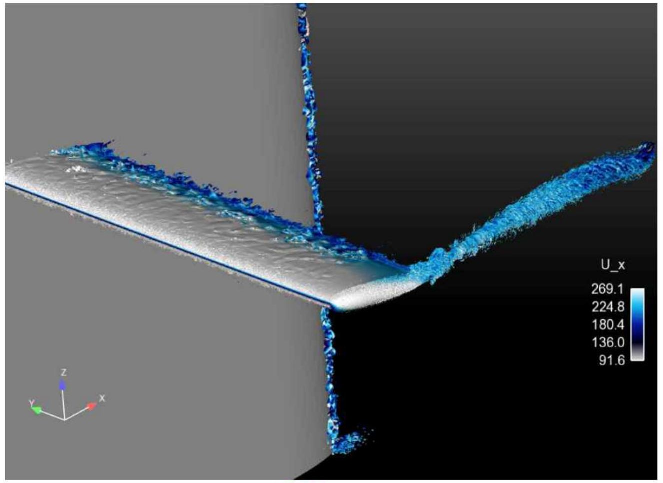
- Potentially very good accuracy for cost
  - Better work load per datum moved ratio

- LES models complicate things
  - Overall error converges between 1^{st}-2^{nd} order
  - Numerical errors affect filter-scale flow physics

- Important structures are resolved well
  - Wakes

Bull and Jameson, 2016

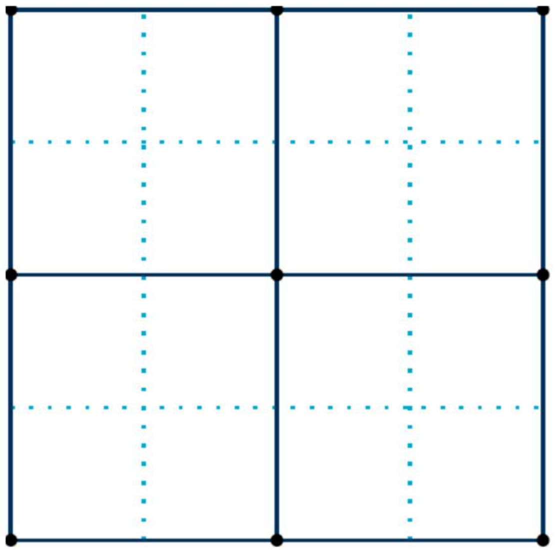


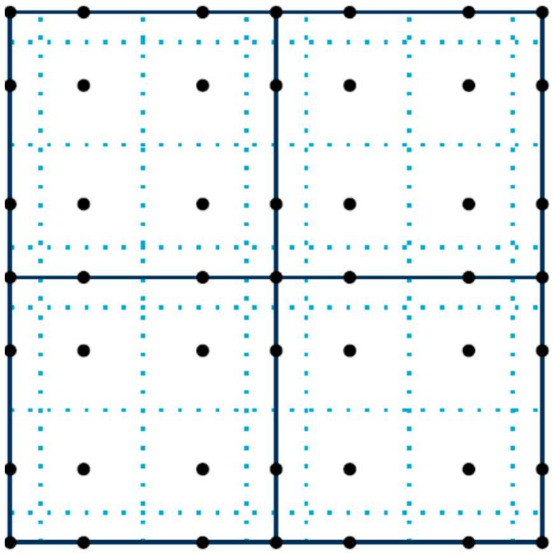


Control volume finite element

- Linear CVFEM is the production discretization in nalu-wind
  - Design is semi-flexible in terms of discretization
  - Node-centered finite volume also implemented

- Basic idea for CVFEM: define a test space of indicator functions on a dual mesh
  - Other names “finite volume element”, “covolume method”, etc.
  - Can generalize node-centered finite volume to high order





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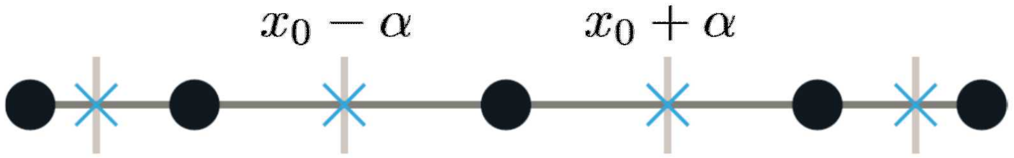
CVFEM

$$\partial_t u + \partial_x F(u) = 0$$

- Around a node, define a dual volume, $\Omega_0^\star = [x_0 - \alpha, x_0 + \alpha]$



- Using Gauss divergence, we have

$$\int_{x_0-\alpha}^{x_0+\alpha} \partial_t q \, \mathrm{d}x = F(q)|_{x_0+\alpha} - F(q)|_{x_0-\alpha}$$

- Introducing a finite element approximation for u: $u_h = \sum u_j(t)\varphi_j(x)$ and a numerical flux, we have

$$\left(\int_{x_0-\alpha}^{x_0+\alpha} \varphi_j(x) \, \mathrm{d}x\right) u_j'(t) = F_h(u_h)|_{x_0+\alpha} - F_h(u_h)|_{x_0-\alpha}$$

High order CVFEM

- Finite volume method with finite element assembly
  - Requires that the dual partition be carefully defined relative to the basis
  - A lot of finite volume machinery still applies (same pressure stabilization)

- Numerical quadrature is complicated due to the test space being discontinuous

- We use a Lagrange basis through the GLL points
  - Another option would be "histopolation" functions, using a Lagrange basis through CVs

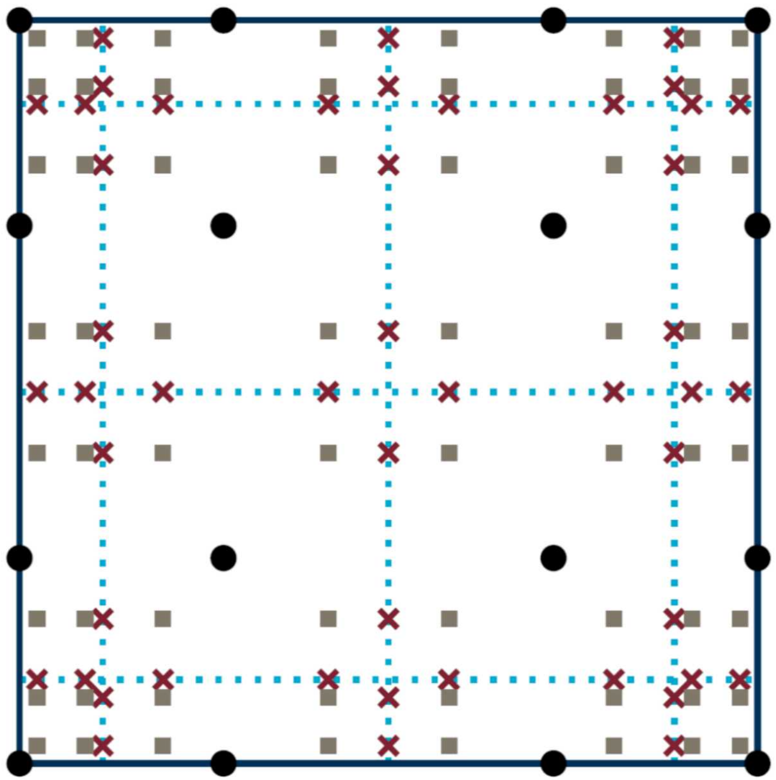
$$h_j(x) = -\sum_{k=0}^{j-1} \ell'_k(x) \Rightarrow \int_{\Omega_i^\star} h_j(x)\,\mathrm{d}x = \delta_{ij}$$

Initial quadrature

- For each section of the dual volume within an element, define an appropriately high order Gauss quadrature (on faces and volumes)
- Explodes with polynomial order very quickly
  - 216 quadrature points for a quadratic element
  - Generally, for even orders,

$$\#(IPs) = \frac{3}{4}p(p+1)^4$$

- Fits in with nalu-wind’s assembly pattern without modification



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New approach

Define matrices:

$$\partial_t u = \Delta u$$

$$W_{ij}^{-1} = h_i\left(x_j^{\text{GLL}}\right), \quad \tilde{D}_{ij} = \varphi_i'\left(x_j^{GL}\right), \quad \tilde{\Delta}_{ij} = \begin{cases} -1 & i = j \\ +1 & i = j - 1 \\ 0 & \text{o/w} \end{cases}$$

For an element in 1D, we have

$$W_{ij} u_j'(t) = \tilde{\Delta}_{ik} \tilde{D}_{kj} u_j$$

For higher dimensions, introduce $\tilde{I}_{ij} = \varphi_i\left(x_j^{GL}\right)$ and $D_{ij} = \varphi_i'(x_j^{GLL})$

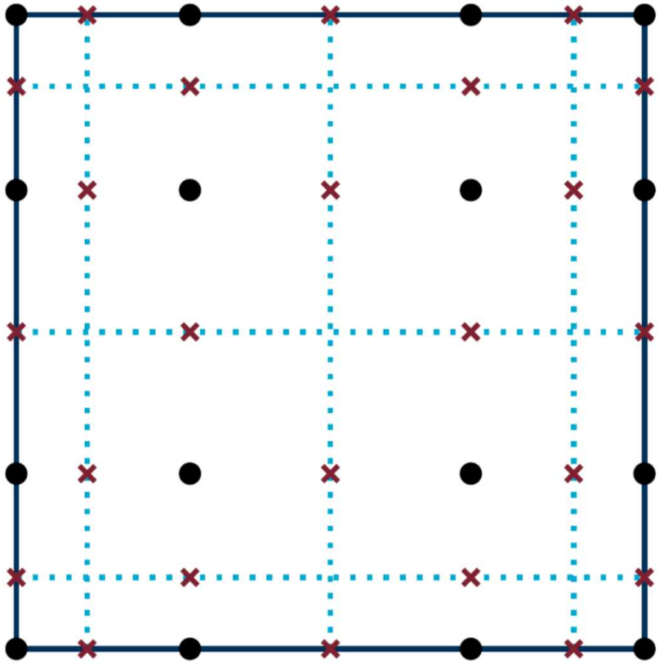
$$M_{\ell p, mq, nr} q_{pqr}'(t) = \sum_{pqr} \widetilde{\Delta}_{\ell p} W_{mr} W_{nr} \left(G_{pqr}^{\hat{x}x} \sum_i \widetilde{D}_{pi} \phi_{iqr} + G_{pqr}^{\hat{x}y} \sum_{ij} \tilde{I}_{pi} D_{qj} \phi_{ijr} + \ldots \right) + \ldots$$

Cost comparison

- Scales properly with polynomial order
  - $3p\,(p+1)^2$ instead of $\frac{3}{4}p\,(p+1)^4$ integration points

Case	New algorithm timing relative to P1
P1	0.97
P2	4.6
P4	26.7

Test case: 32^3 mesh, momentum assembly (lhs/rhs)



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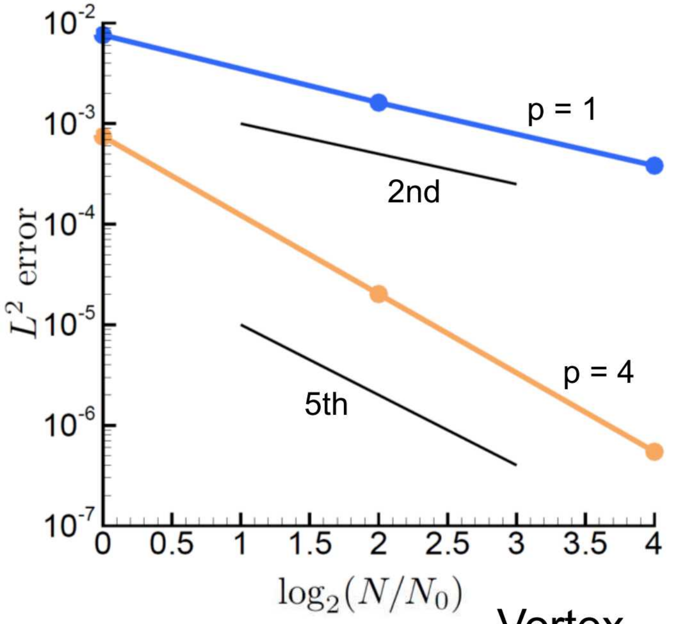
Nalu "kernels"

- Responsible for evaluating "terms" in the governing equation
  - GPU pathforward for nalu-wind, easily testable
  - Explicit outerloop SIMD vectorization



Vortex transport

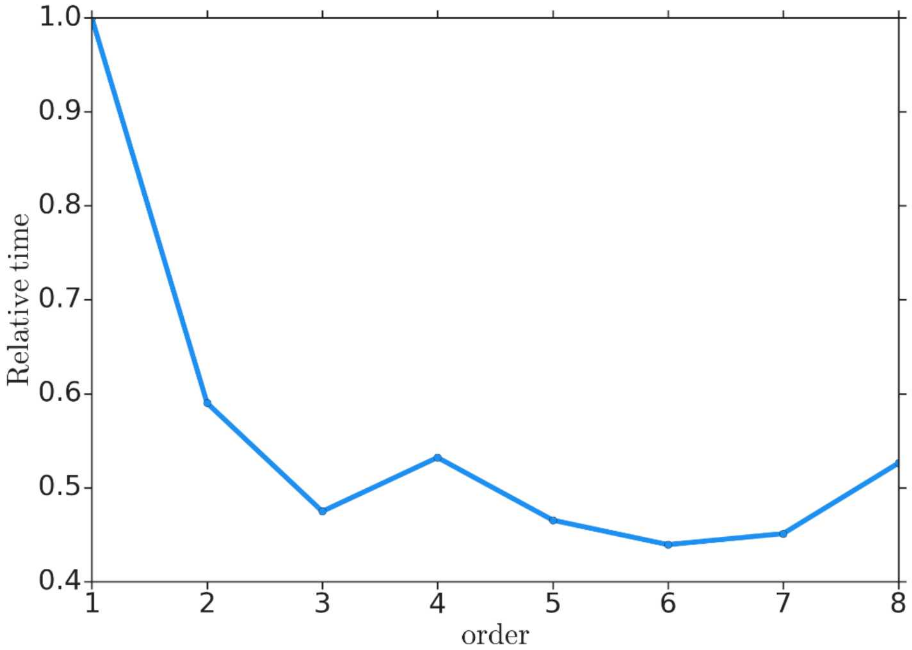
```
void run_algorithm(...)
{
  ...
  auto team_exec = nalu::host_team_policy(len, bytes_per_team, bytes_per_thread);
  Kokkos::parallel_for(team_exec, [&](const nalu::TeamHandleType& team)
  {
    ...
    Kokkos::parallel_for(Kokkos::TeamThreadRange(team, simdBucketLen),
    [&](const size_t& bktIndex)    {
      nalu::fill_pre_req_data(...)
      nalu::execute_all_kernels(...);
      nalu::apply_coeff(...)
    });
  });
}
```

Effect of polynomial order on residual evaluation

- Tested on Skylake (avx512)
  - Normalized by number of nodes (~500k)
  - Includes interleaving costs

- Effect of explicit outerloop vectorization

Order	Speedup
P1	2.83
P2	2.64
P3	2.2
P4	2.2



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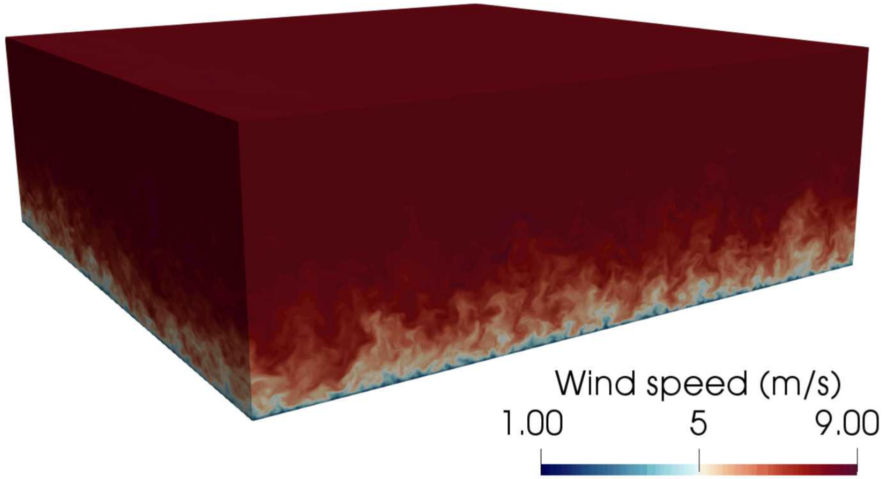
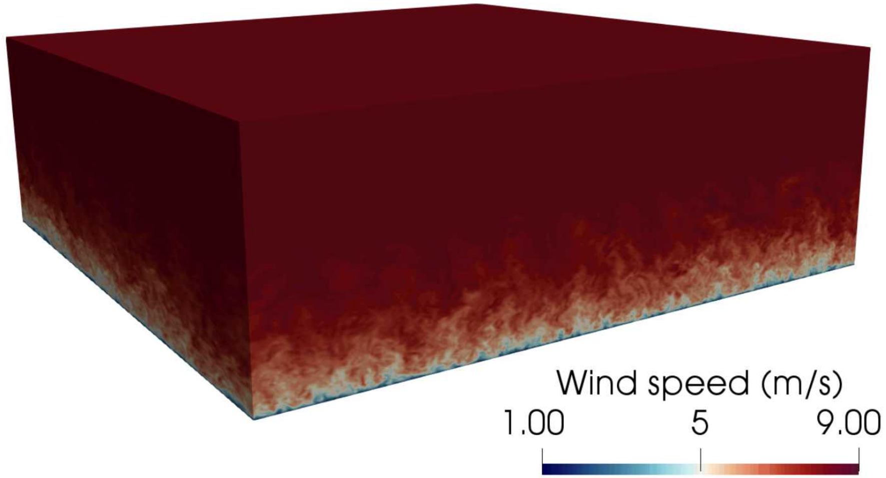
Atmospheric boundary layer

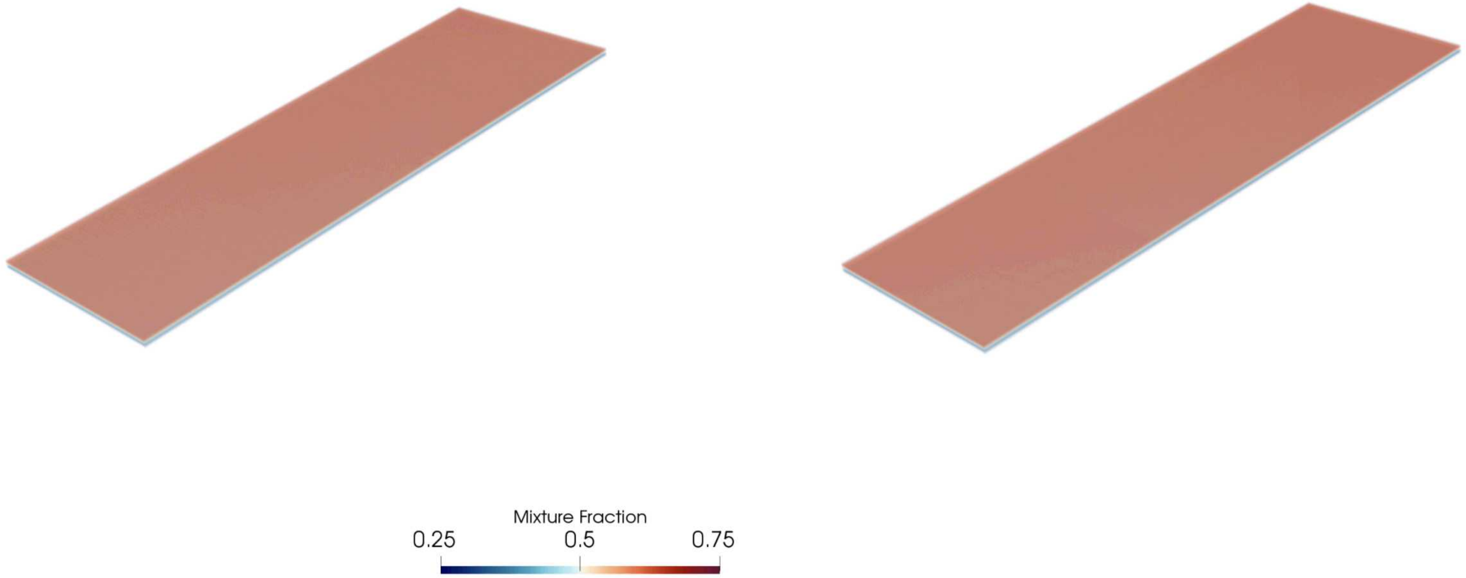


Polynomial order 3



Node-centered finite volume

Mixing layer



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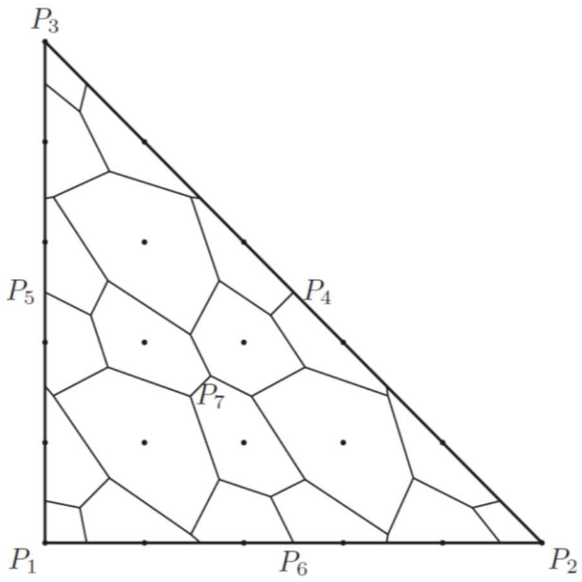
Closing

- Still a work in progress
  - Active milestone
  - Can't afford matrix in 3D, storage or cost

- Really only a pathforward for high order hexs for CVFEM
  - Tetrahedral/wedge elements are possible but unlikely to be efficient



Fifth-order element
Wang, Xiang, and Yonghai Li , 2016

Acknowledgement

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Citations

- Wang, Xiang, and Yonghai Li. "L^2 Error Estimates for High Order Finite Volume Methods on Triangular Meshes." *SIAM Journal on Numerical Analysis* 54.5 (2016): 2729-2749.
- Bull, Jonathan R., and Antony Jameson. "Explicit filtering and exact reconstruction of the sub-filter stresses in large eddy simulation." *Journal of Computational Physics* 306 (2016): 117-136.

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