

Towards Industrial Large Eddy Simulation of Vortex Dominated Flow Using High-Order Methods

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Outline

- Introduction
- Pacing items towards industrial LES
  - High order methods and high order meshes
  - Equilibrium wall model
  - Scalable time marching algorithms
  - GPU implementation
- Study of vortex-dominated flows
  - Benchmark problem
  - Turbomachinery flow
  - NASA CRM High-lift configurations
- Summary and future work





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Turbulent Flow Prediction Key for Sustainable Aviation

- Air Traffic is expected to double in the next 20 years
- How do we sustain this level of growth?
  - Continuously improve performance (aircraft and engine) to reduce fuel burn
  - Dramatically reduce greenhouse gas emissions and noise

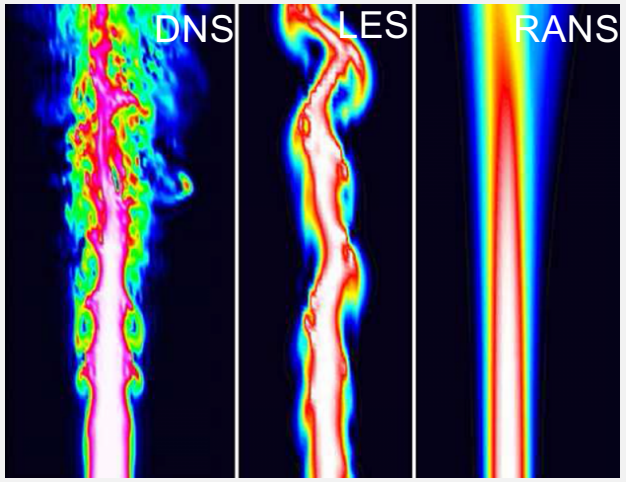




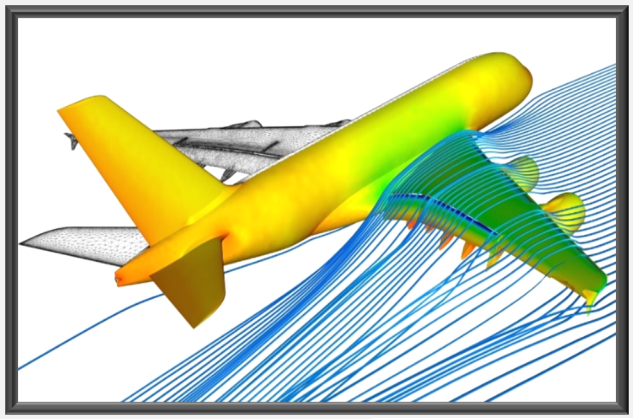
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Introduction

- Approaches to compute turbulent flows
  - RANS: model all scales
  - LES: resolve large scales while modeling small scales
  - DNS: resolve all scales
- NASA's 2030 CFD Vision
  - "The use of CFD in the aerospace design process is severely limited by the inability to accurately and reliably predict turbulent flows with significant regions of separation."
  - Call for scale resolving simulations

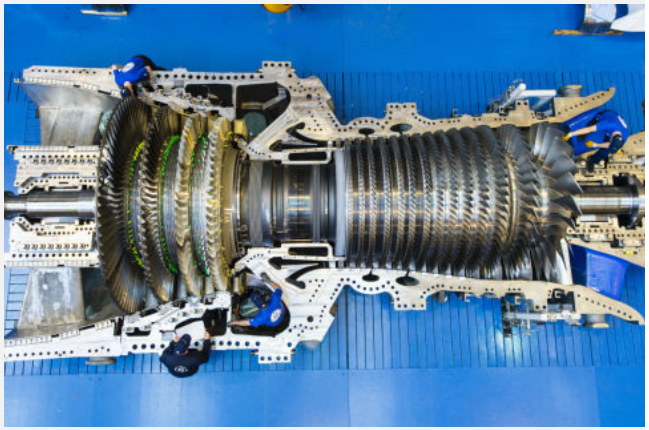


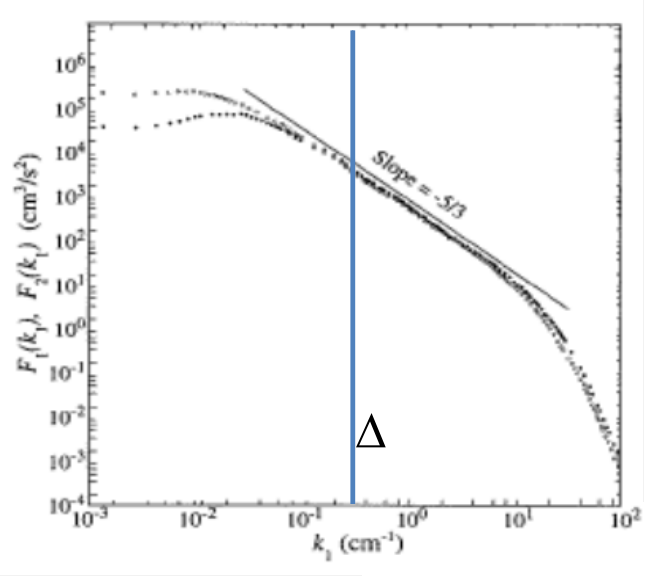
A. Maries, University of Pittsburgh



LES – the Challenges

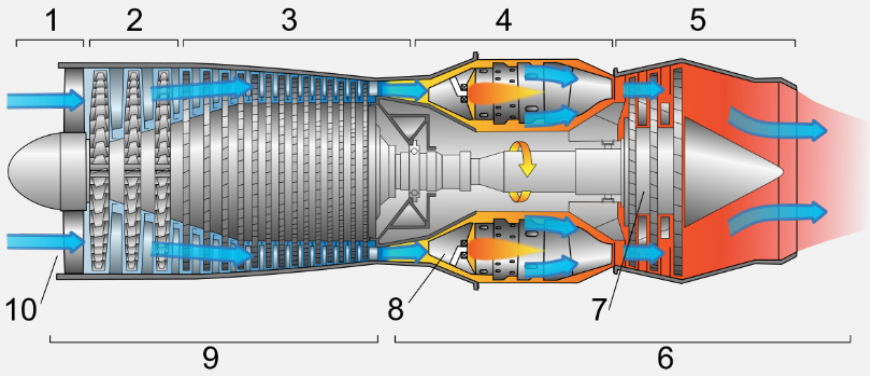
- Cost!
  - 3D time accurate simulations
  - Disparate turbulent length and time scales at high Reynolds numbers
  - Wall Modeled LES ~ $Re^{1.3}$
  - Wall Resolved LES ~ $Re^{2.5}$
- Other challenges
  - Complex geometries
  - Wall and subscale stress models
  - Scalable and efficient time integration schemes
  - How to choose filter width



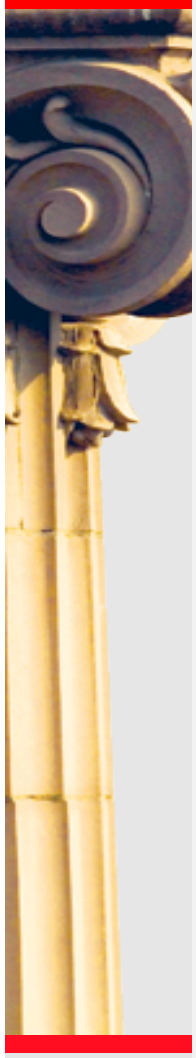


How We Address the Challenges

- Cost
  - High-order methods in space
  - Implicit time integration approaches on CPU/GPU clusters
- Other challenges
  - Complex geometries
    - High-order unstructured meshes
  - Wall and SGS models
    - Equilibrium wall model and implicit LES
  - High performance computing
    - Scalable space and time discretization algorithm
- Vision
  - High-order methods + GPU computing for industrial LES



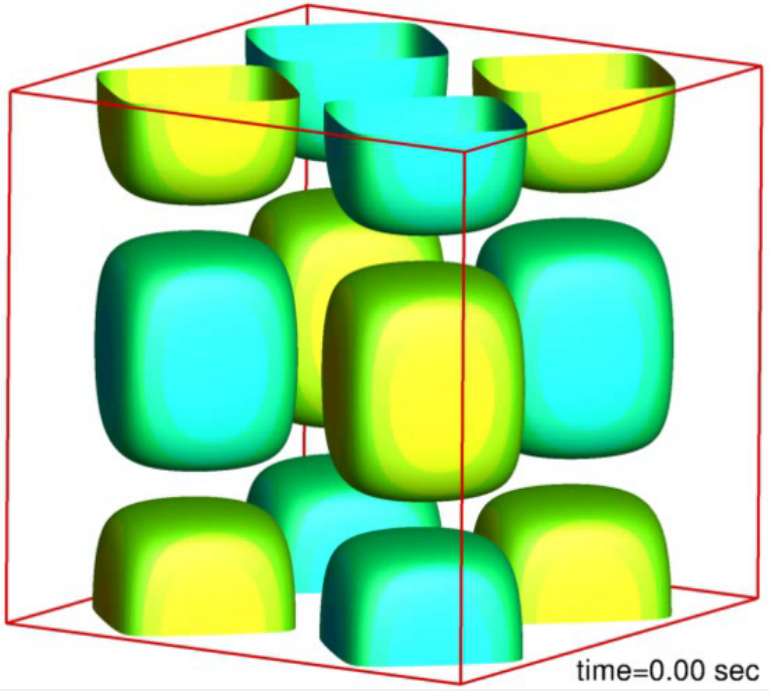
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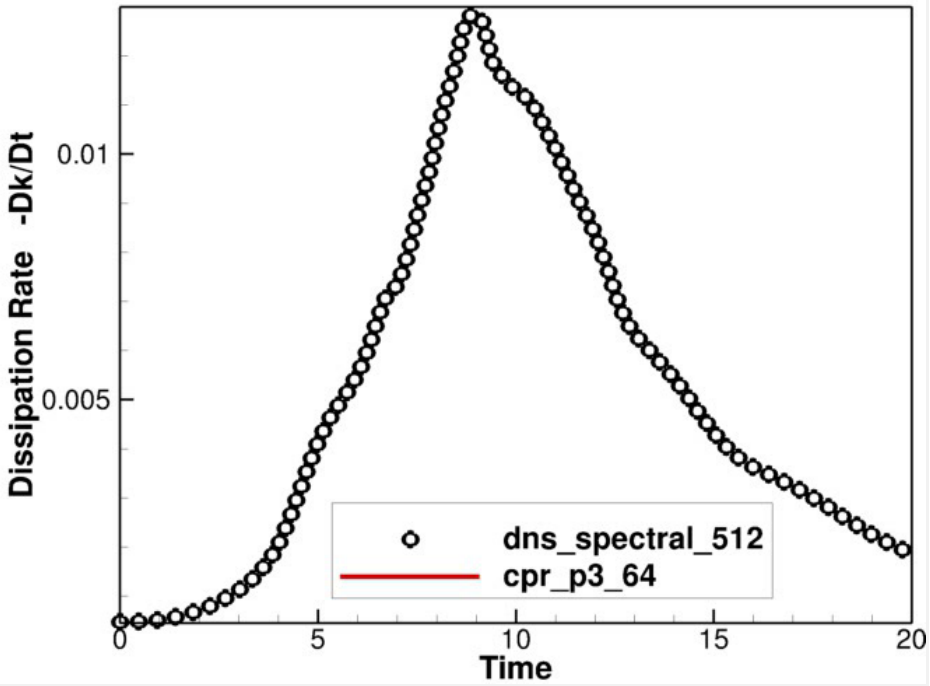


High-Order Methods and High-Order Meshes

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Why High-Order CFD Methods - Taylor-Green Vortex Problem

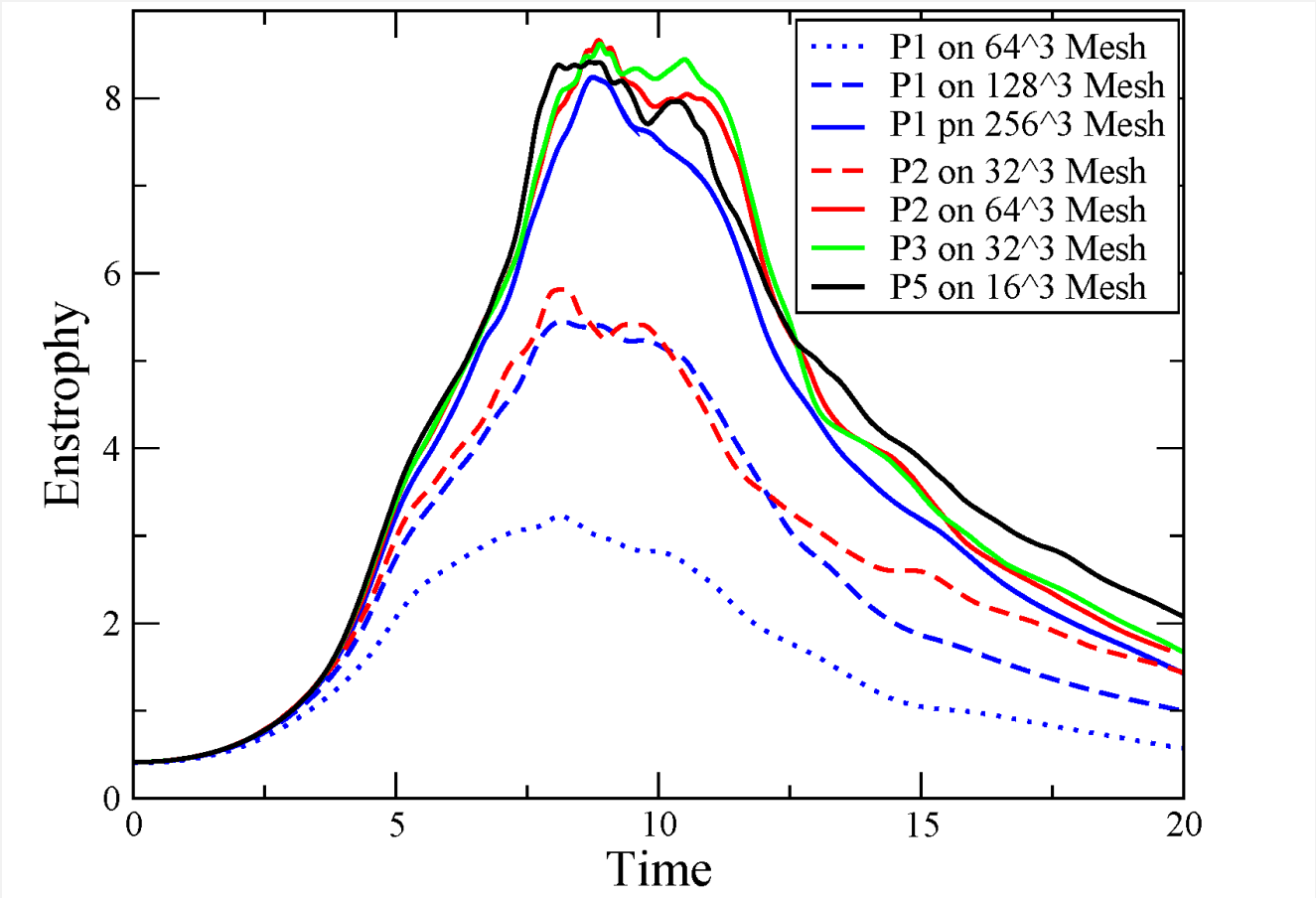




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Taylor-Green Vortex Problem – Enstrophy History

$$\mathcal{E}(\omega) \equiv \int_S |\omega|^2 \, dS \, .$$



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How Much Faster for Similar Accuracy?

- Same time integration scheme: SSP RK3 with maximum time step

	Mesh Size	DOFs/equ	Estimated Cost	Observed Cost
P = 1	256x256x256	1.34E+08	1	1
P = 2	64x64x64	1/19 of P1	1/46	1/55
P = 3	32x32x32	1/64 of P1	1/219	1/376
P = 5	16x16x16	1/151 of P1	1/663	1/596

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How to Achieve High-Order Accuracy

- Extend reconstruction stencil
  - Finite difference, compact
  - Finite volume, ENO/WENO, …



- Add more internal degrees of freedom (like FE)
  - Spectral element
  - Discontinuous Galerkin
  - Spectral difference/spectral volume
  - Flux reconstruction (FR) or correction procedure via reconstruction (CPR), …
  - Advantages in scalability, boundary condition treatment, et al



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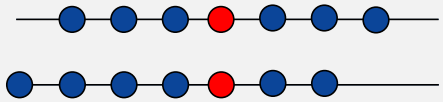
Key Summaries from High-Order Workshops

- Hp-adaptation showed big payoff for steady state benchmark problems
- For scale-resolving simulations (LES and DNS), higher order methods are more efficient/accurate than low order ones
- High-order RANS solvers are still not as robust as 2nd order ones
- Pacing items:
  - High-order mesh generation (Pointwise and GridPro produced commercial high-order mesh generators)
  - Robust, accurate and parameter-free shock-capturing
  - Low-memory, efficient implicit time-marching
  - Hp-adaptations for large eddy simulation



A Comparative Fourier Analysis

- Spatial discretization
  - 6th order central difference scheme
  - 6th order upwind-biased scheme
  - 6th order compact difference scheme with a low pass filter
  - 6th order DG or FR/CPR-DG



- Same time discretization scheme
  - SSP RK3
- Comparisons are made with the same number of total degrees of freedom (DOFs)

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FR/CPR Method

- Flux reconstruction developed by Huynh in 2007. It is a differential formulation like “finite difference” for

$$\frac{\partial u}{\partial t}+\frac{\partial f(u)}{\partial x}=0$$

- The DOFs are solutions at a set of “solution points”

$$\frac{\partial U_i(x)}{\partial t}+\frac{\partial F_i(x)}{\partial x}=0,\quad U_i(x)\in P^k,\quad F_i(x)\in P^{k+1}$$

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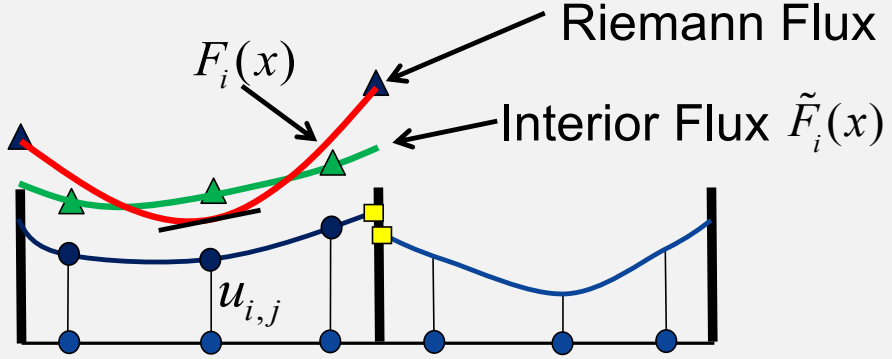
FR/CPR (cont.)

- Find a flux polynomial $F_i(x)$ one degree higher than the solution, which minimizes

$$\left\| \tilde{F}_i(x) - F_i(x) \right\|$$

- The use the following to update the DOFs

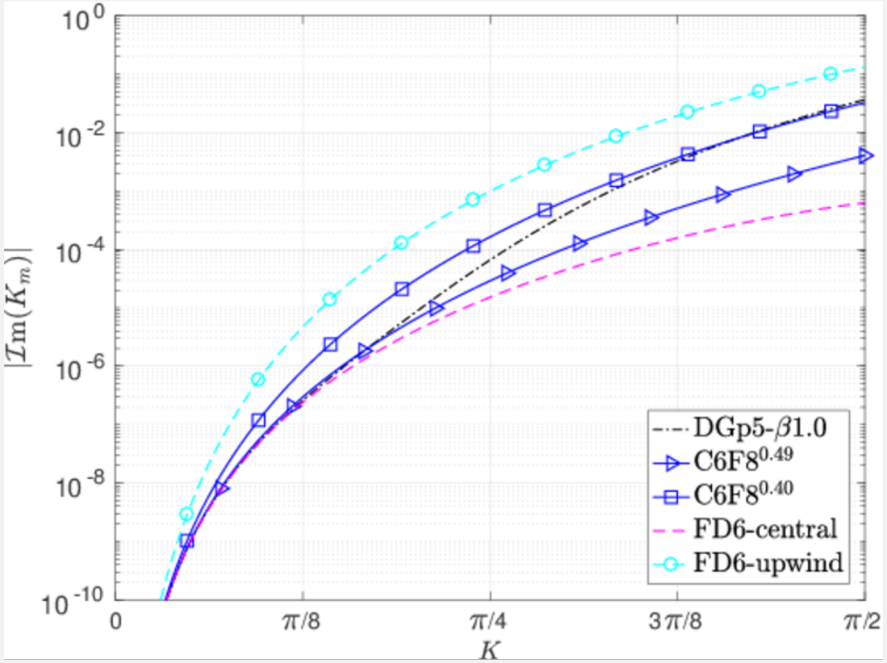
$$\frac{du_{i,j}}{dt} + \frac{dF_i(x_{i,j})}{dx} = 0$$



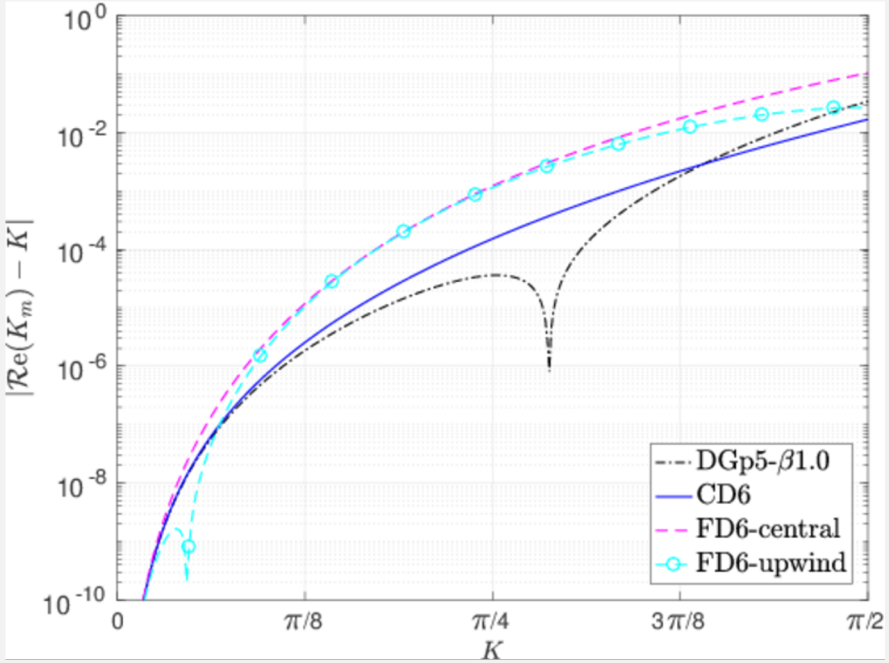
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Fixed Δt to the one of DGp5 at r_DG=0.9

3 Stage SSP Runge-Kutta scheme for time



Dissipation error

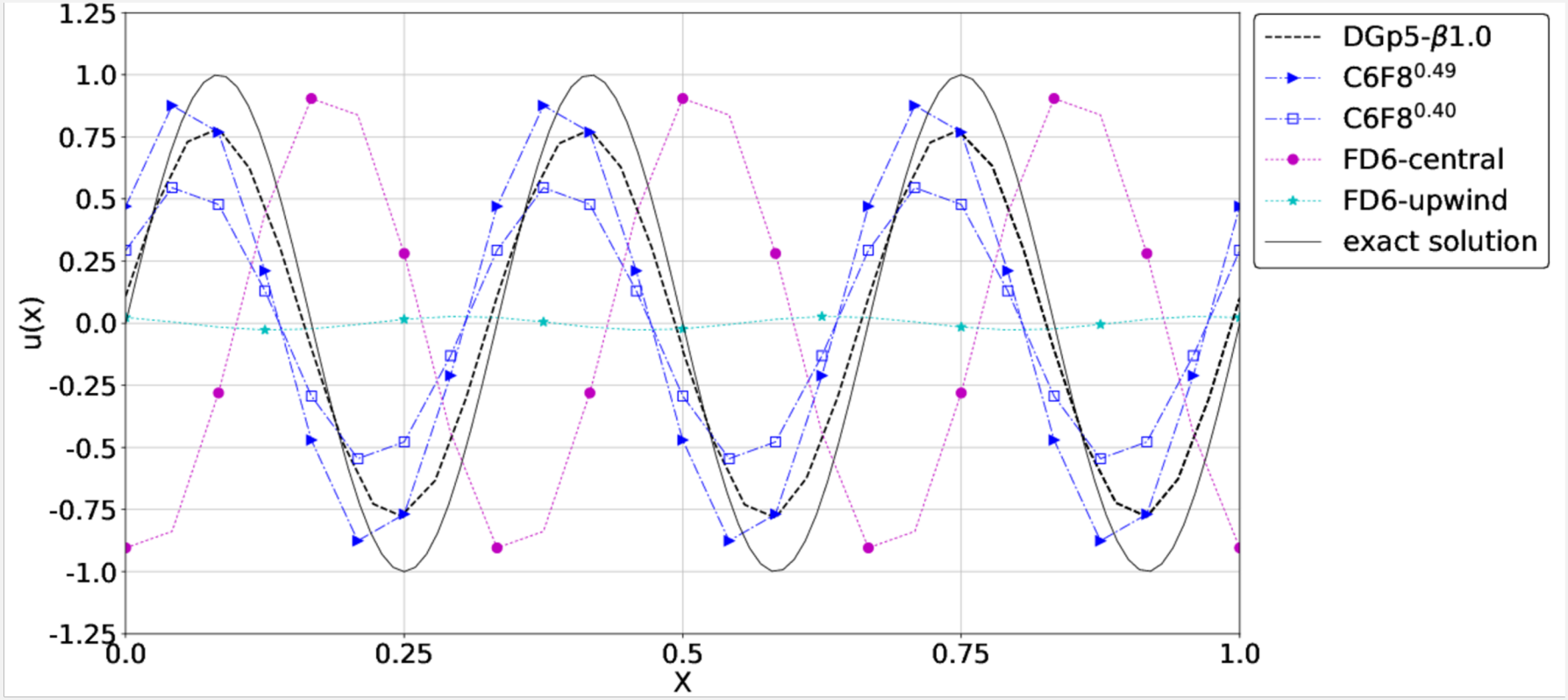


Dispersion error

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Performance for the Linear Wave Equation

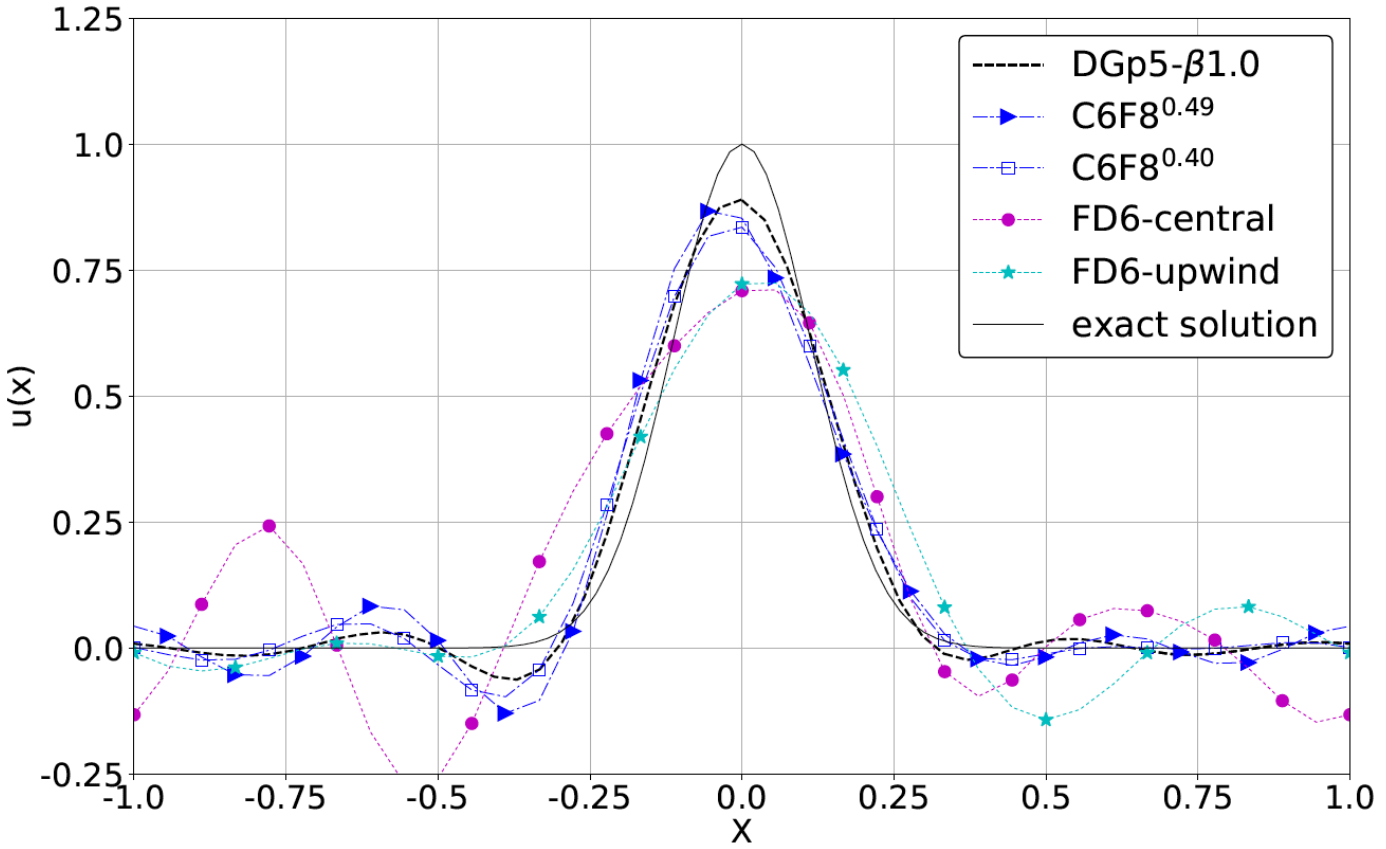
Same Δt, t = 150T



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Performance for the Linear Wave Equation

Same Δt



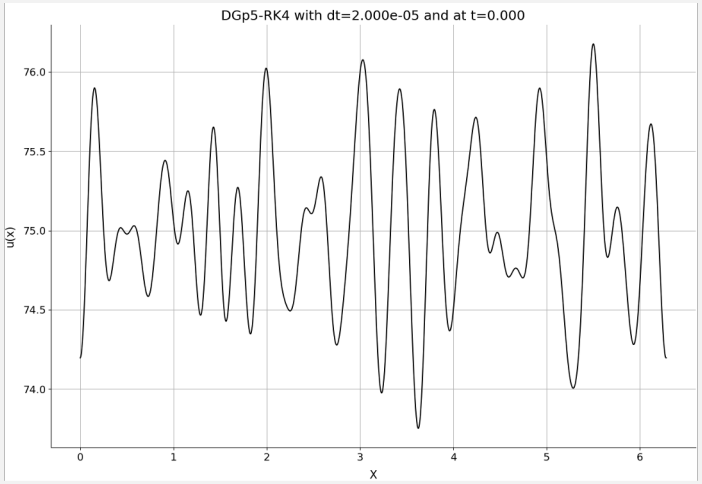
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Burgers Turbulence

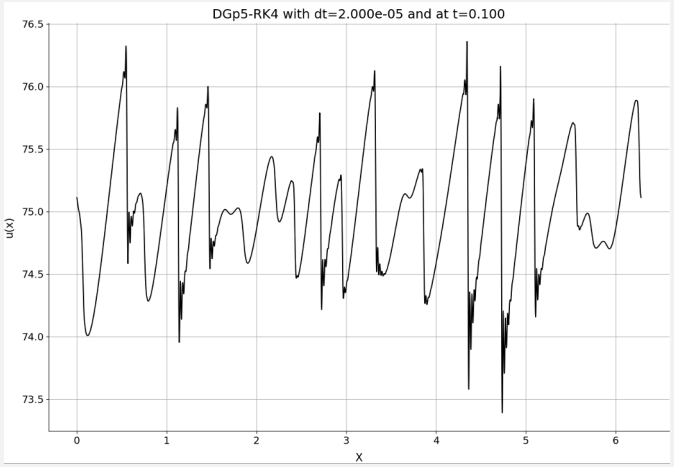
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \qquad \nu = 2x10^{-4}$$

Initial Energy Spectrum

$$E(k, 0) = E_0(k) = Ak^4\rho^5 e^{-k^2\rho^2}$$



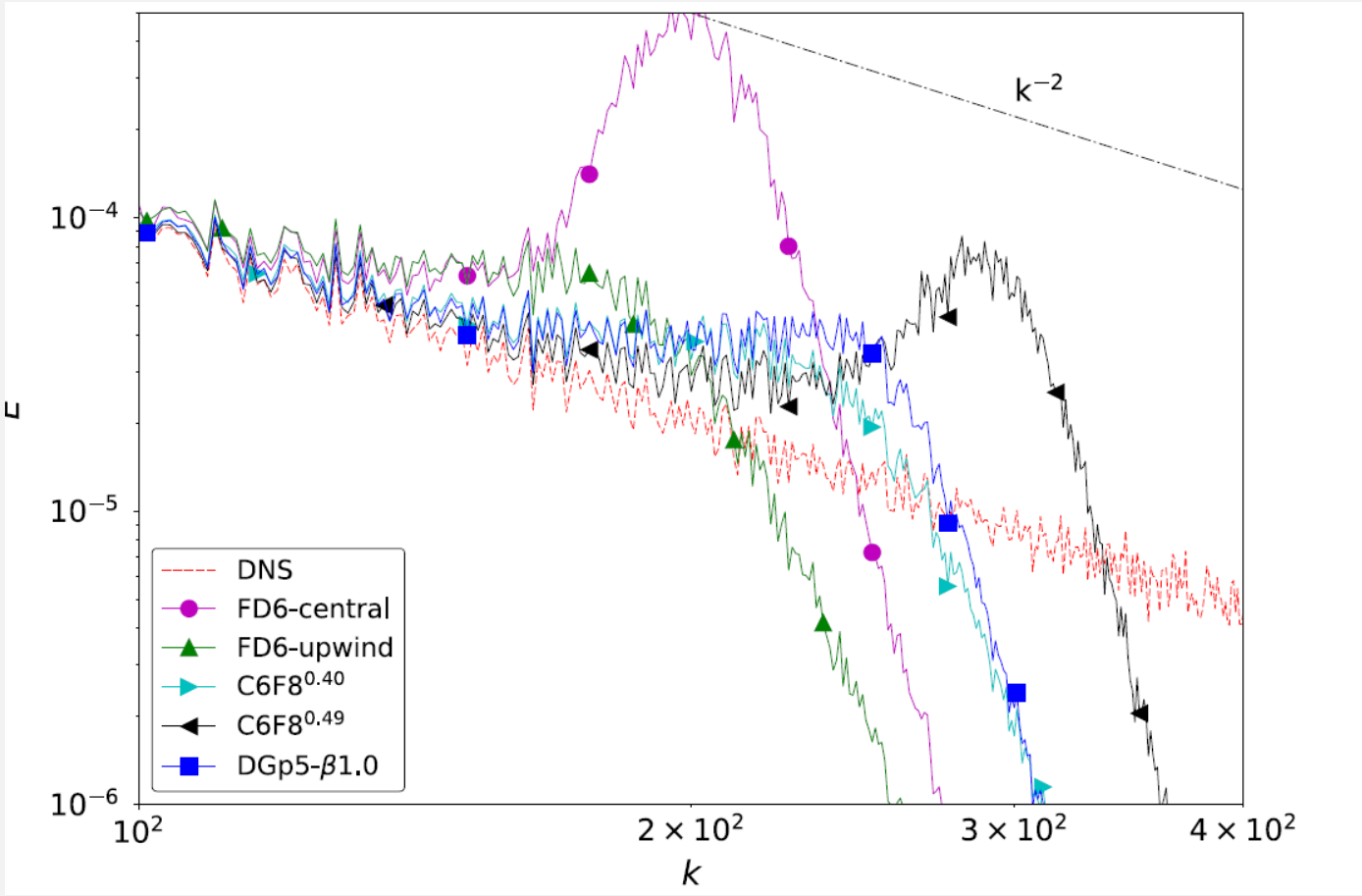
t = 0.



t = 0.1

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Performance for Burgers Turbulence (Fixed Δt)

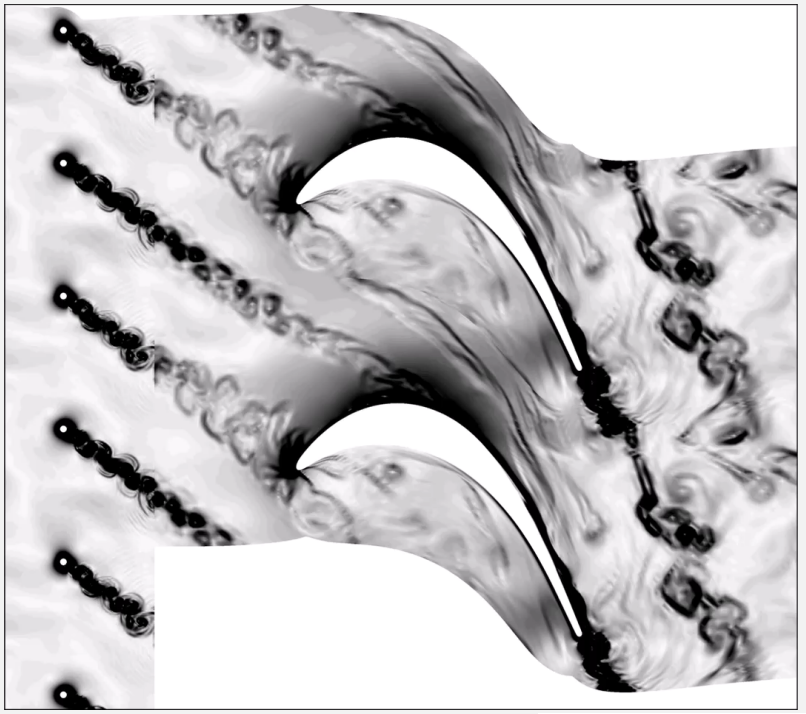


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Development of hpMusic

- Decades of research on high-order CFD methods leads to hpMusic for LES
  - Mixed meshes in CGNS or Gmsh format
  - High-order accuracy (up to 6th)
  - Overset and sliding meshes for moving grids
  - Highly scalable on CPU and GPU clusters
  - Implicit LES, wall-resolved or wall modeled
  - Explicit and implicit time integration schemes

hp-adaptive MUlti-physics
SImulation Code

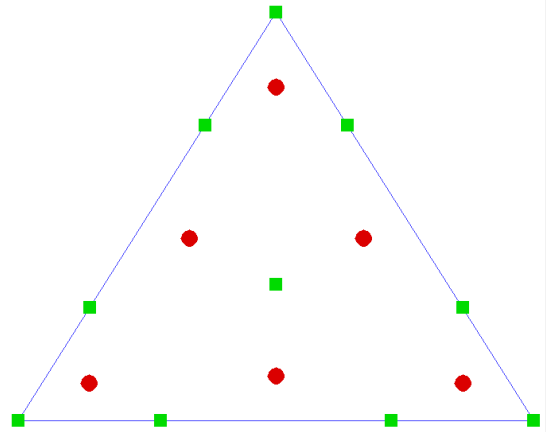


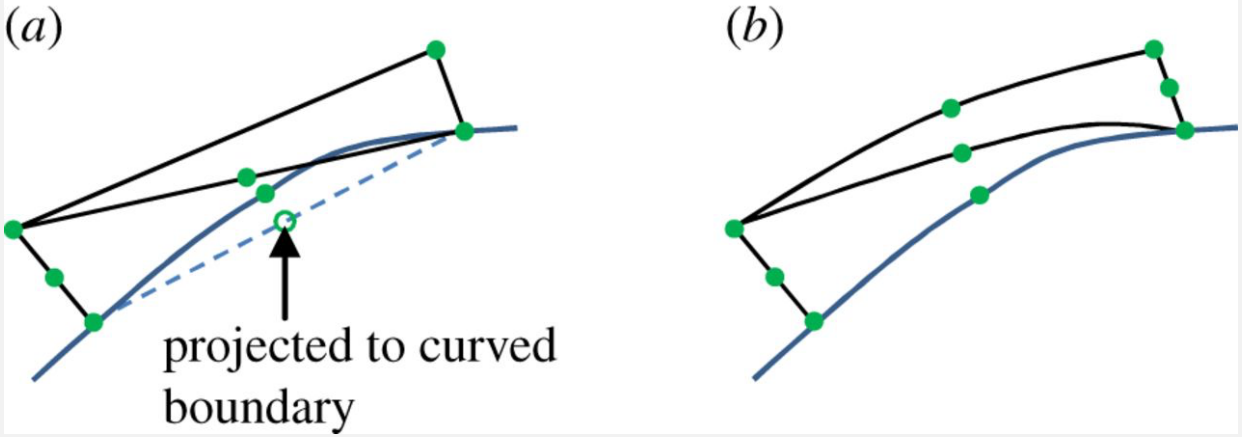
The Need for Coarse, High-Order Meshes

- Internal degrees of freedom are added such that meshes with ~1,000,000 elements may be sufficient to achieve engineering accuracy
- If boundaries are still represented by linear facets, large errors are generated

1M Hex Mesh

P	nDOFs at 2nd Order
2	513M
3	4.1B
5	32.6B

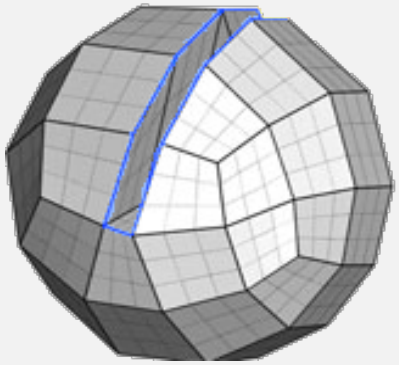




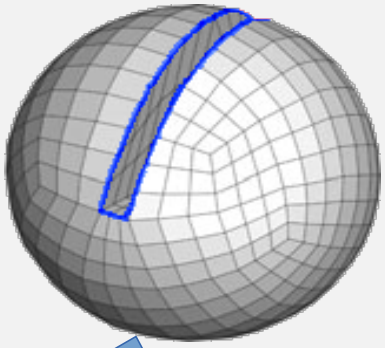
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The Mission

For high-order CFD simulations, we need to



change this



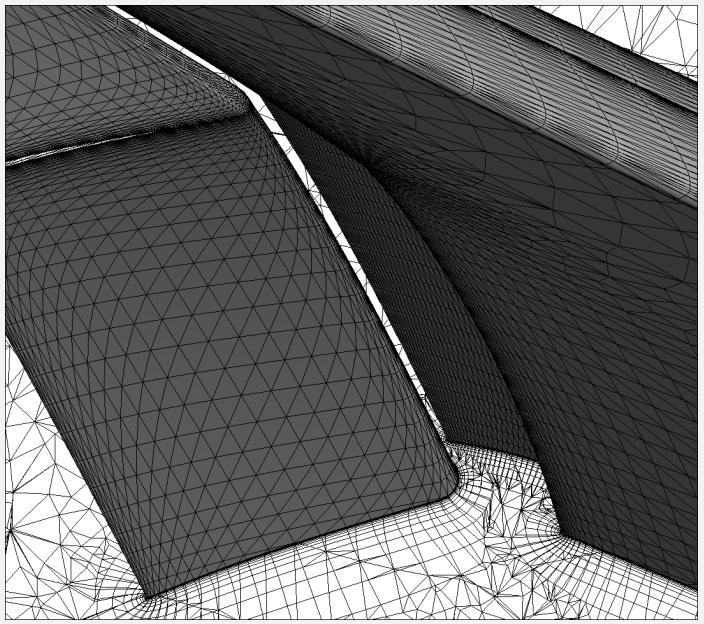
to this

without smoothing away edges.

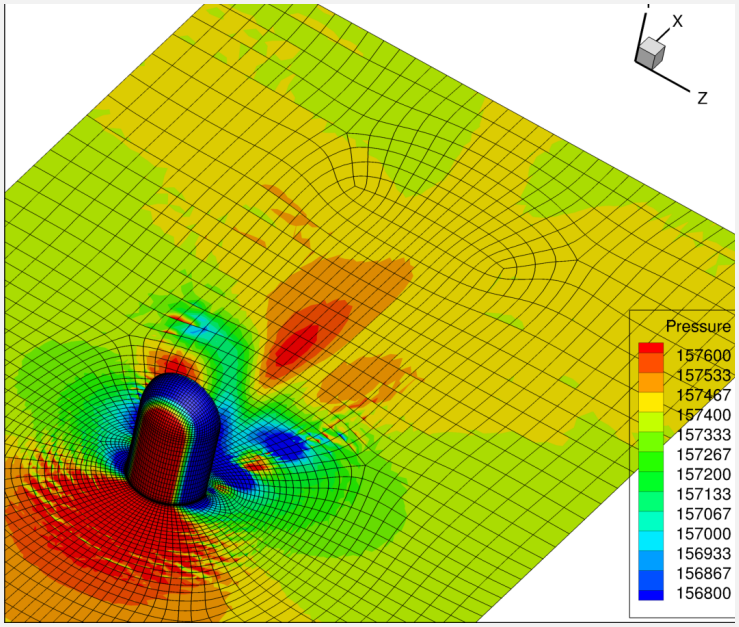
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Commercial High-Order Mesh Generators

- Pointwise, mixed meshes
- GridPro, hexahedral meshes

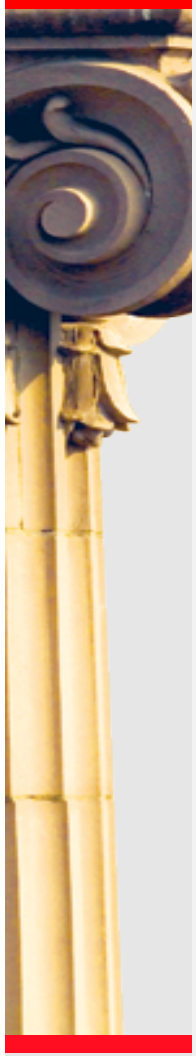


CRM High Lift, Pointwise



Generic mirror, GridPro

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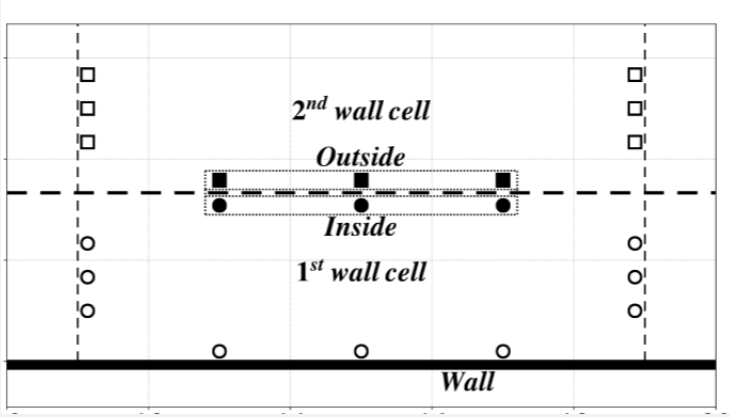


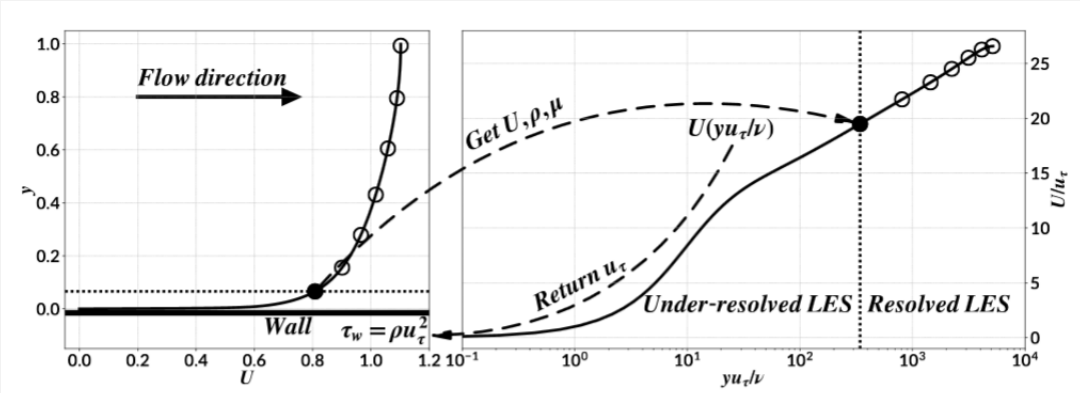
Equilibrium Wall Model

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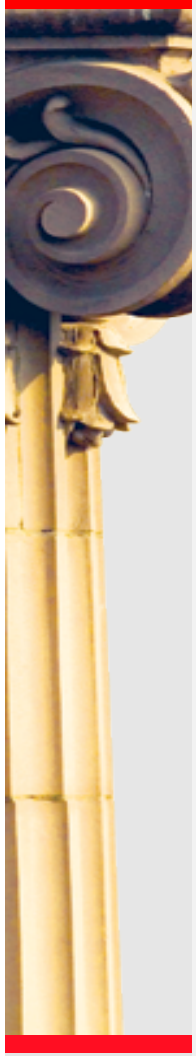
Schematic of the Wall Model

- The wall stress computed based on velocity obtained from the 2nd cell
- The wall stress is then used in the momentum equations
- Since the first cell does not have the proper resolution, a slip wall boundary condition is imposed at the wall
- The law of the wall is derived from the Spalart-Allmaras turbulence model





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Scalable Time Integration Schemes

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Need for Low Memory Implicit Schemes

- Explicit schemes
  - Good performance demonstrated for Runge-Kutta schemes with 1 element per core if p is reasonably high
  - Time step limited by the smallest cell with global time-stepping
  - Time accurate local time-stepping viable alternative, but not trivial to parallelize
- Implicit schemes
  - Time discretization
    - BDF2, optimized BDF2, DIRK, IRK, …
  - Linear (non-linear) solvers
    - GMRES with various preconditioners (memory depends on the preconditioner)
    - Block LU-SGS approach (but memory ~ p6)

Experience with Various Time Integration Schemes

Scheme	Time Step	Memory Use	Throughput
GMRES + ILU(n)	Largest $\sim\Delta t_{physical}$	Most (CPUs) $\sim p^6$	~3rd
GMRES + Block Jacobi	Large $\sim 0.1\Delta t_{physical}$	Medium (CPUs) $\sim p^6$	~2nd
BLU-SGS	Medium $\sim 10\text{-}100\Delta t_{explicit}$	Medium (CPUs) $\sim p^6$	~1st
GMRES + No Precond	Medium $\sim 10\text{-}50\Delta t_{explicit}$	Little (CPUs + GPUs)	~4th
RK3	Small $\sim\Delta t_{explicit}$	Least (CPUs + GPUs)	~5th

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Some Time Scales for a Real-World Problem: NASA CRM-HL

- Characteristic time scale

$$t_c = \frac{MAC}{V_\infty} = 0.1s$$

- Estimated dominant turbulent time scale

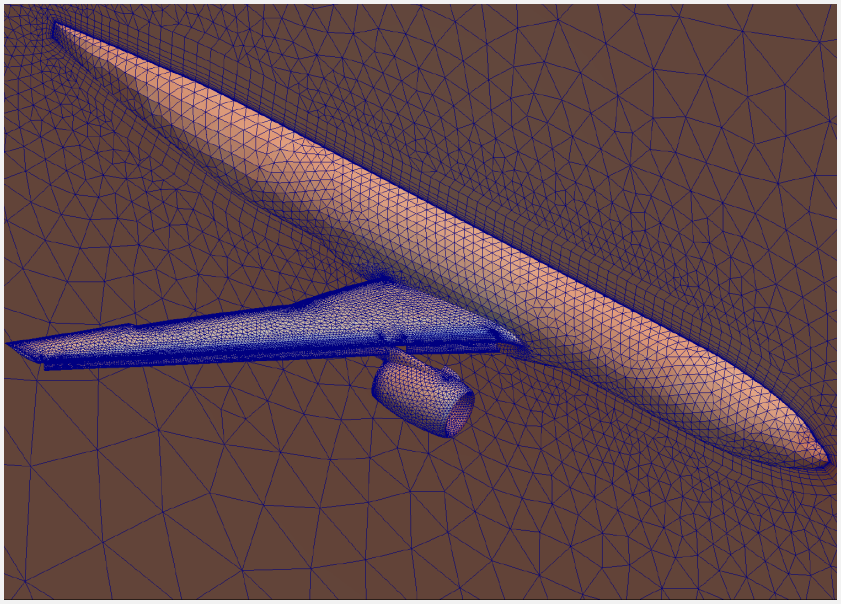
$$\Delta t_{physical} = 10^{-4}s$$

- Explicit time step (p = 2)

$$\Delta t_{explicit} = 8.1x10^{-10}s$$

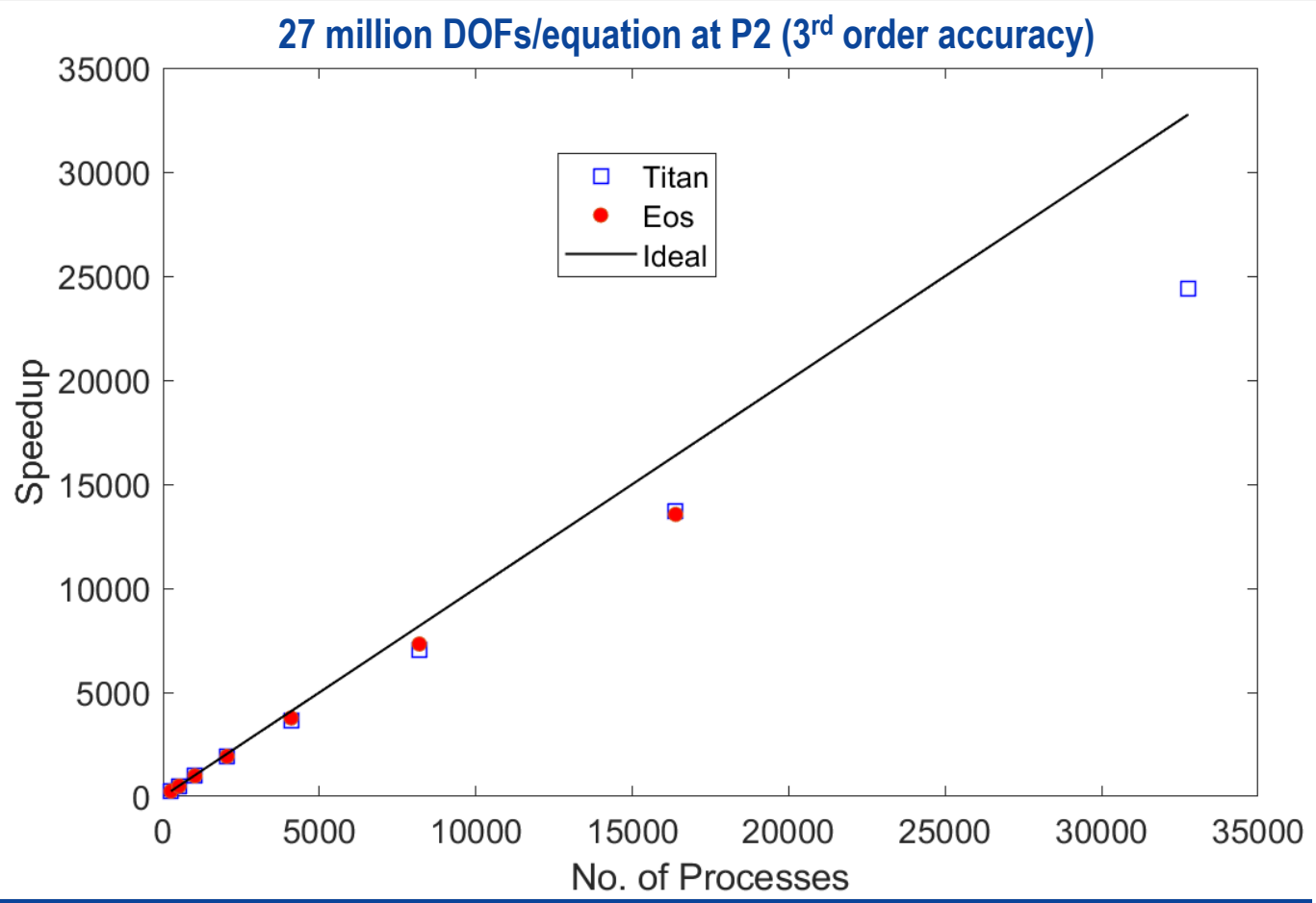
- Time step for LU-SGS (p = 2)

$$\Delta t_{LU-SGS} = 10^{-6}s$$

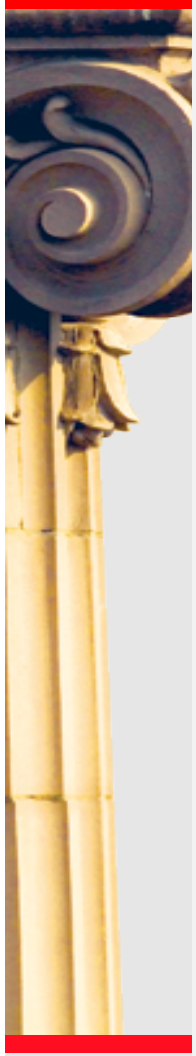


2.37M cell mesh by Dr. Steve Karman

Strong Scalability for LU-SGS on DOE's Titan and EOS



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Implementation on GPU clusters

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The FR/CPR Method

Consider

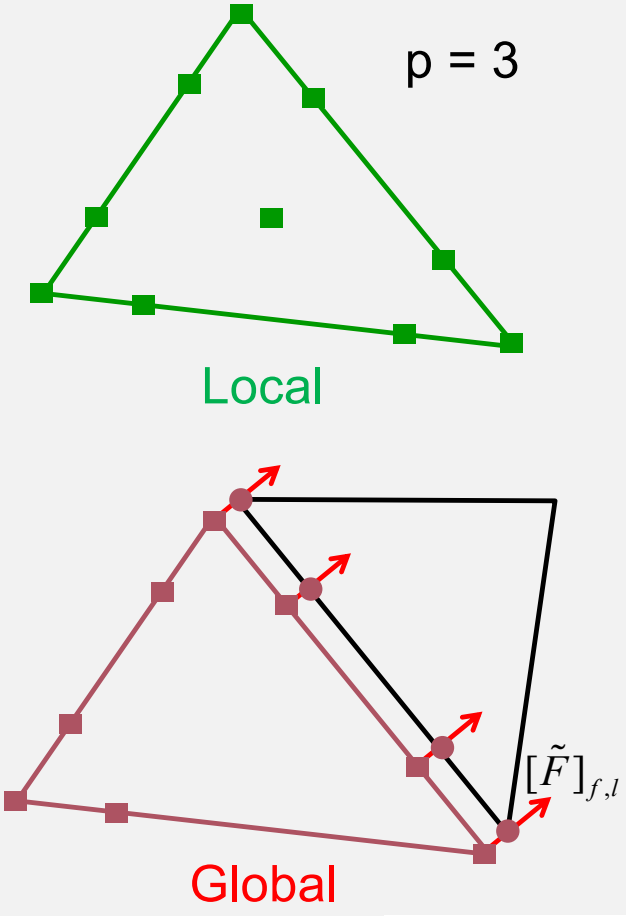
$$\frac{\partial Q}{\partial t} + \nabla \cdot \vec{F} = 0$$

The FR/CPR method can be written as

$$\frac{\partial Q_{i,j}^h}{\partial t} + \nabla \bullet \vec{F}(Q_{i,j}^h) + \frac{1}{|V_i|} \sum_{f \in \partial V_i} \sum_l \alpha_{j,f,l} [\tilde{F}]_{f,l} S_f = 0.$$

RK3 and matrix-free GMRES/no preconditioner for time integration.

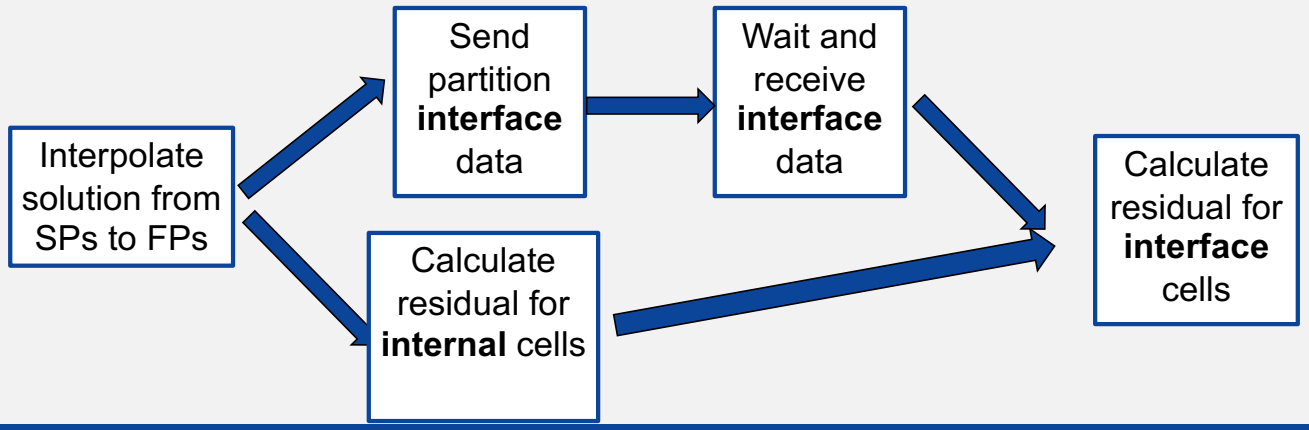
$$Aq = \frac{R(\hat{Q} + \varepsilon q) - R(\hat{Q})}{\varepsilon}$$



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Basic Parallel Strategy

- Domain decomposition and message passing (MPI)
- All computations performed on the GPUs
  - Only interface data transferred between CPU/GPU for communication
  - Communication and computation overlap
- The entire solution is transferred to CPU for post-processing only



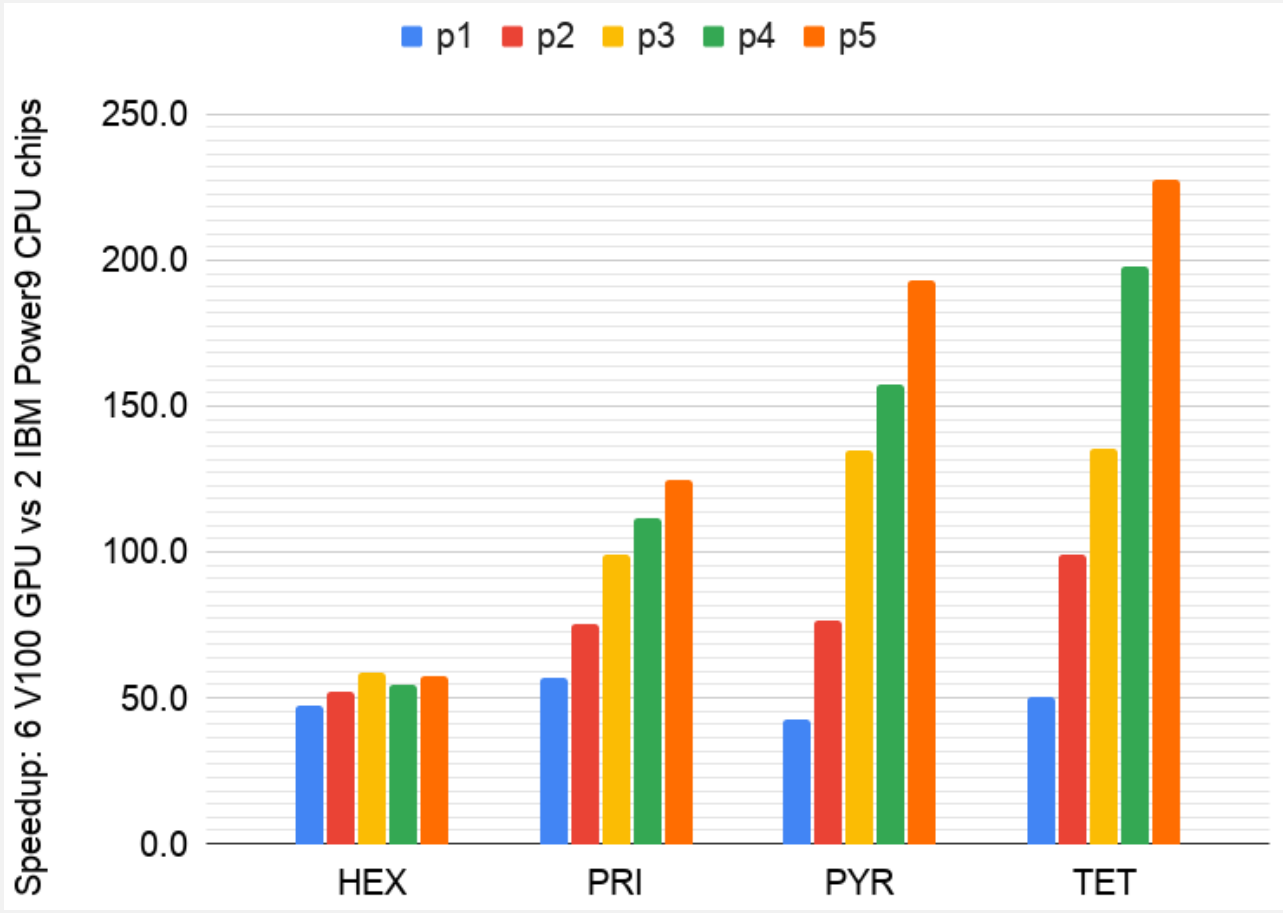
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Finer Details - Data Structure

- Multiple solution points (SPs) per element.
- 5 equations/variables per SP.
- Thread/block strategy:
  - Threads -> SP
  - Block -> elements (more than one element per block)
- 1-D solution array:
  - CPU: element x SP x equations
  - GPU: element x equations x SP (coalesced access)
- Consecutive threads access consecutive SPs and therefore consecutive memory positions in the array: coalesced memory access.

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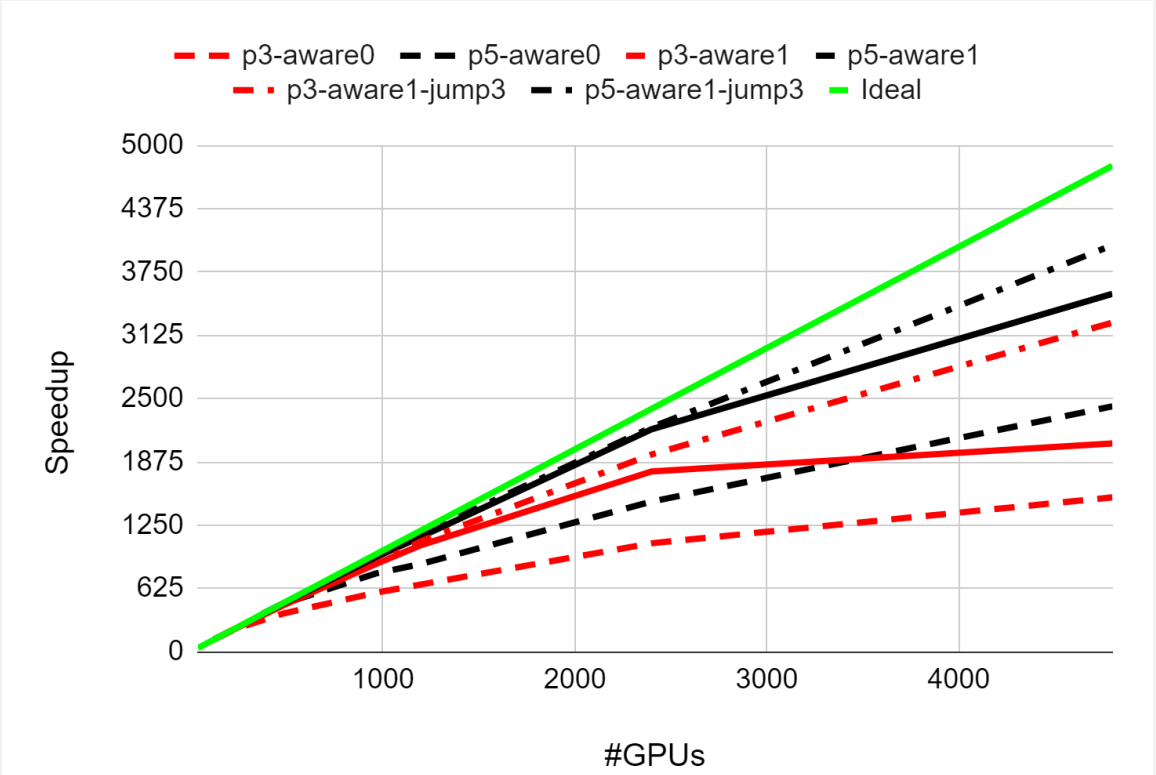
Node Performance (6 GPU /44 CPUs on Summit)



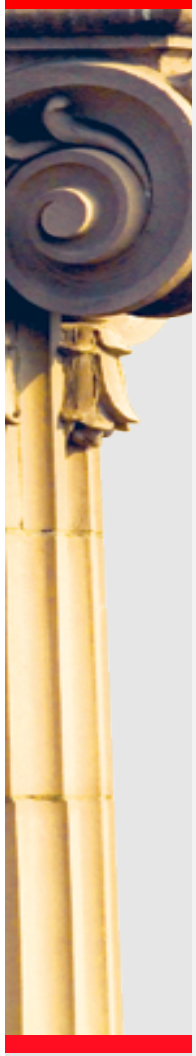
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Multi-GPU Performance (Summit/Oak Ridge National Lab.)

- Tet mesh with 36.7M cells.



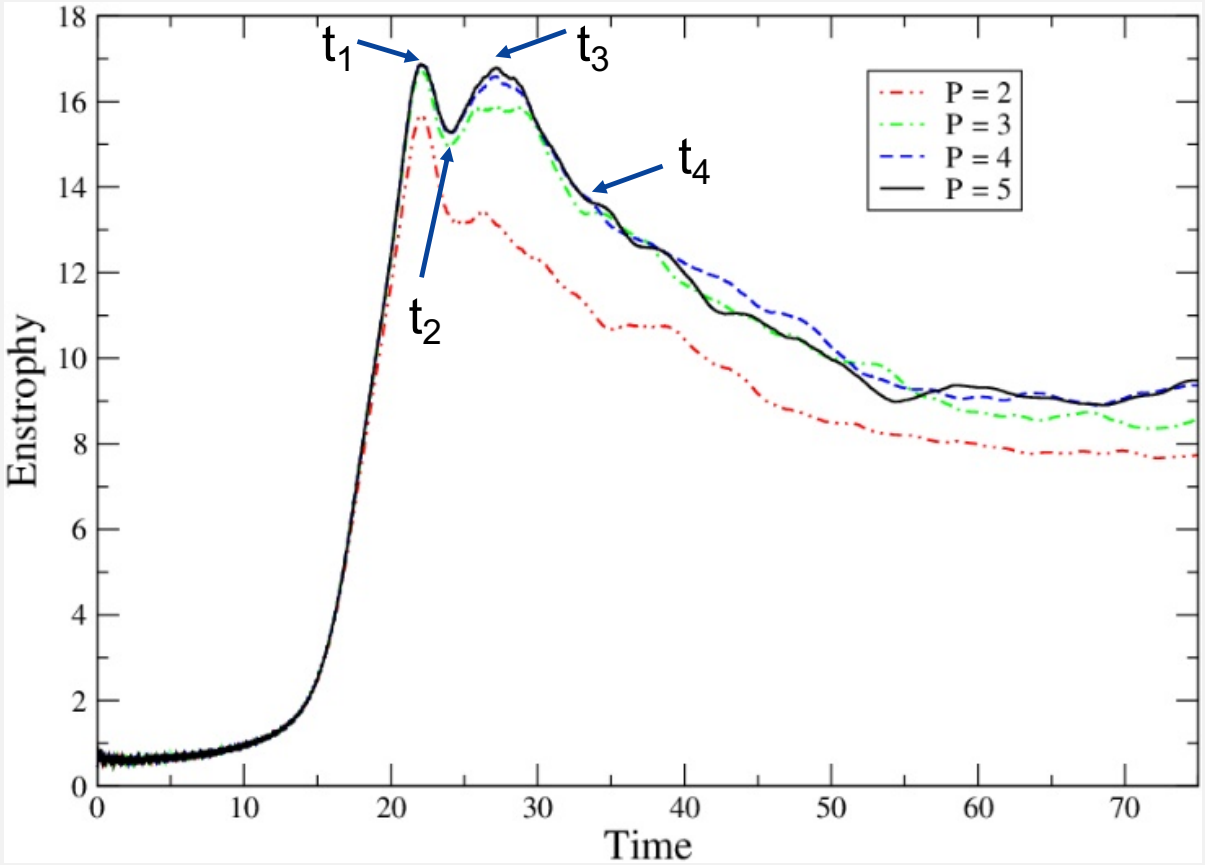
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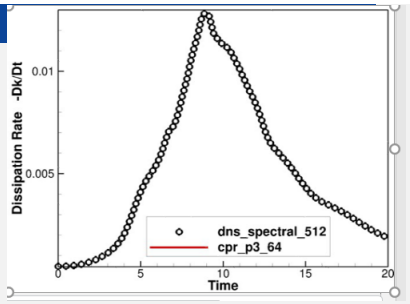


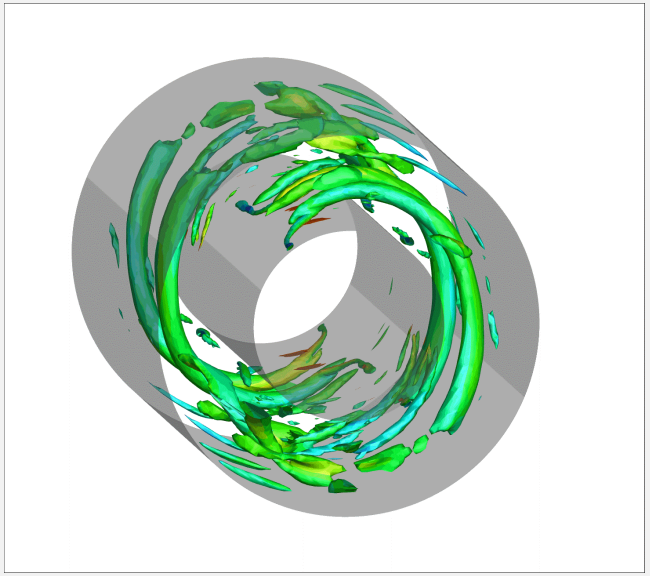
Study of Vortex-Dominated Flows

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Another Benchmark - Taylor-Couette Flow





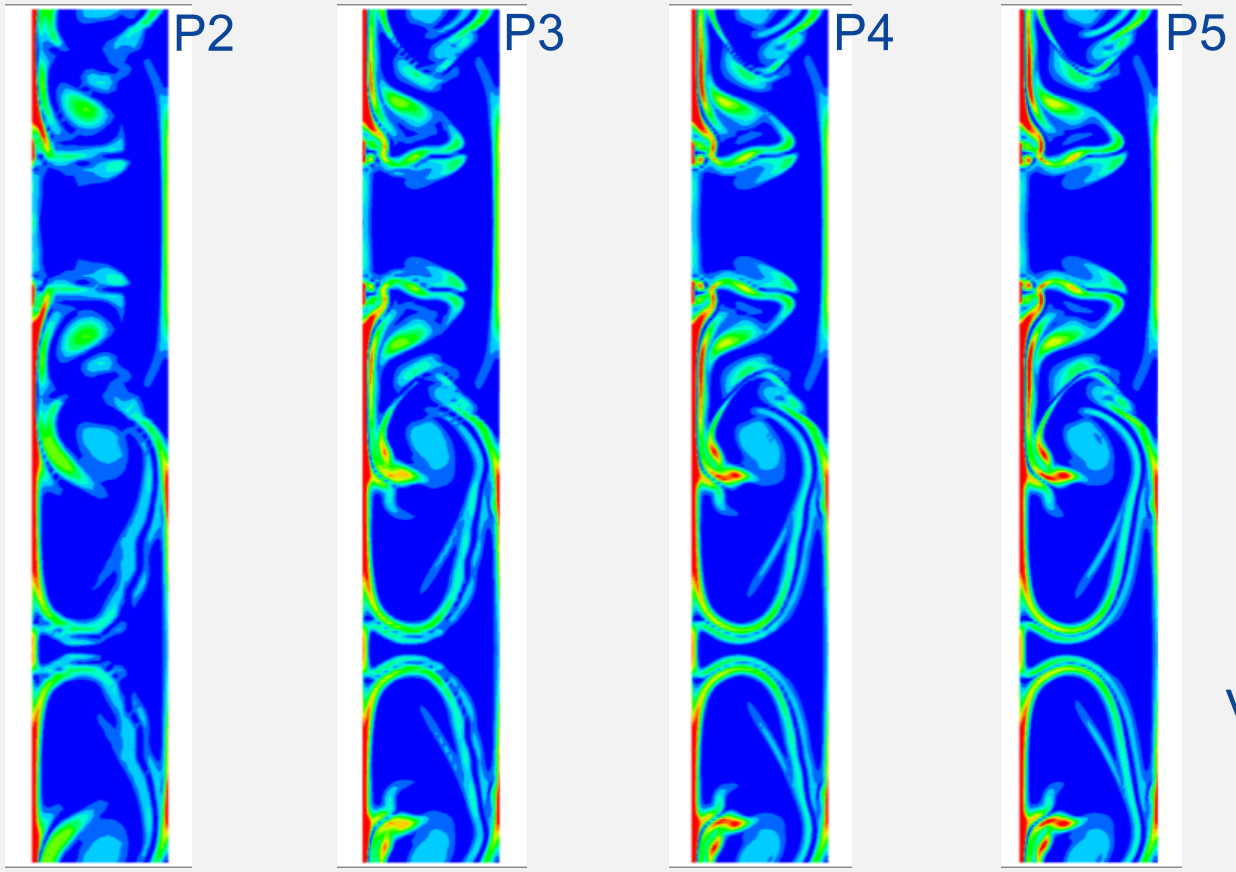


Re = 4,000

$\eta = r_i/r_o = 0.5$

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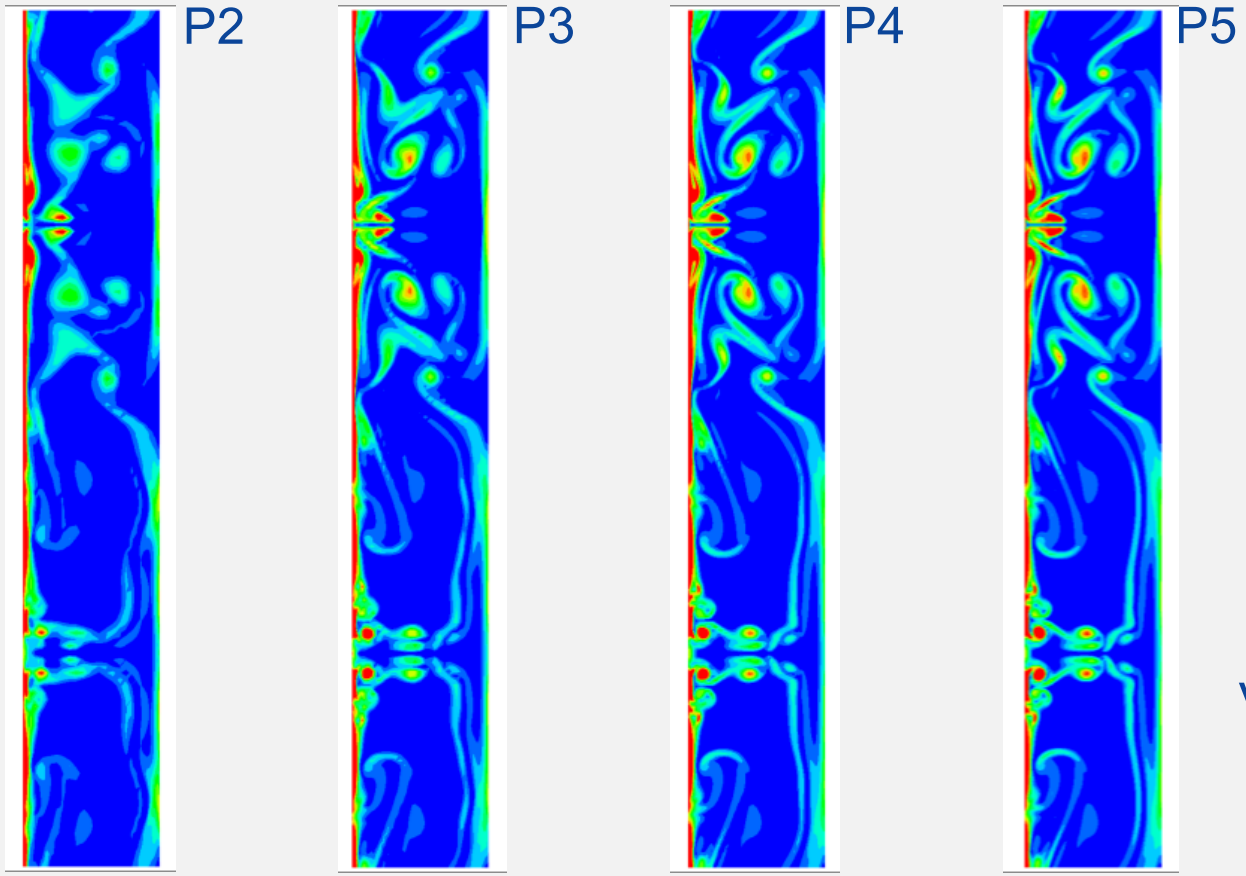
Taylor-Couette Flow – Vorticity Magnitude at t_1



Vortex sheet stretching

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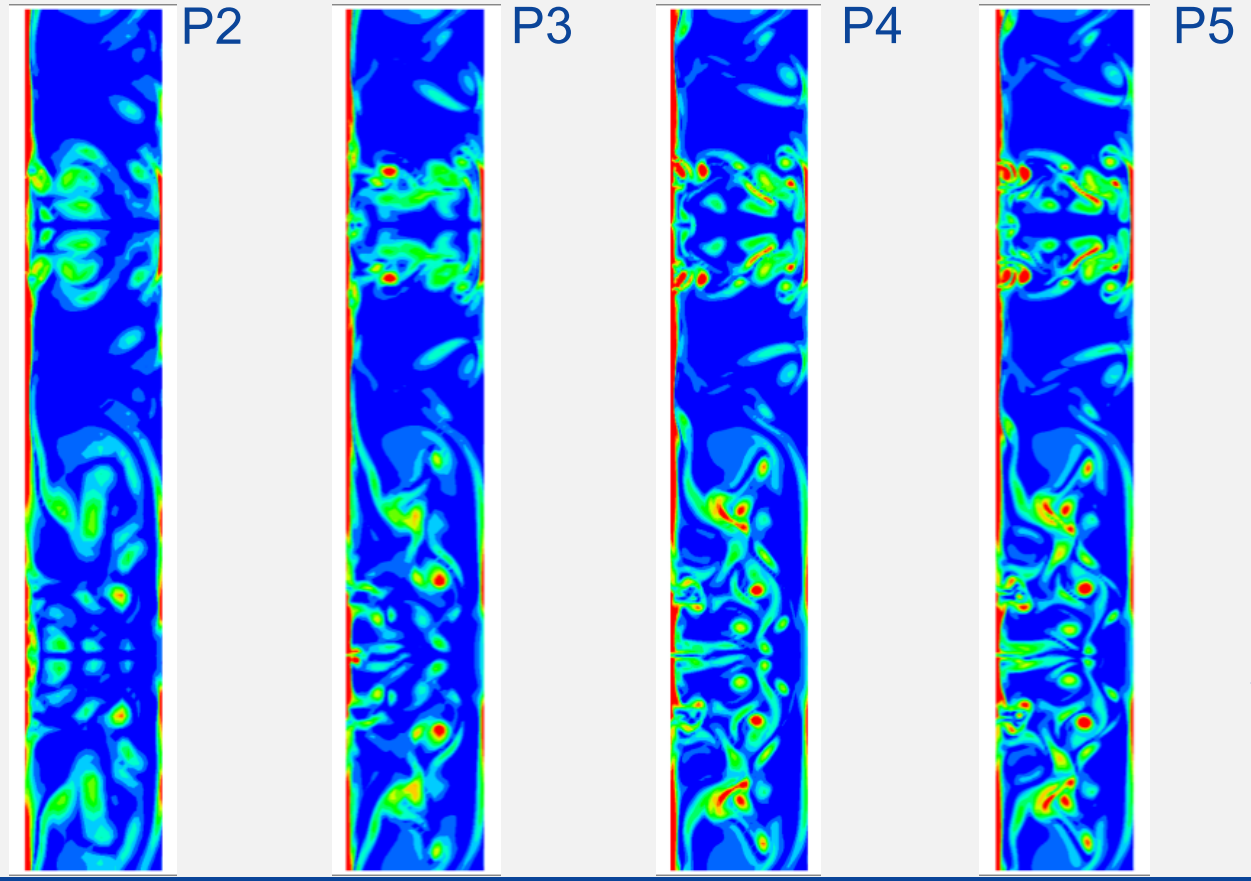
Taylor-Couette Flow – Vorticity Magnitude at t_2



Vortex sheet breakdown

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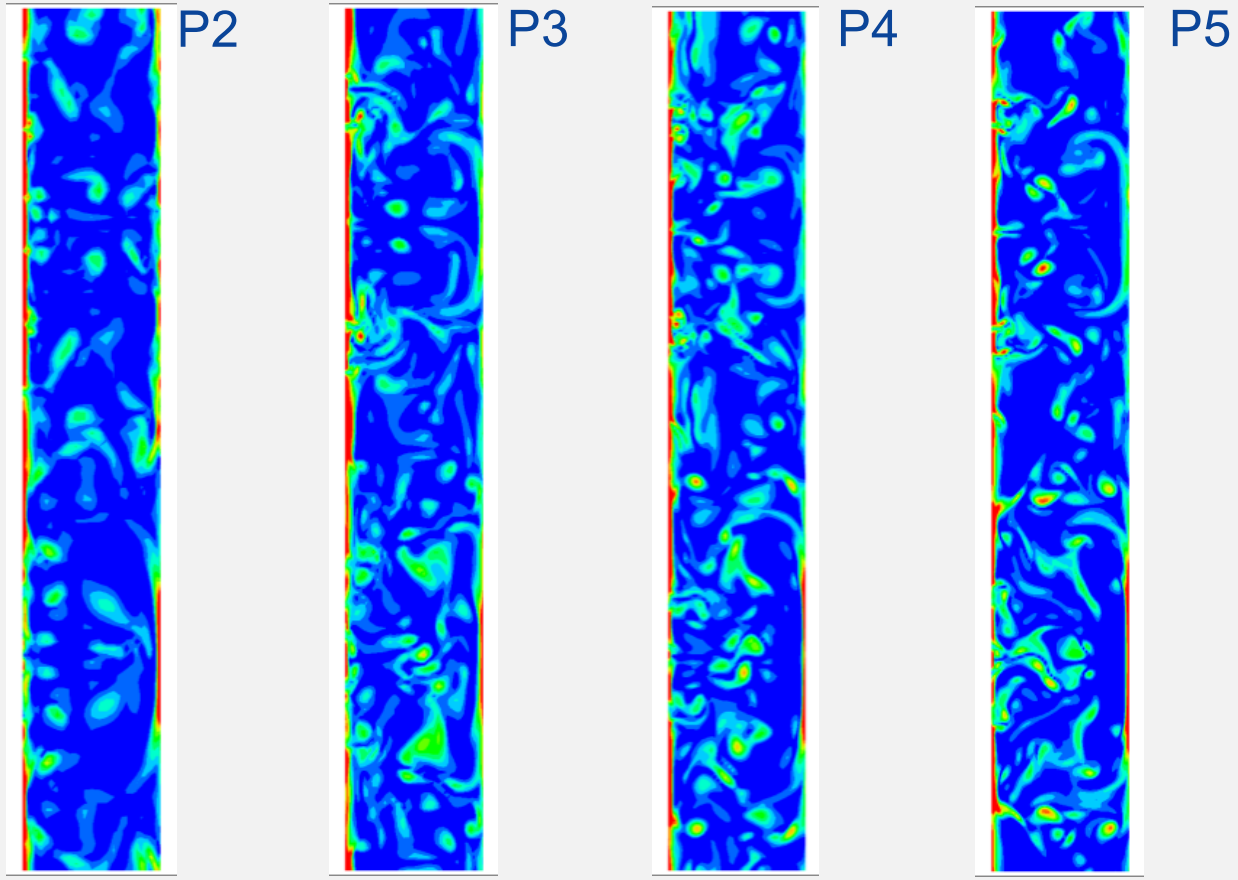
Taylor-Couette Flow – Vorticity Magnitude at t_3



Vortex-wall interaction

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Taylor-Couette Flow – Vorticity Magnitude at t_4

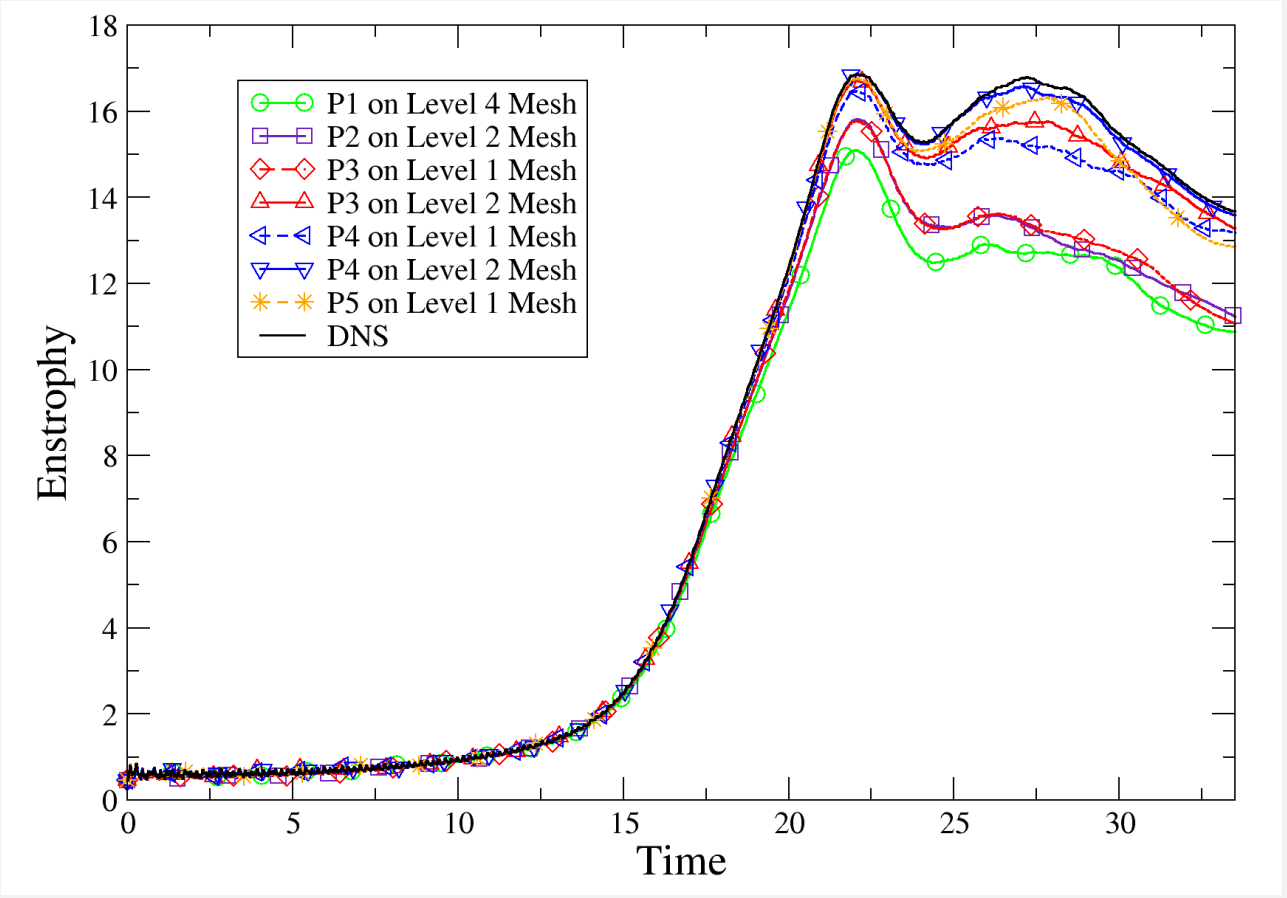


Turbulent

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Taylor-Couette Flow – Enstrophy History

$$\mathcal{E}(\omega) \equiv \int_S |\omega|^2 \, dS \, .$$



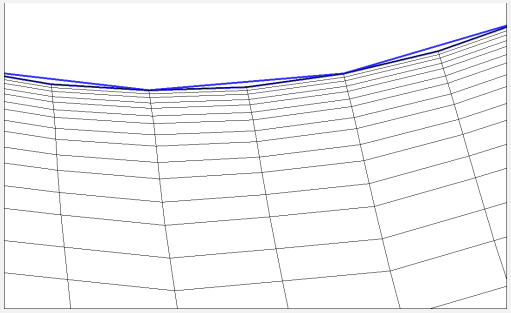
With a wall, higher order schemes preferred more!

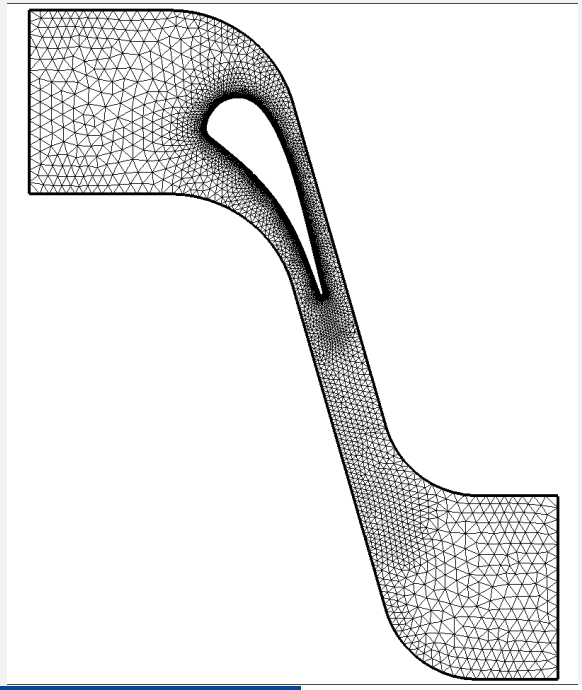
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Turbomachinery Benchmark – VKI HPT Heat Transfer

Case	Num. of cells	Cell type	Span layers	Span/chord	Mach	Reynolds	Avg. Y+
MUR129	448,175	Hex/Prism	35	16.6%	0.84	1.16M	3.3

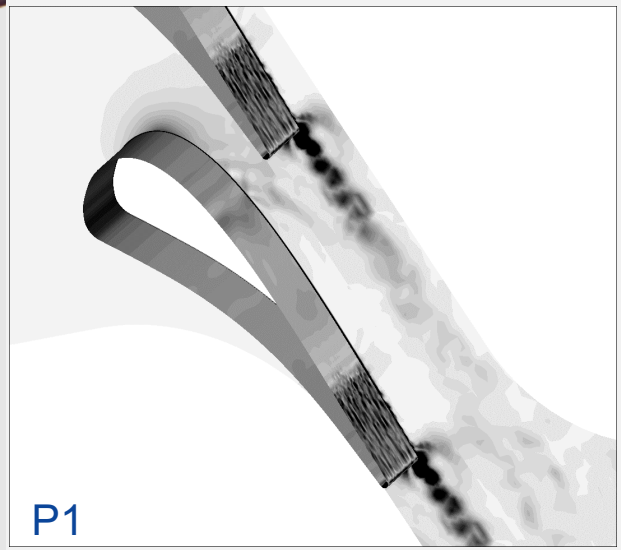
- P refinement performed with hpMusic
- Key physics
  - Laminar and turbulent boundary layers
  - Transition
  - Heat transfer
  - Shock waves and acoustic waves
  - Turbulent wake

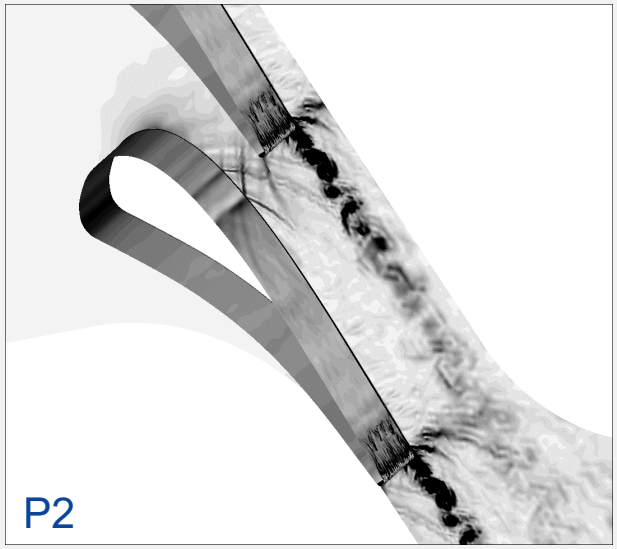




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Schlieren Movies: P-refinement

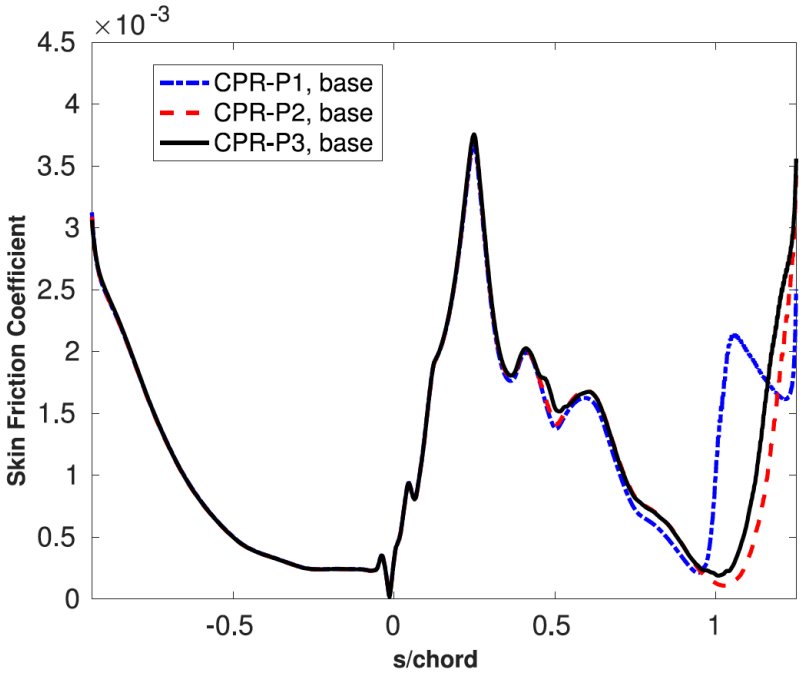


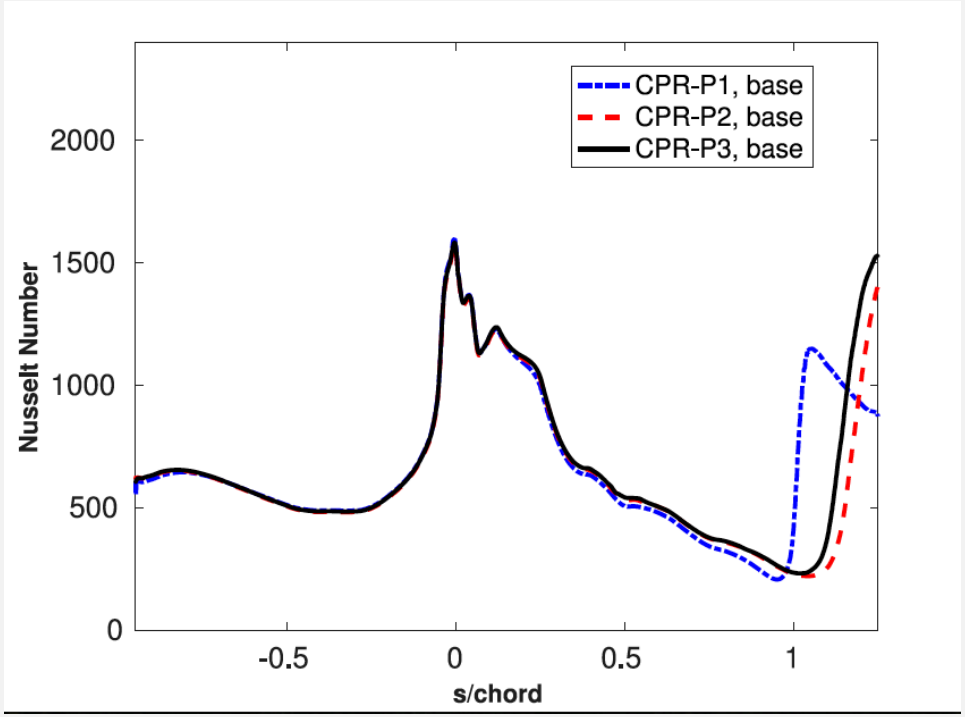




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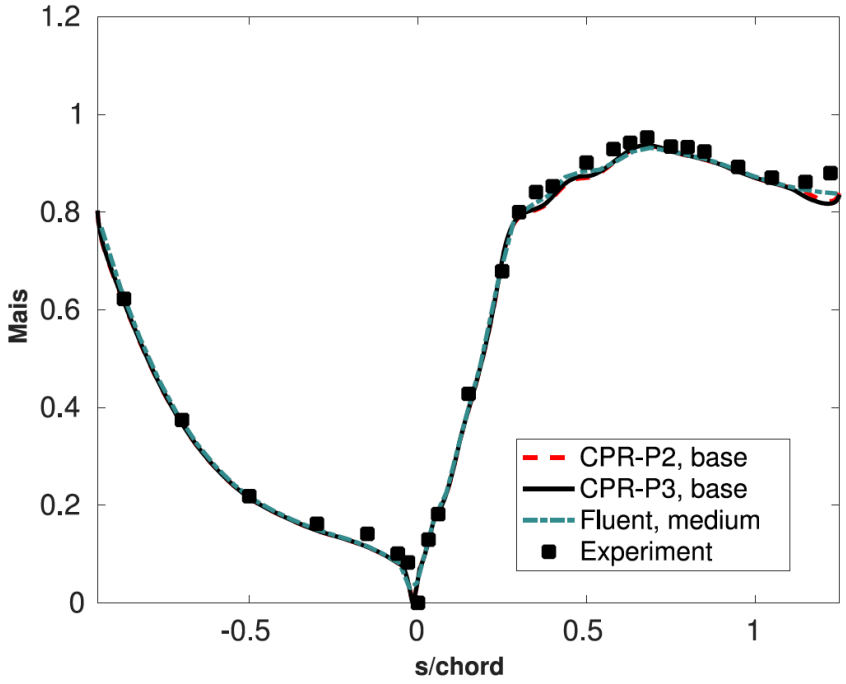
Numerical Results: P-refinement

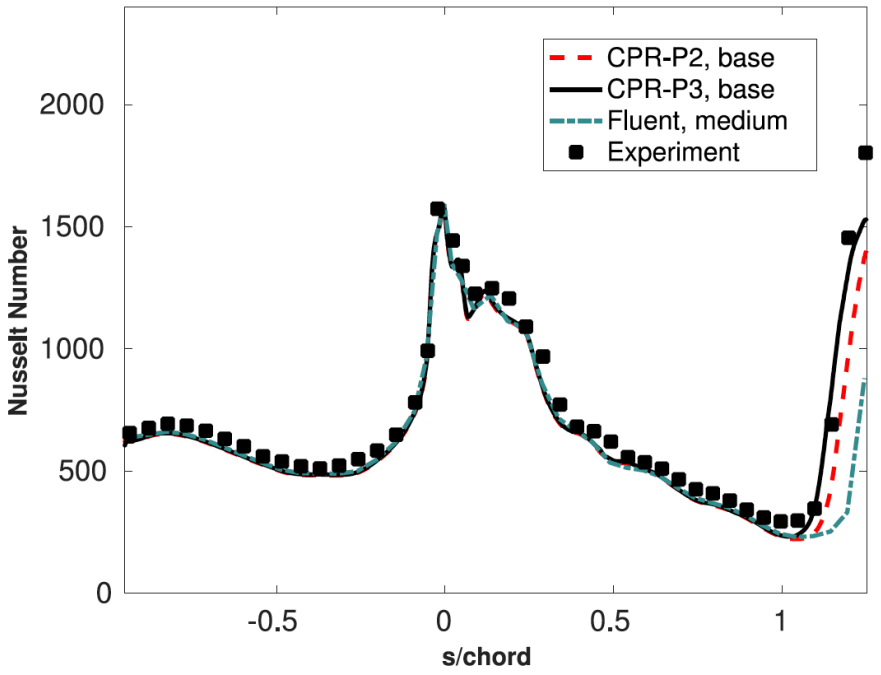




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Comparison with Experimental Data

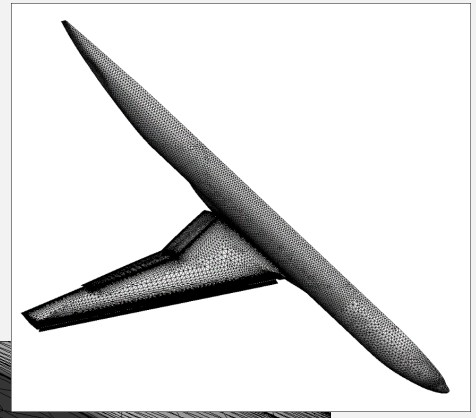


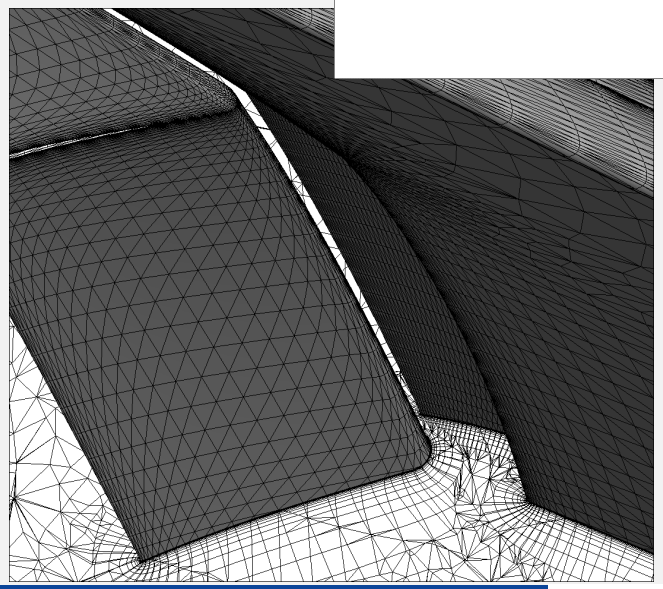


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ILES of CRM-High Lift Configuration (3rd AIAA Workshop)

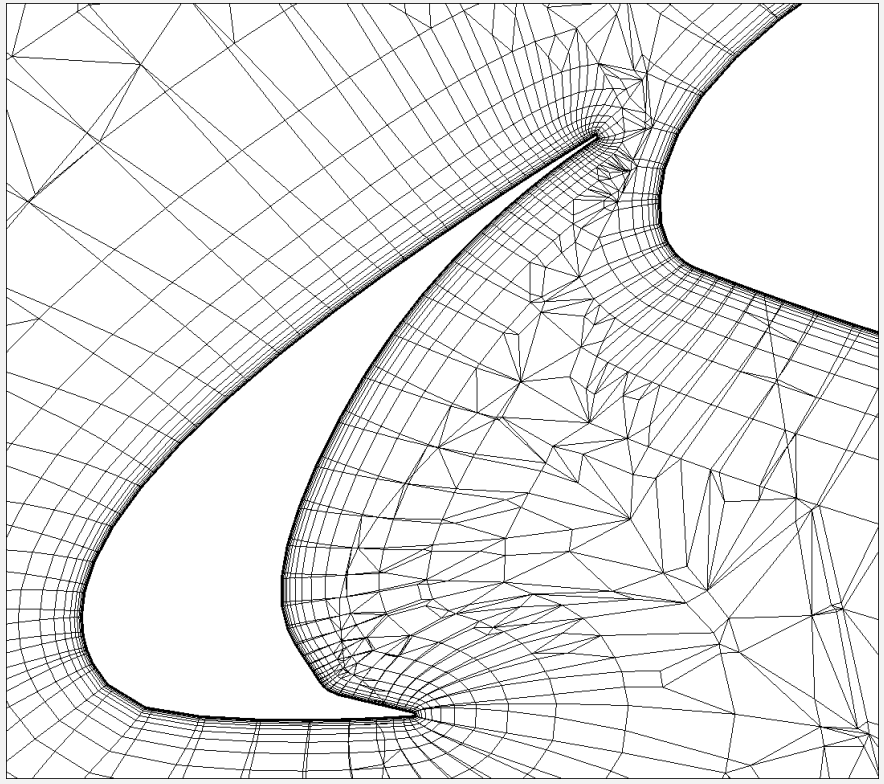
- Mach = 0.2
- Re = 3.26E6 based MAC
- AOA = 16 degrees (at stall)
- Mesh: ~2.23M mixed elements, generated by Pointwise, quadratic mesh
  - ~18M DOFs/equ at p = 1 (2nd order)
  - ~60M DOFs/equ at p = 2 (3rd order)
  - ~143M DOFs/equ at p = 3 (4th order)
  - Y+ <1 near the wall (RANS like mesh)
  - No wall-model used



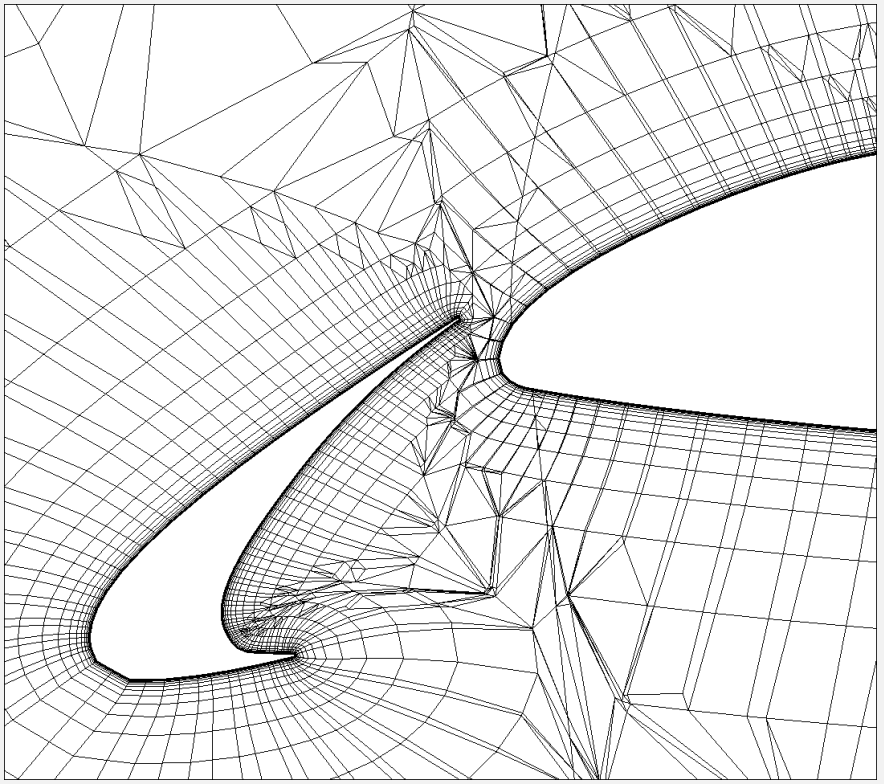


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Meshes at Different Span Locations



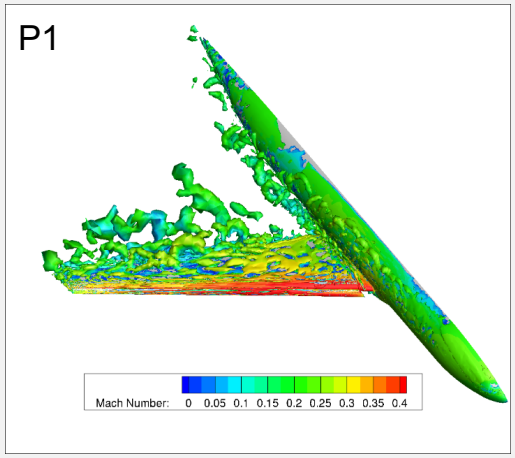
η = 0. 24

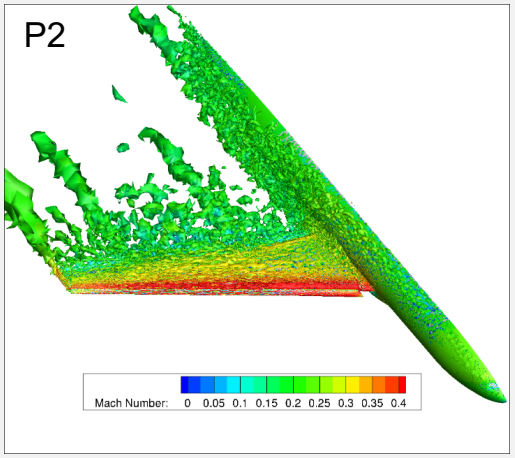


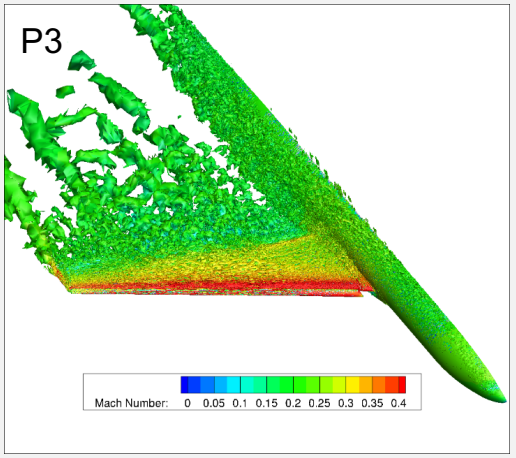
η = 0. 552

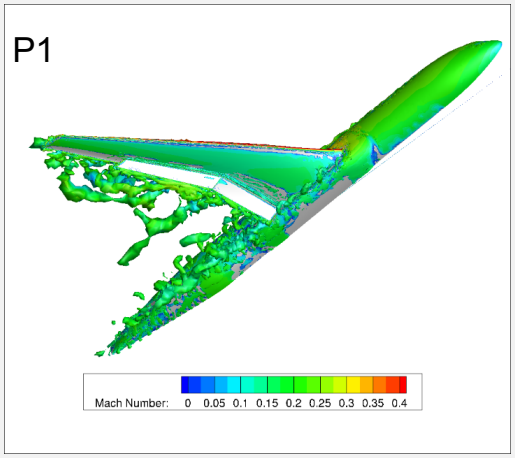
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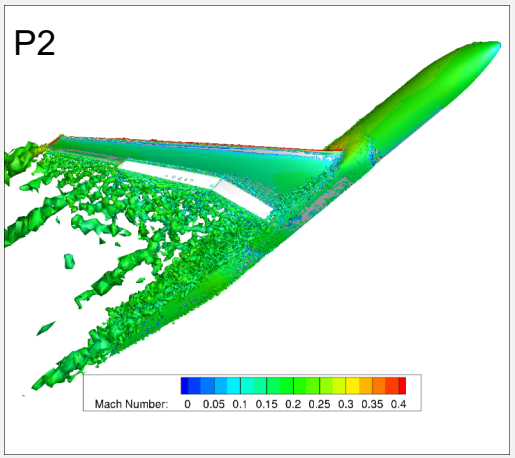
Comparison of Q-Criterion Colored by Mach

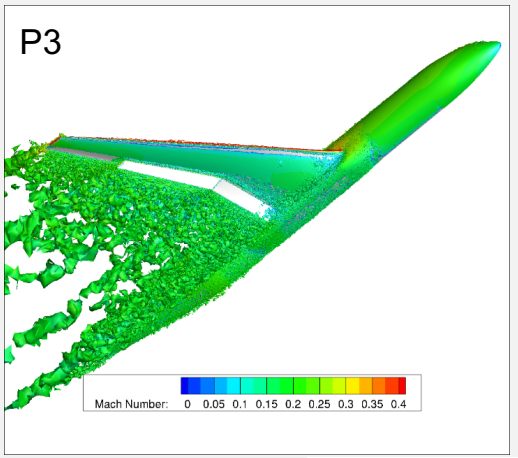






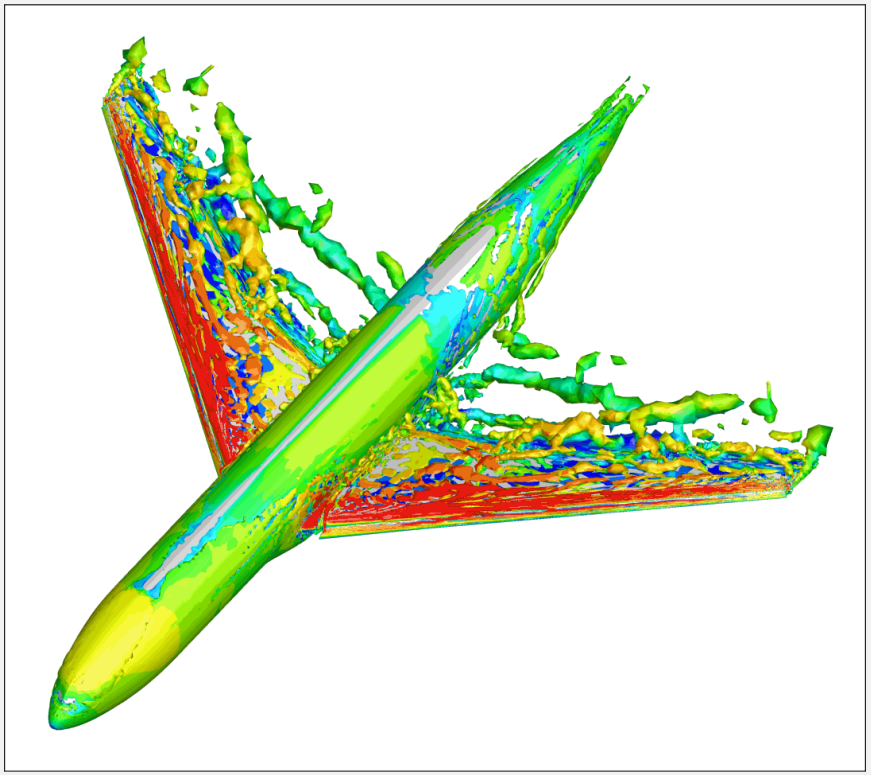






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Q-criterion Colored by Stream-wise Velocity

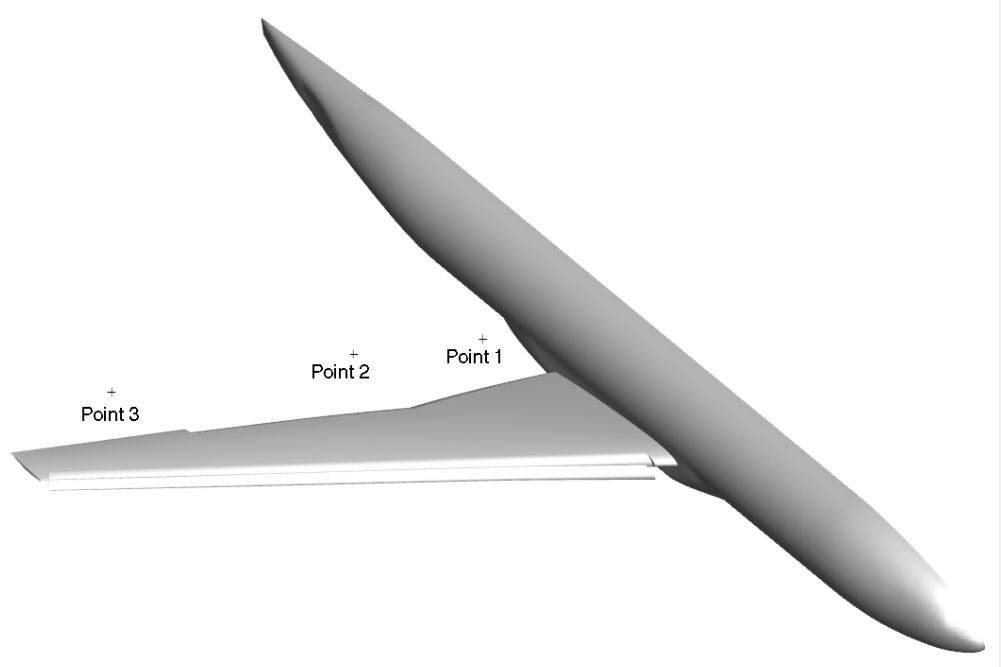


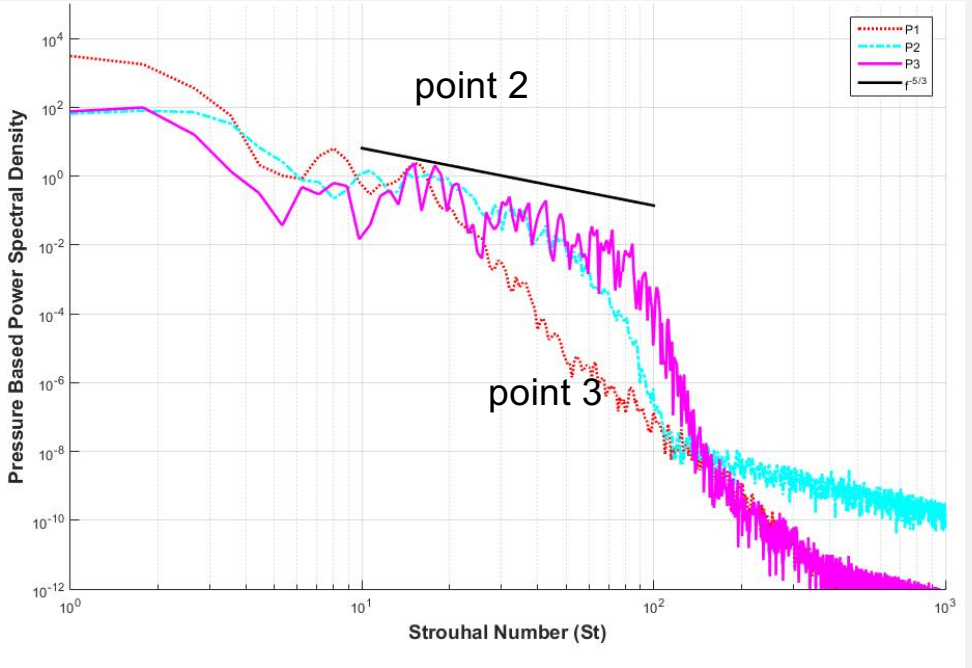
P1, 18M DOFs/equation

P2, 60M DOFs/equation

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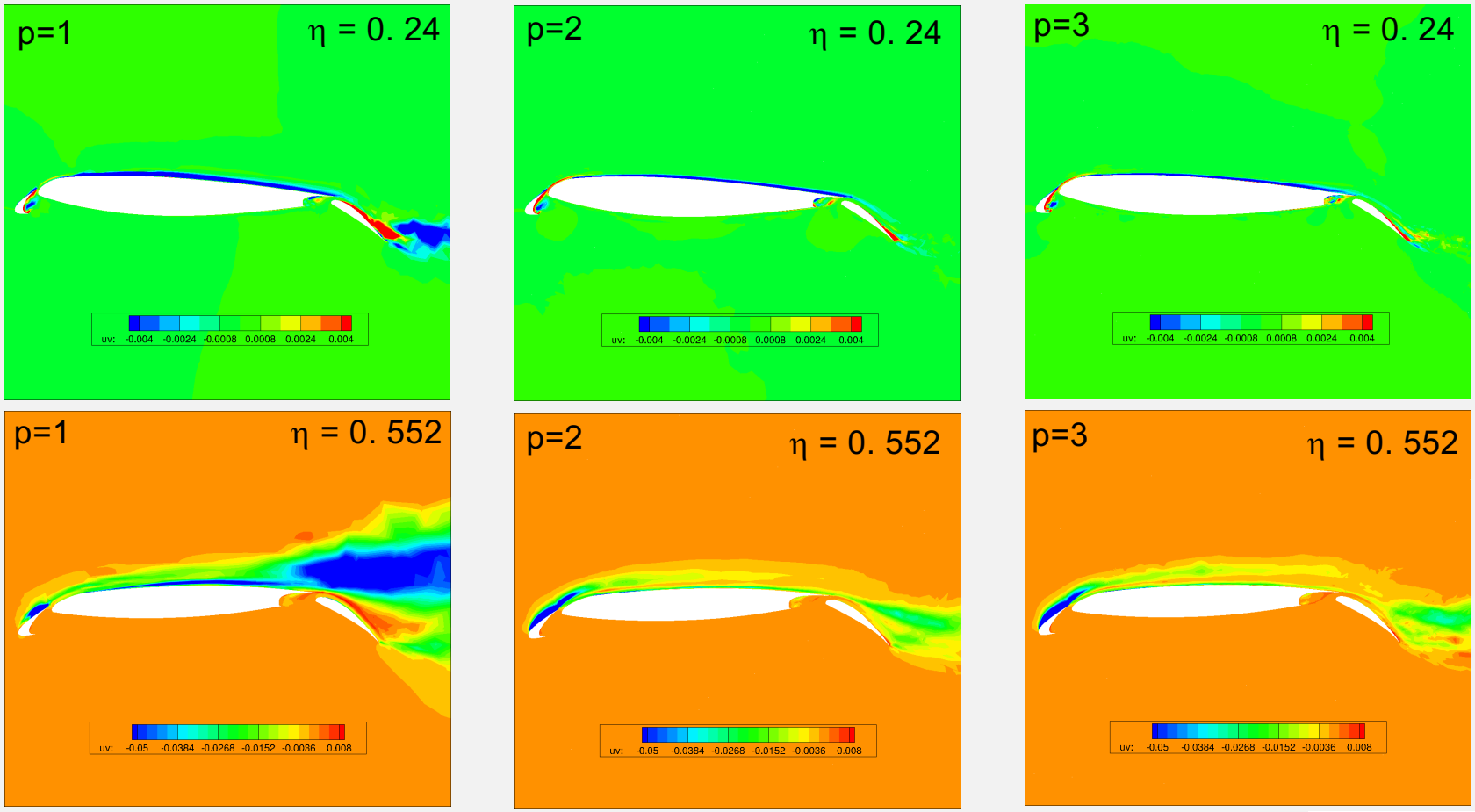
Comparison of Power Spectral Density





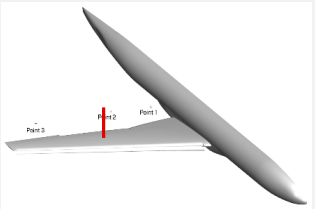
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Comparison of Reynolds Shear Stress

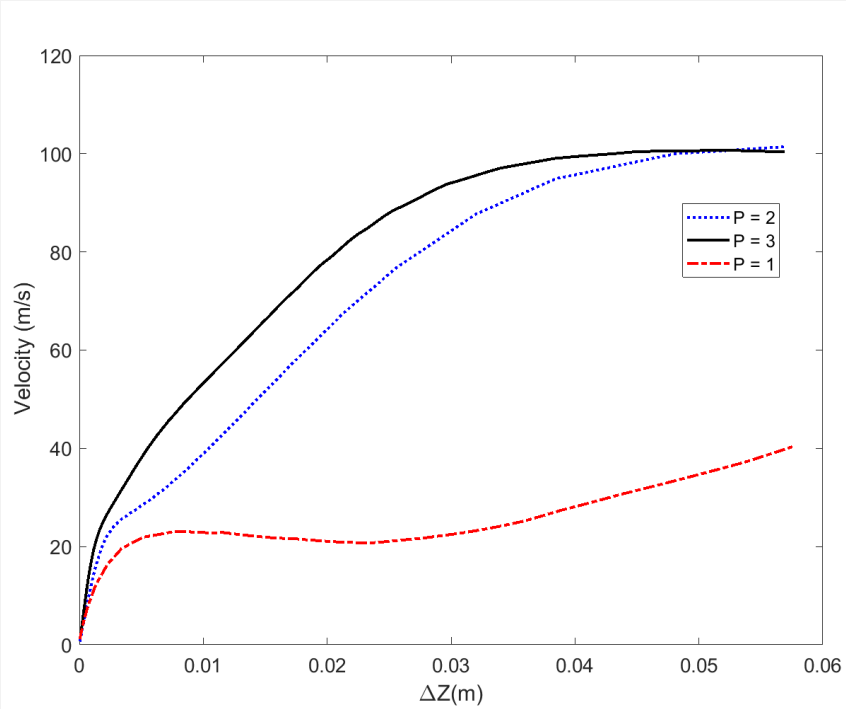


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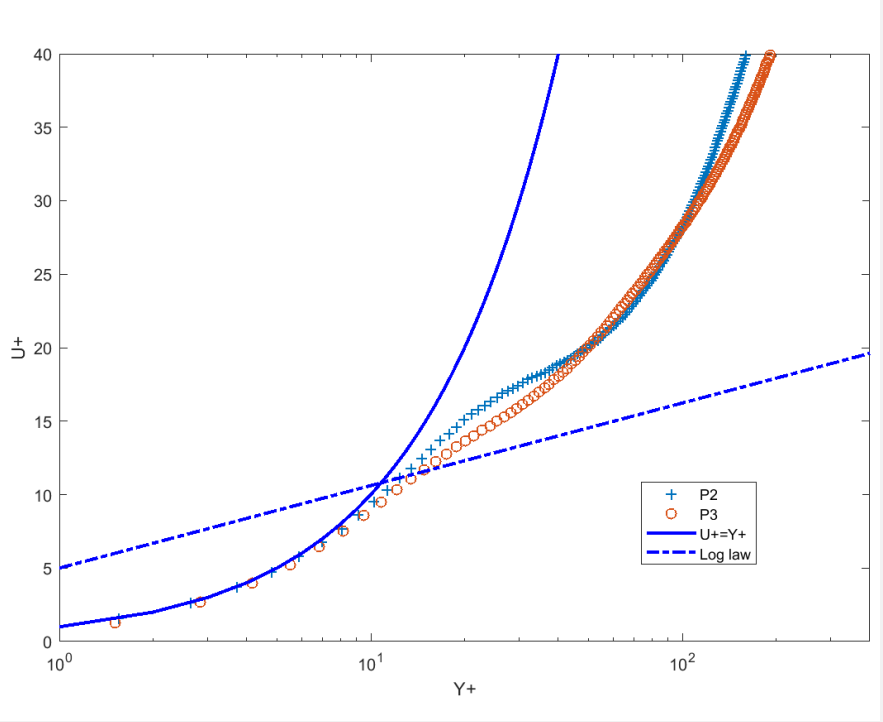
Boundary Layer Velocity Profiles (Suction Side)



At ½ chord point of span location η = 0. 552



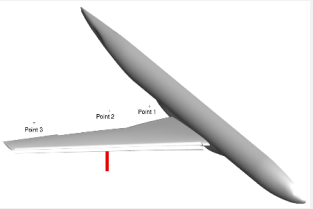
Dimensional



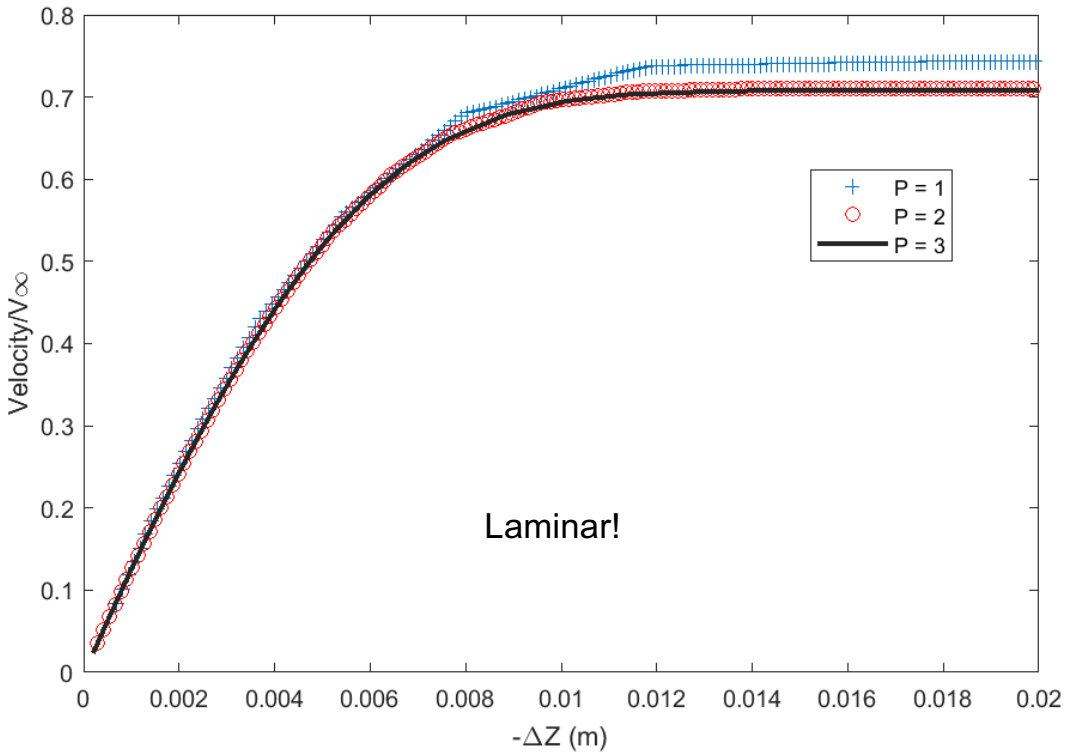
Non-dimensional

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Boundary Layer Velocity Profiles (Pressure Side)

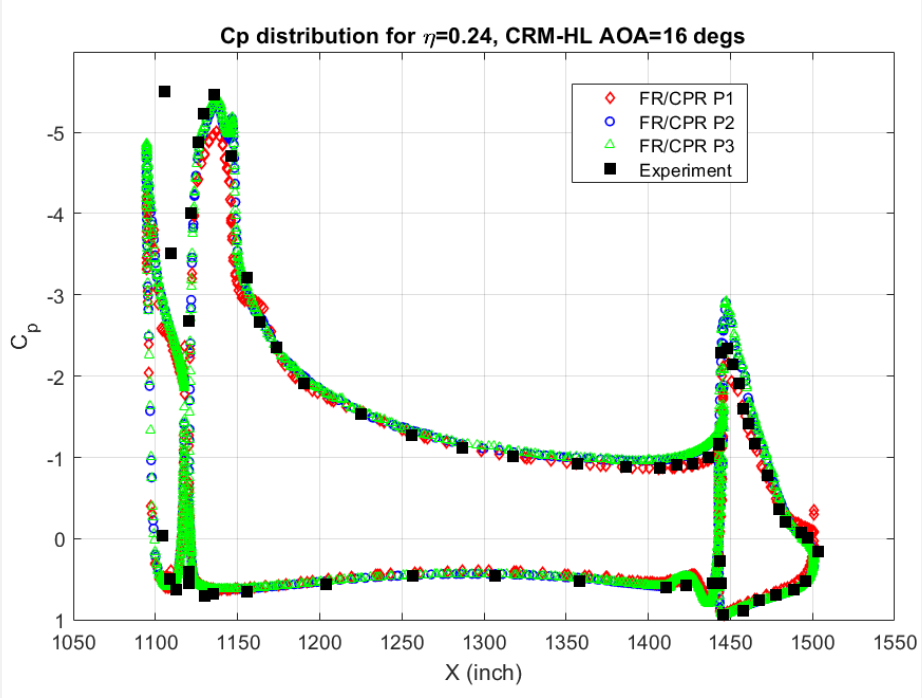


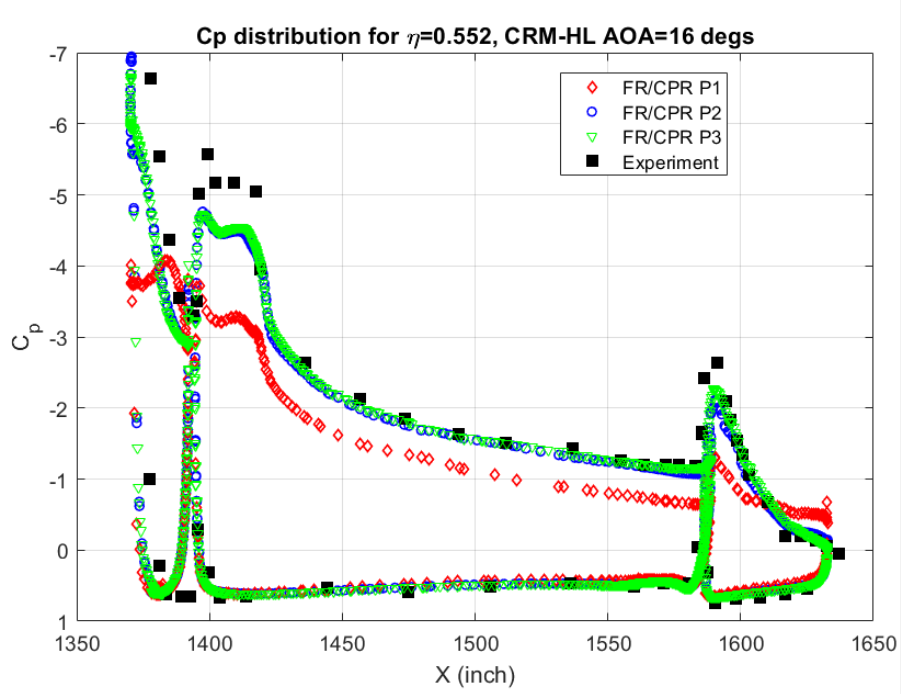
At ½ chord point of span location η = 0. 552



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Cp Comparisons at Two Spanwise Locations





Lin J.C., Melton L.P., Hannon J.A., Andino M.Y., Koklu M., Paschal K.B., and Vatsa V.N., "Wind Tunnel Testing of Active Flow Control on High-Lift Common Research Model," AIAA-2019-3723.

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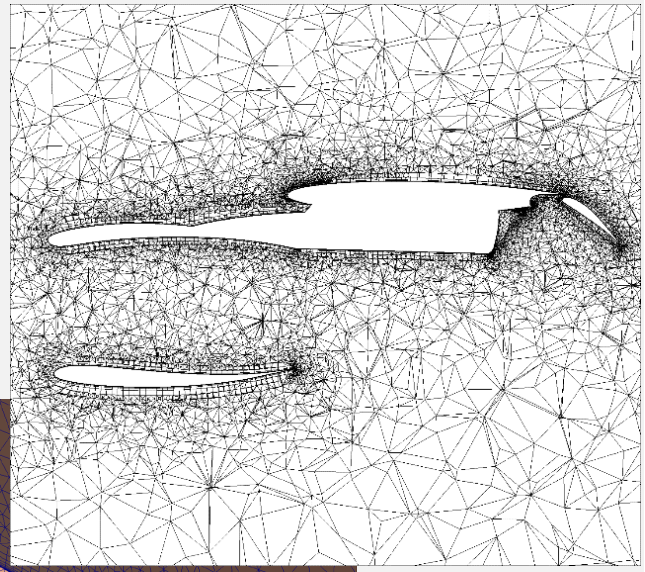
Force Comparison with Experiment (Blind Test)

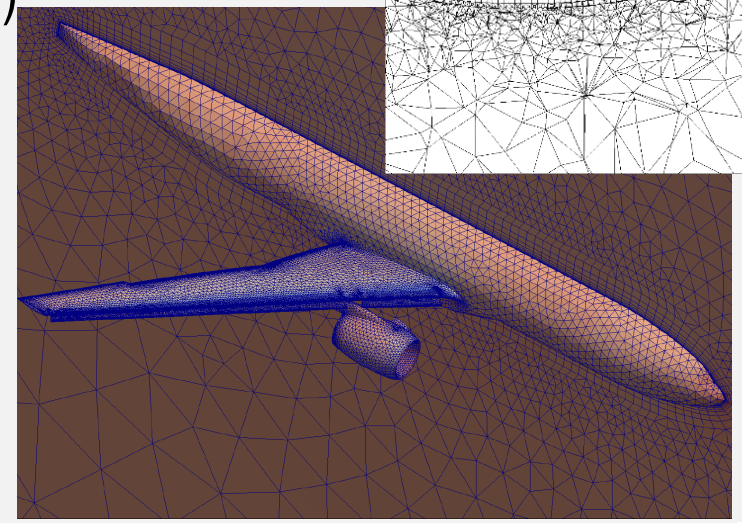
	C_L	C_D
P = 1	2.020	0.293
P = 2	2.411	0.282
P = 3	2.413	0.283
Experiment [1]	2.479	0.252
Experiment (wall-corrected) [2]	2.405	0.287

1. Lin, J. C., Melton, L. P., Hannon, J. A., Andino, M. Y., Koklu, M., Paschal, K. B., and Vatsa, V. N., "Wind Tunnel Testing of Active Flow Control on the High Lift Common Research Model," AIAA AVIATION 2019 Forum, AIAA Paper 2019-3723, 2019. doi: 10.2514/6.2019-3723
2. Lin J.C., Melton L.P., Hannon J.A., Andino M.Y., Koklu M., Paschal K.B., and Vatsa V.N., "Testing of High-Lift Common Research Model with Integrated Active Flow Control," AIAA J. of Aircraft, Volume 57, Number 6, November 2020. https://doi.org/10.2514/1.C035906.

Wall-Modeled ILES of CRM-HL Configuration (4th AIAA Workshop)

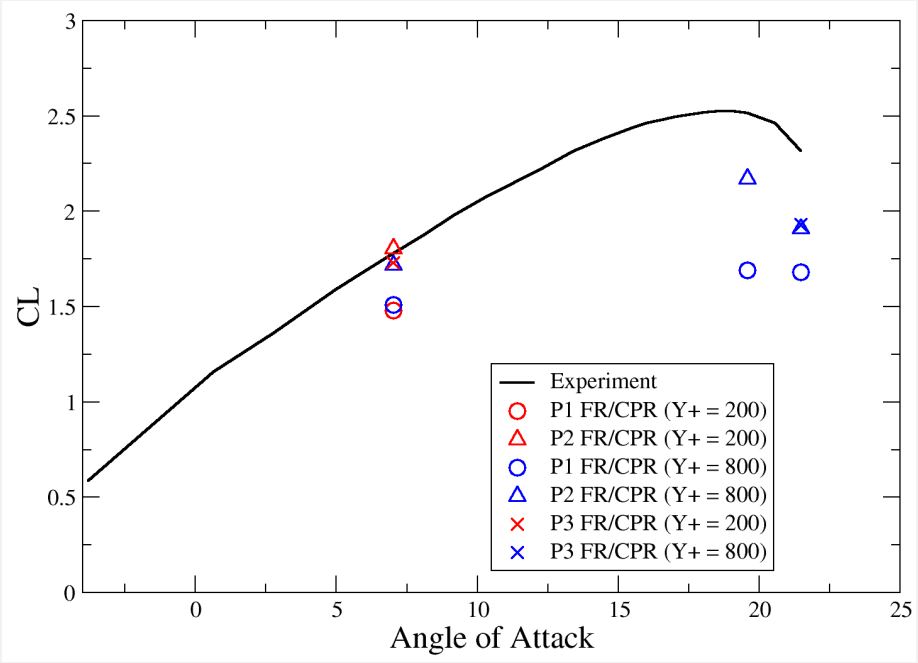
- Mach = 0.2
- Re = 5.49E6 based on MAC
- AOA = 7.01 & 21.47 degrees
- Mesh: ~1.3M Q2 coarse mixed elements, generated by Dr. Karman (Pointwise)
  - ~ 6.5 M DOFs/equ at p = 1
  - ~18 M DOFs/equ at p = 2
  - ~ 39 M DOFs/equ at p = 3
  - Y+ ~ 200 & 800 near the wall (5.4 & 21.5 mm)
  - Equilibrium wall-model used

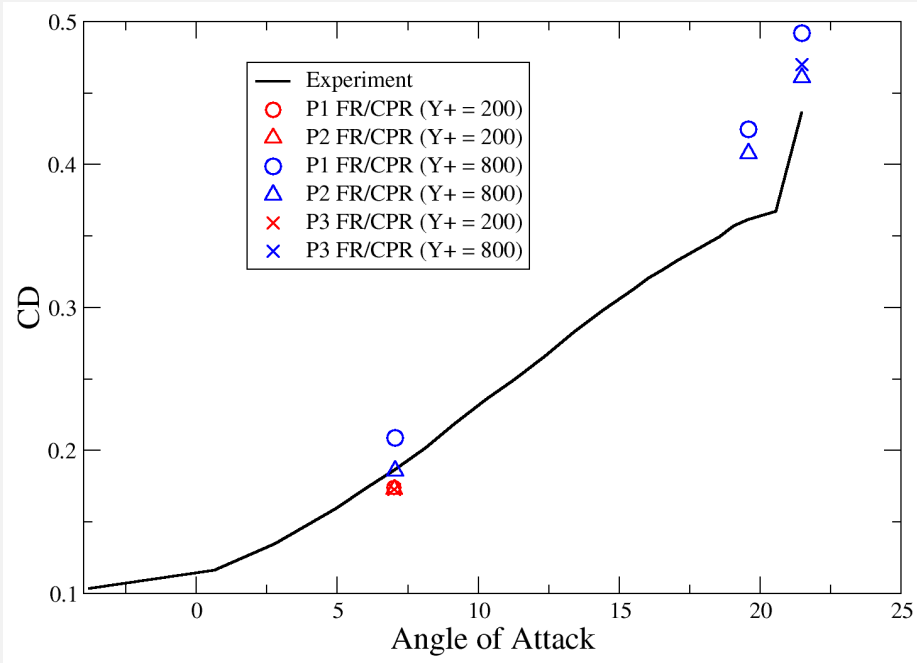




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Comparison with Experimental Data

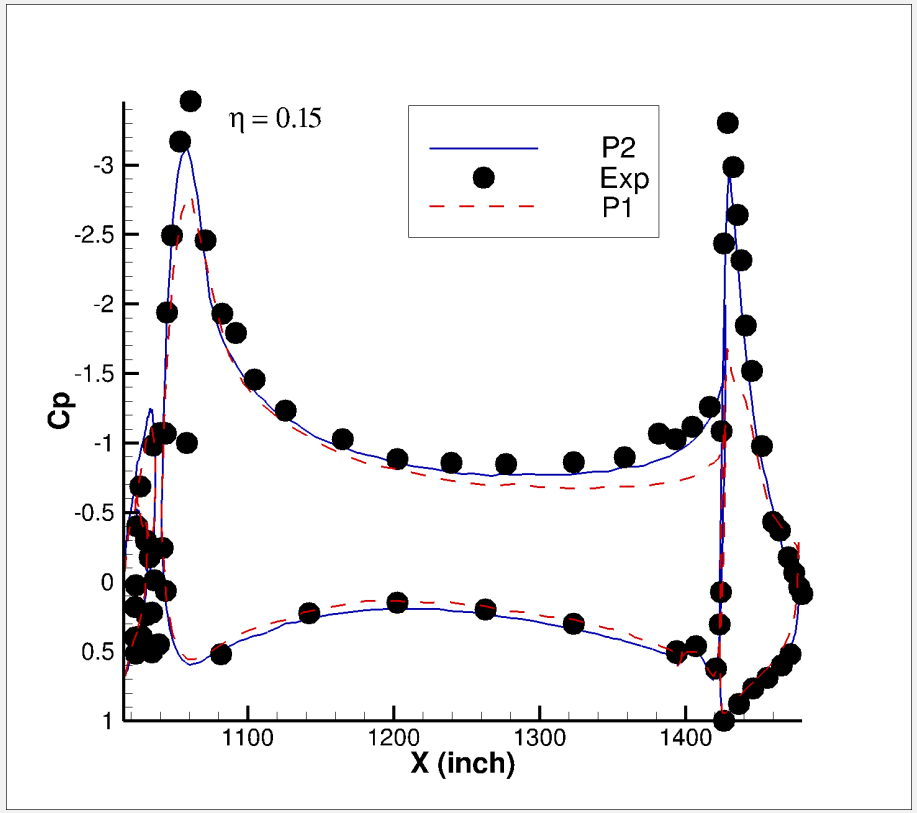


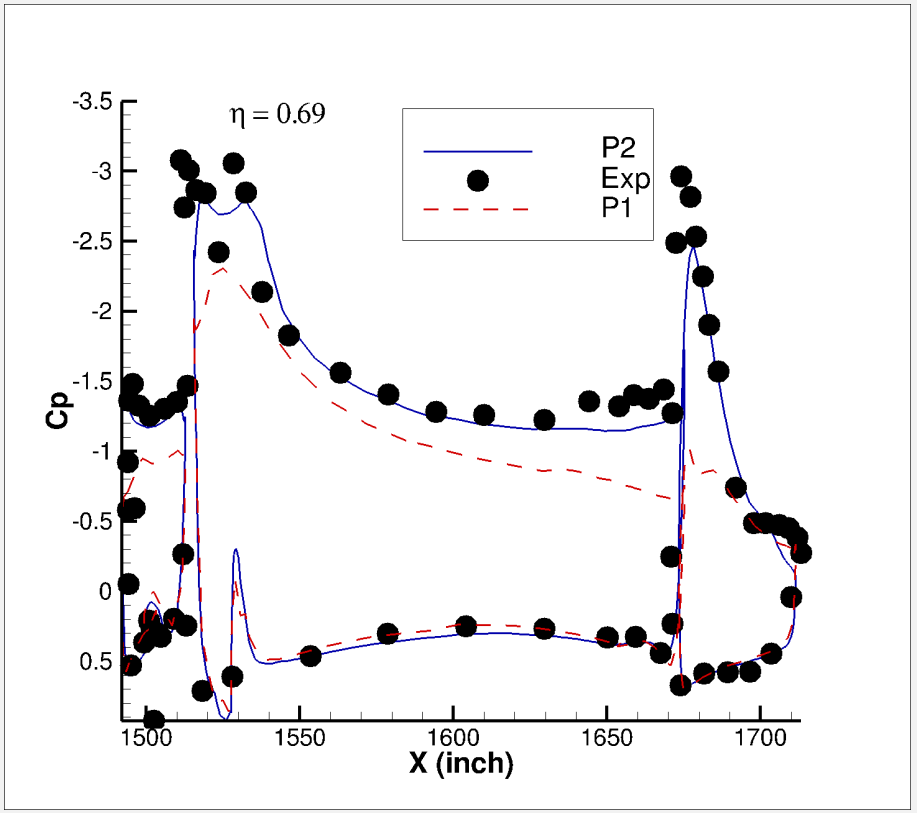


Disagreement at high AOA
- Lack of resolution? Equilibrium wall model? Wind tunnel wall?

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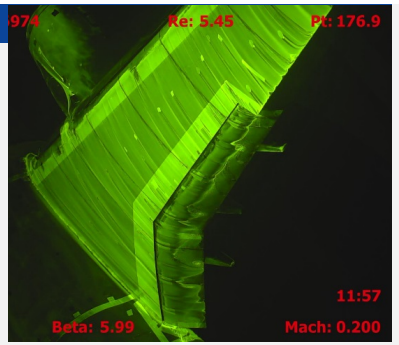
Comparison with Experiment (AOA – 7.01º)



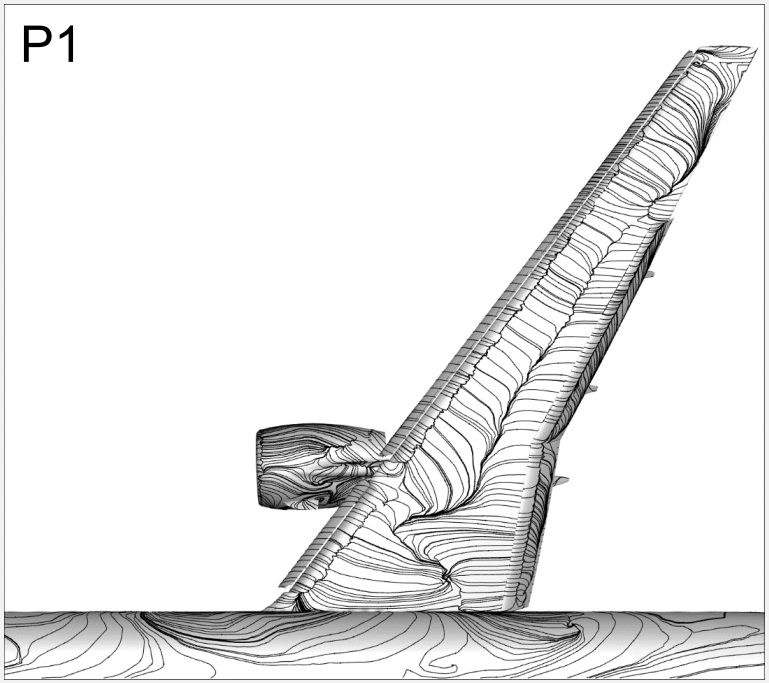


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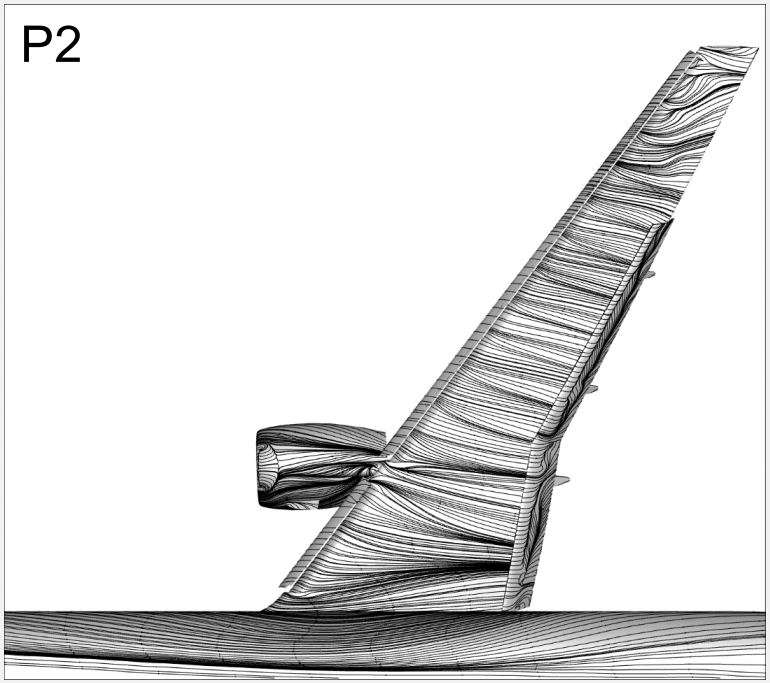
Oil Flows (AOA – 7.01º) (V1)



P1

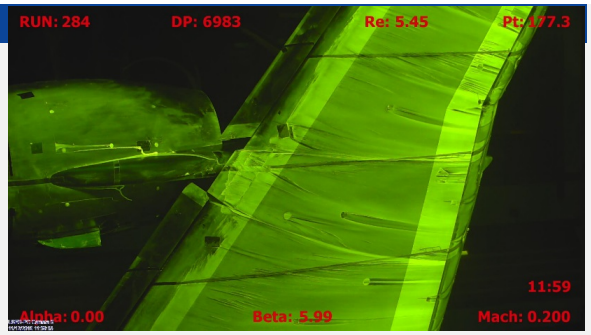


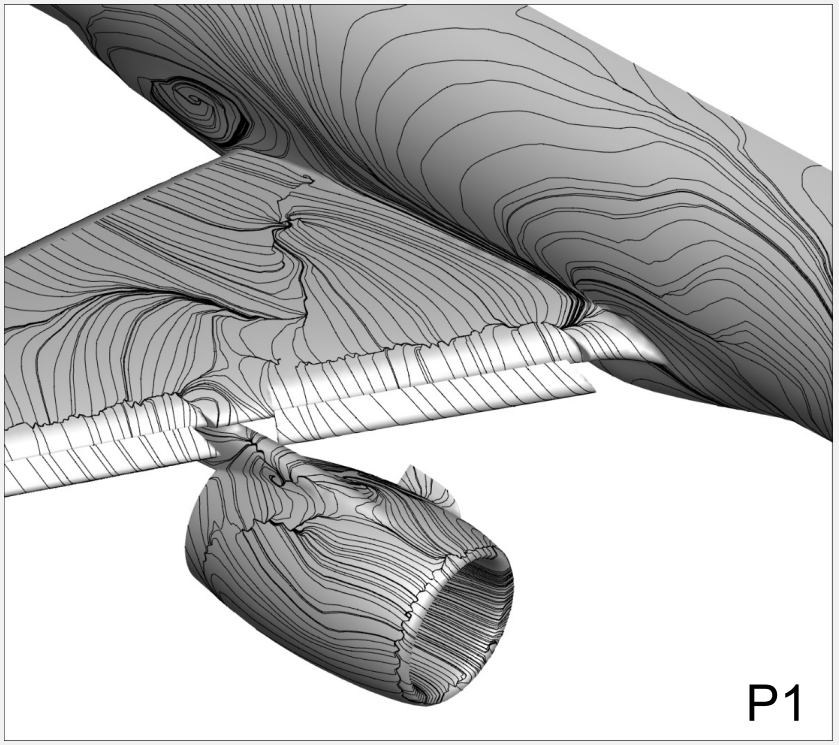
P2

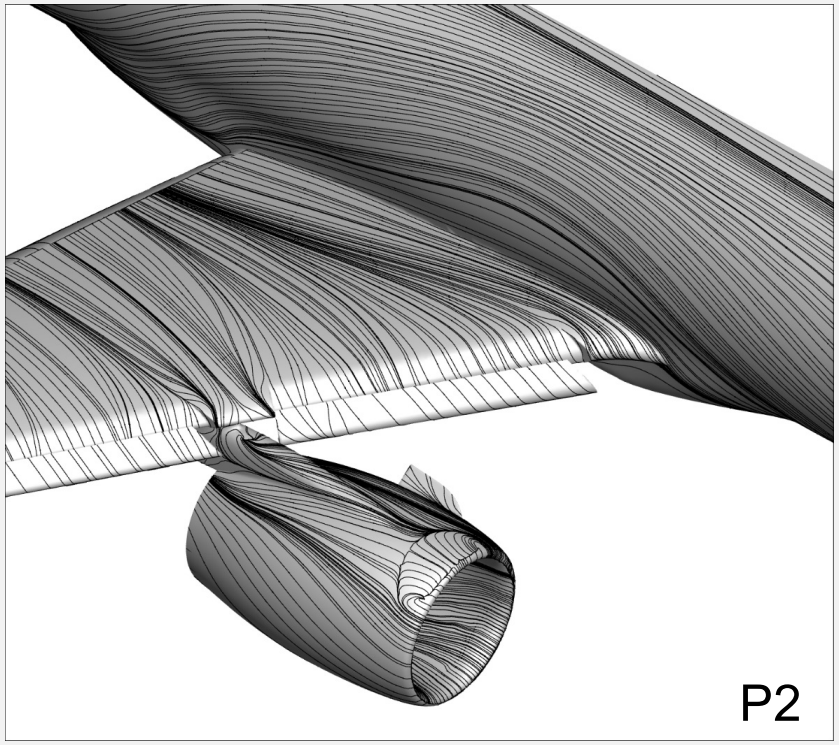


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Oil Flows (AOA – 7.01º) (V5)

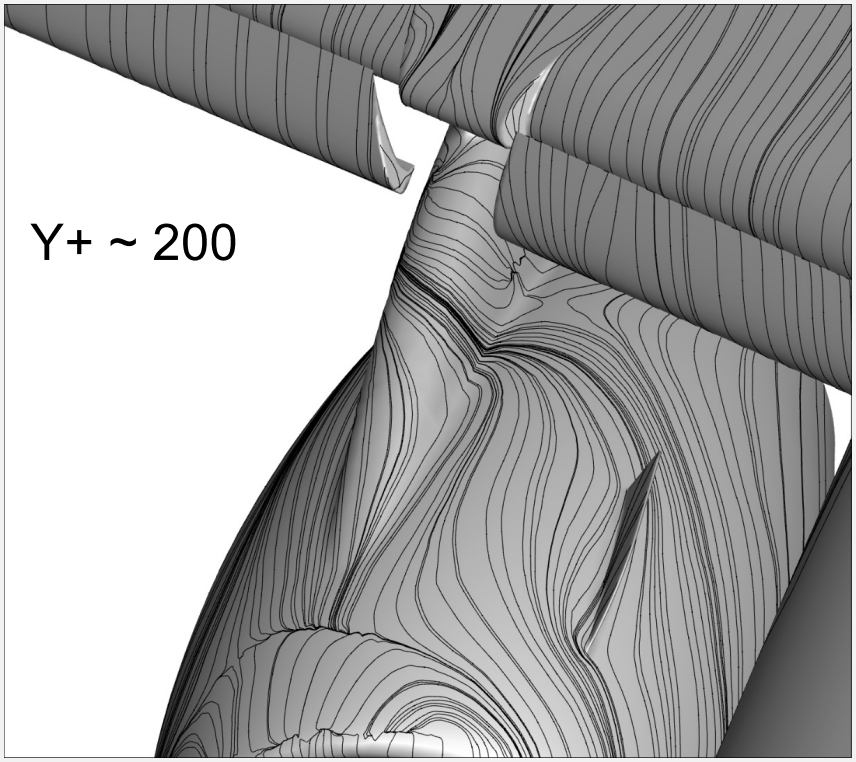


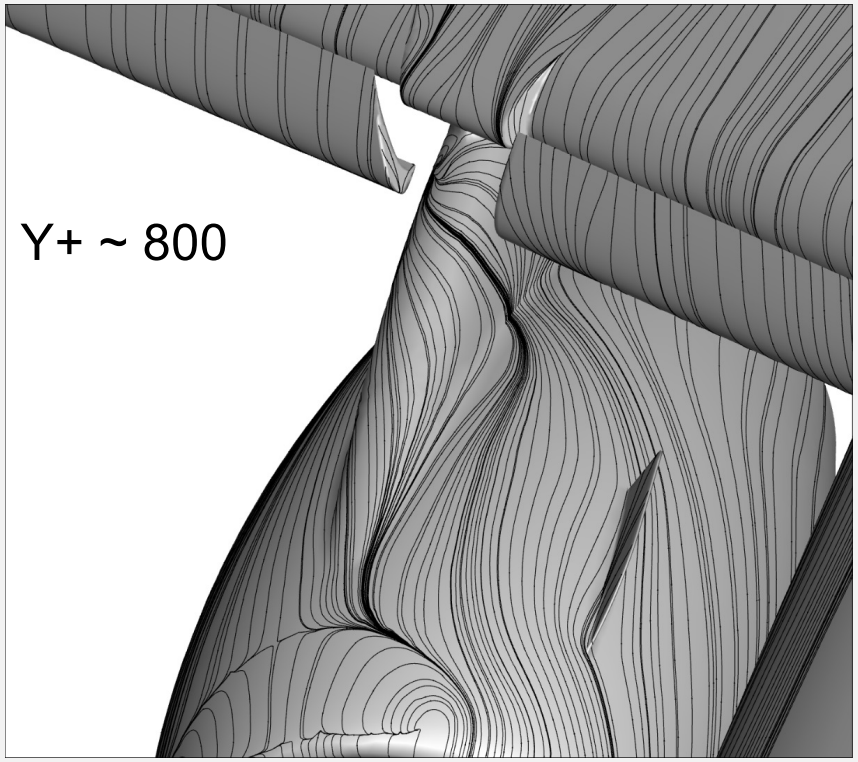




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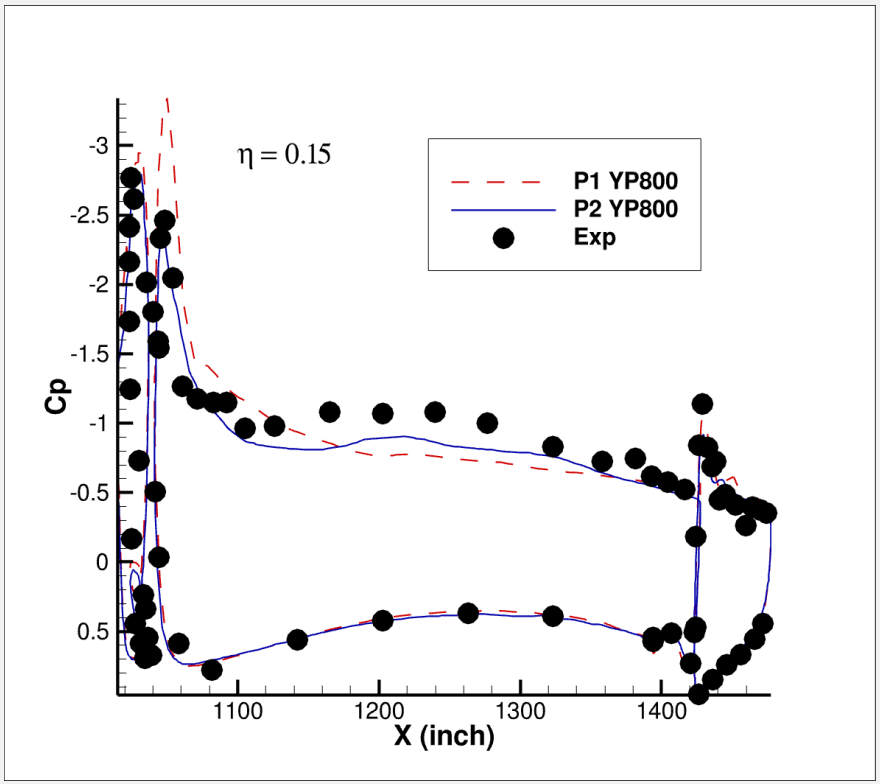
Oil Flows (AOA – 7.01º) P2 (V9)

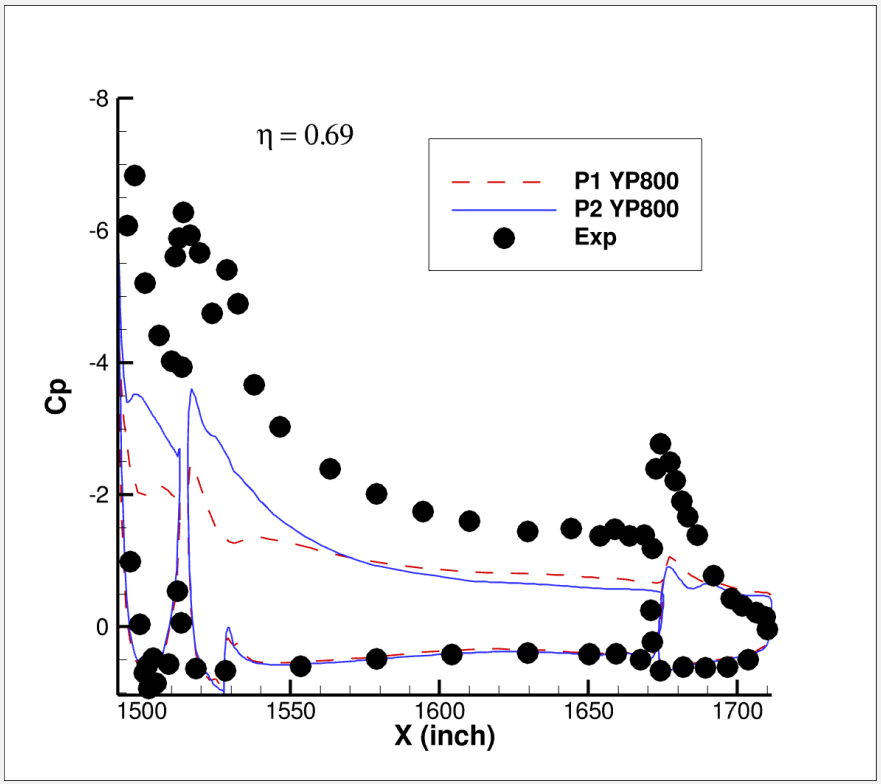




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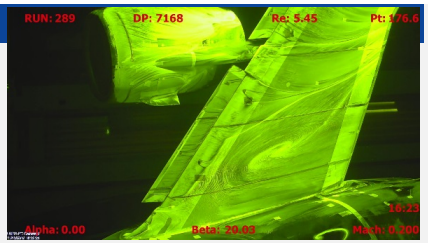
Cp Comparison with Experiment (AOA – 21.47º)



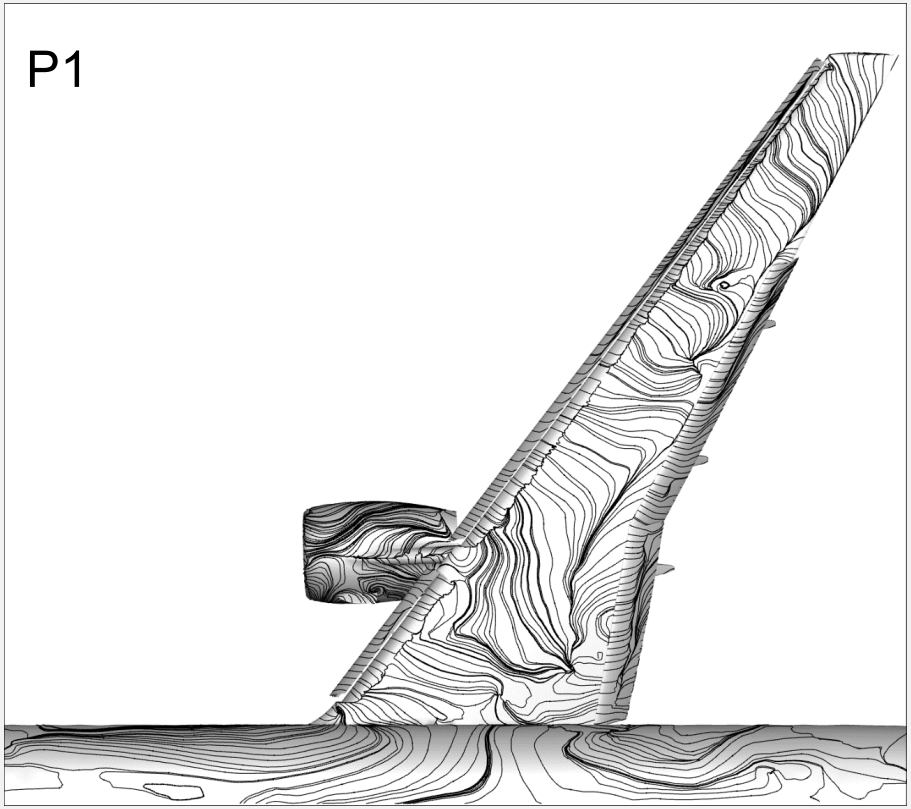


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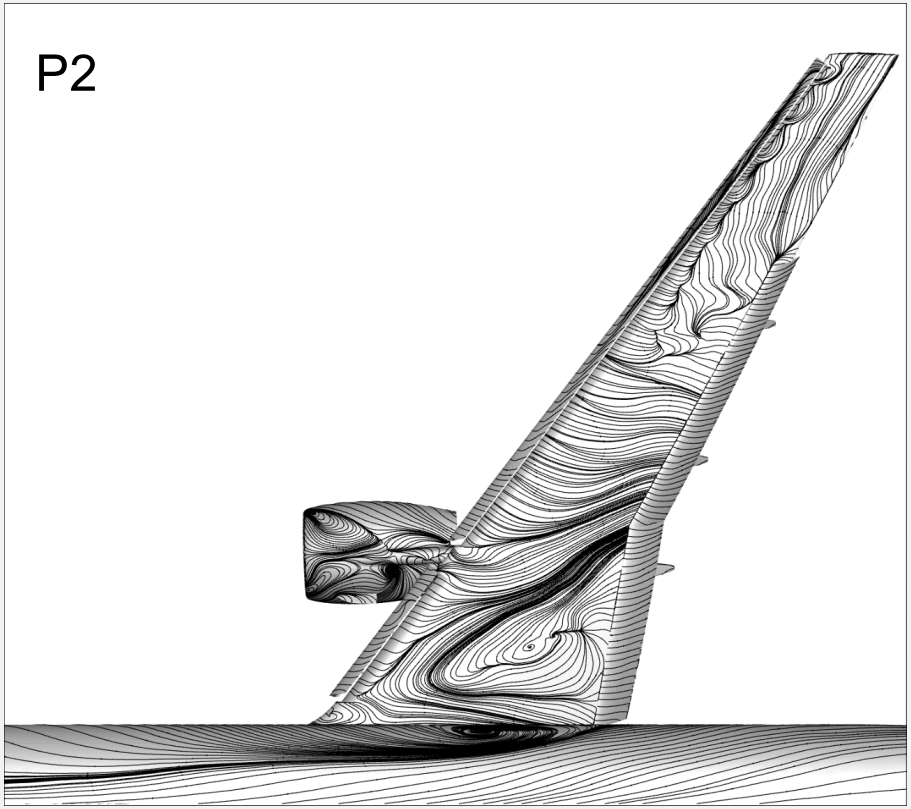
Oil Flows (AOA – 21.47°) (V1)



P1

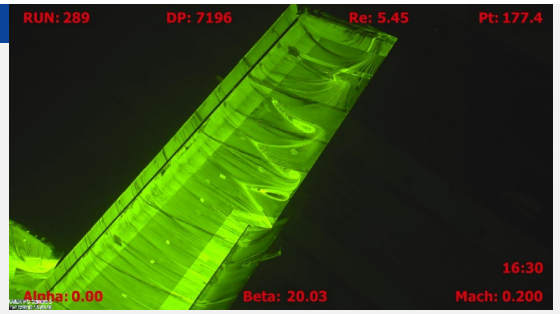


P2

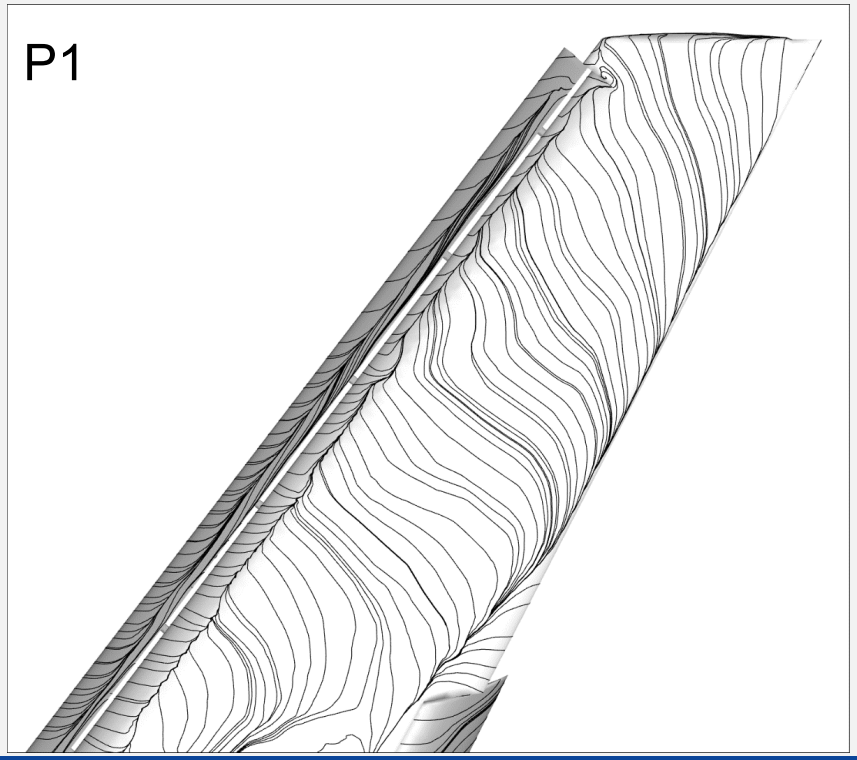


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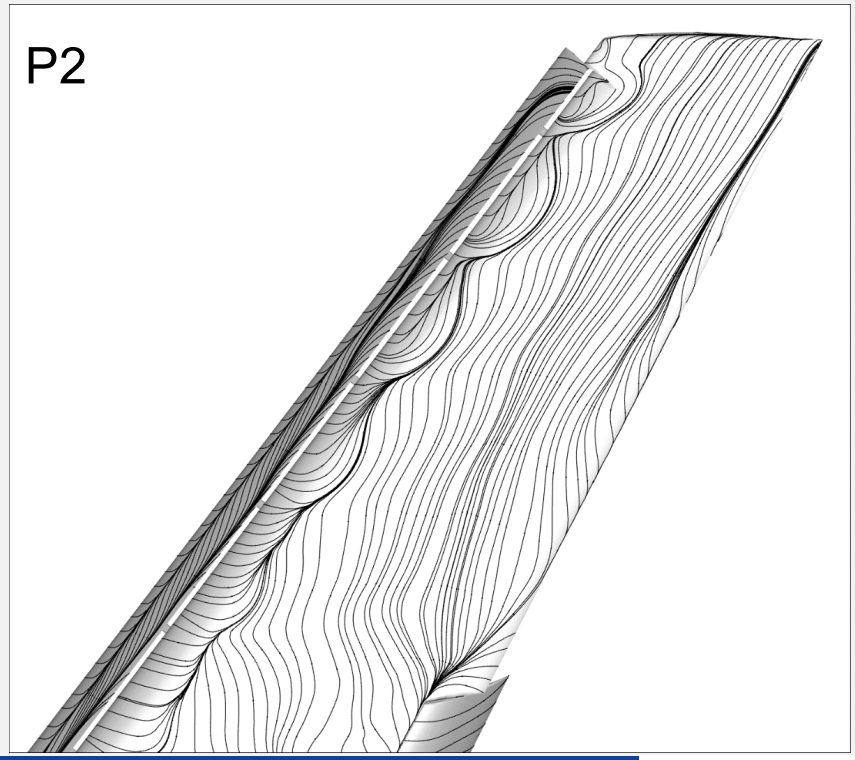
Oil Flows (AOA – 21.47°) (V4)



P1

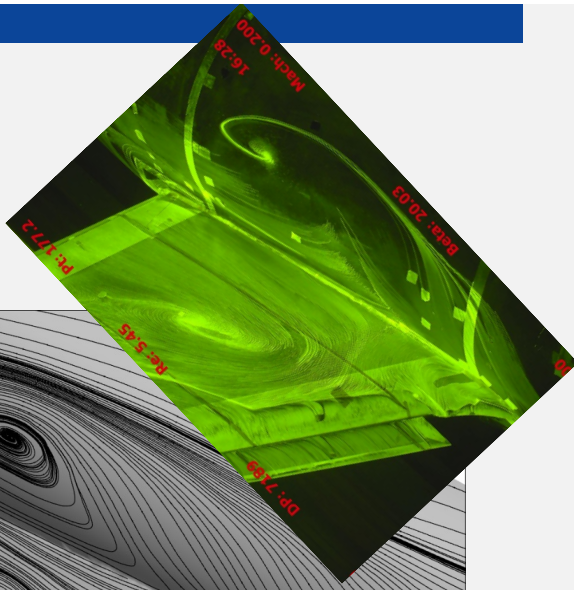


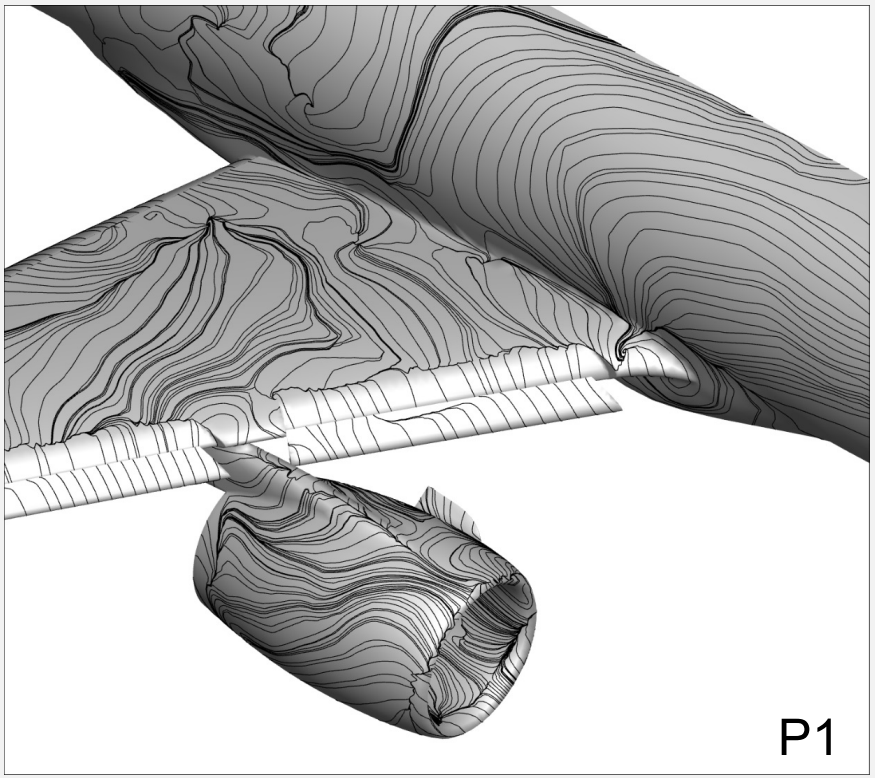
P2

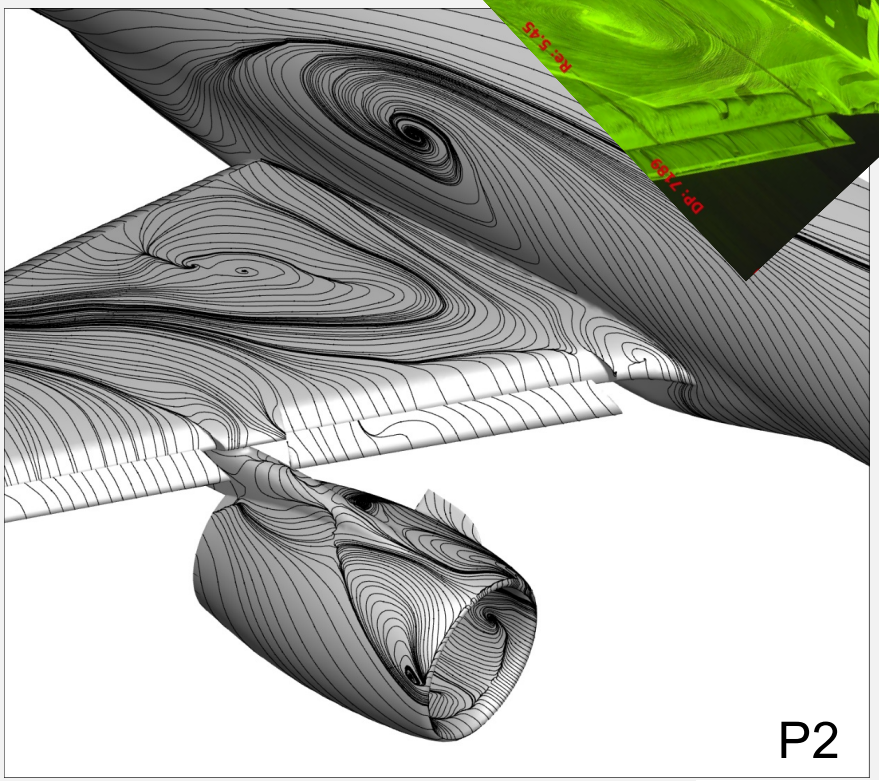


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Oil Flows (AOA – 21.47°) (V5)







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Summary and Outlook

- Progress in the last 6 years (high-order mesh generation, low memory implicit schemes) has enabled high-order LES being used more in industry especially in turbomachinery
- GPU implementation on the recent V100/A100 cards has made overnight LES turnaround possible on small GPU clusters (~100 V100 GPUs)
  - ~50-100M DOFs running p2 (~ 950M – 1.9B DOFs for 2nd order codes)
- Future work
  - Mesh adaptation for LES
  - Non-equilibrium wall-models,
  - More efficient low memory time integration schemes
  - Multi-physics, …

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- HpMusic is a KU-protected software, and is available for use by US government, academia and industry (If interested, please contact me zjw@ku.edu).

