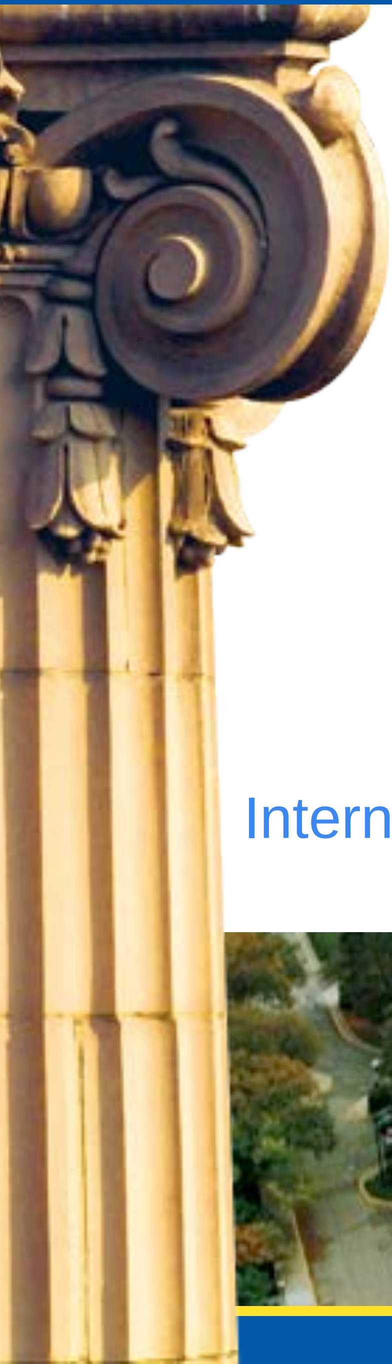

Towards Large Eddy Simulation for Turbo-machinery Flows

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Presented at
International Conference on Flow Physics and Its Simulations
In Memory of Prof. Jaw-Yen Yang

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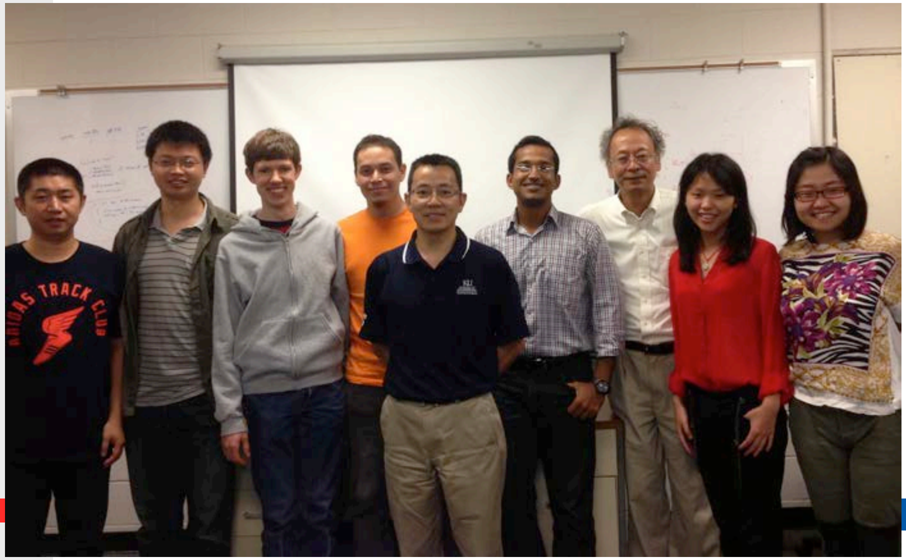
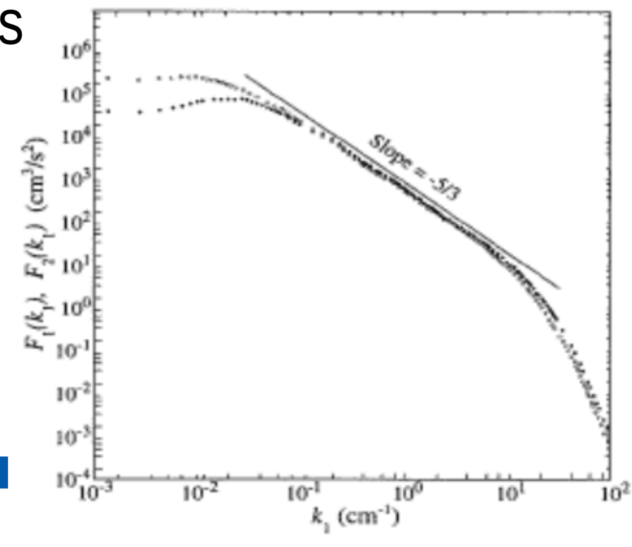


Outline

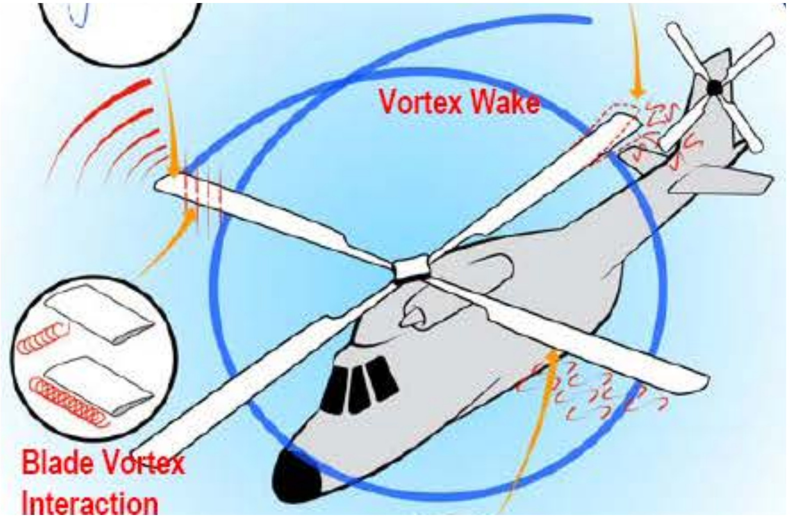
- Introduction to large eddy simulations (LES)
- Key pacing items enabling LES with high-order adaptive methods
  - High-order methods
  - High-order mesh generation
  - SGS models
- Sample demonstrations
- Conclusions

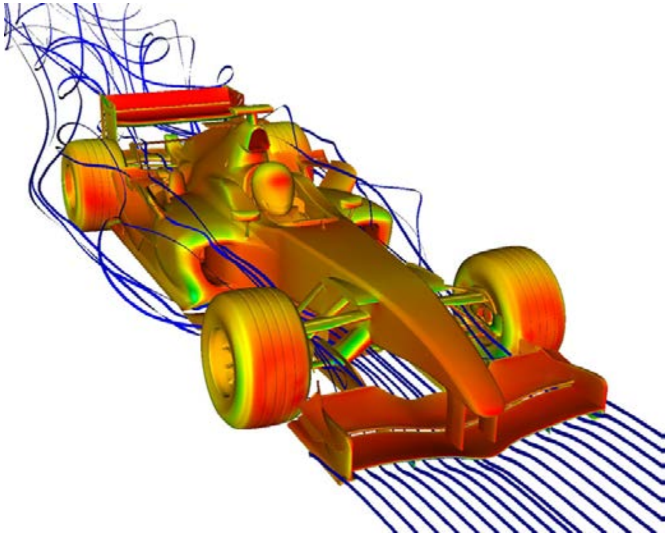
Introduction

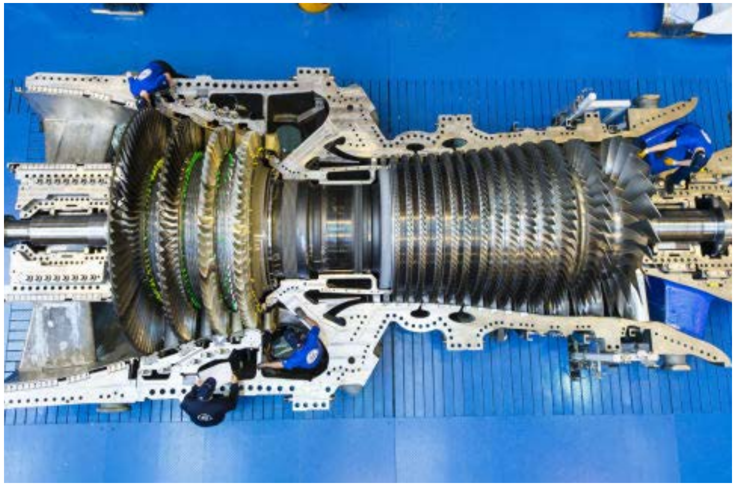
- Approaches to compute turbulent flows
  - RANS: model all scales
  - LES: resolve large scales while modeling small scales
  - DNS: resolve all scales
- What is LES
  - Partition all scales into large scales and small sub-grid scales with a low pass filter with width Δ
  - Solve the filtered Navier-Stokes equations with a SGS closure model
  - A compromise between RANS and DNS

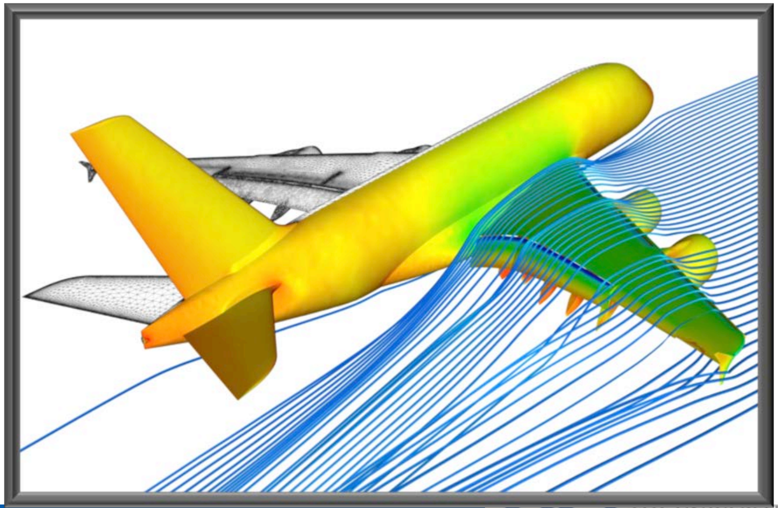


RANS Inadequate for Many Applications



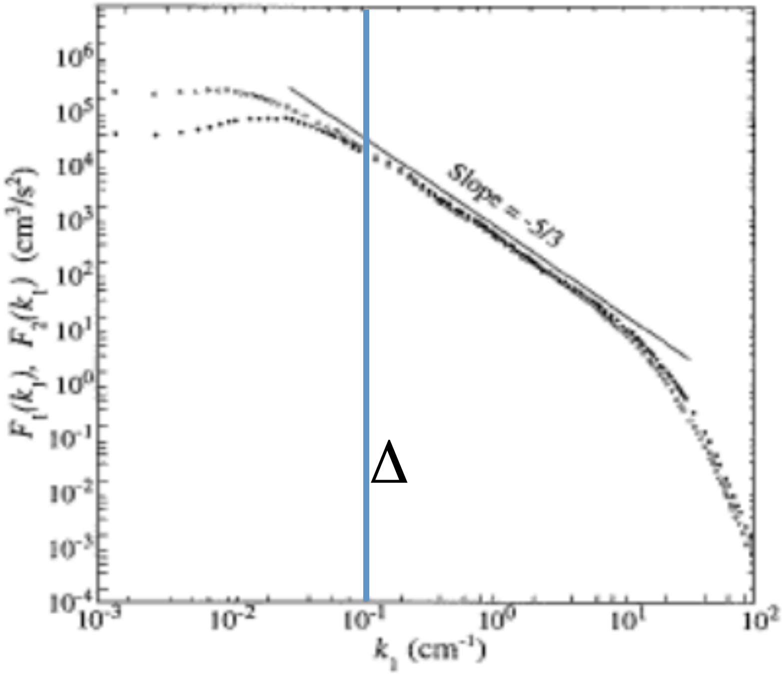






LES – the Challenges

- How to choose the filter width Δ
- How to resolve the disparate length and time scales in the turbulent flow field
- How to handle complex geometries
- How to resolve very small turbulence scales in the boundary layer
- Discontinuity capturing
- Parallel performance on extreme scale computers
- Post-processing and visualization of large data sets



Key Pacing Items in LES

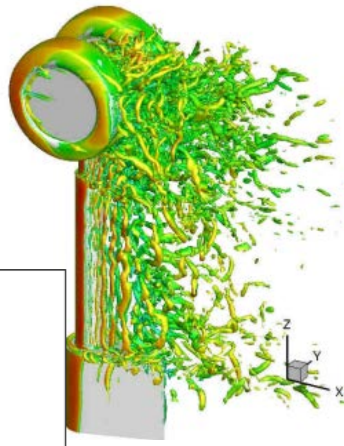
- High-order methods capable of handling unstructured meshes to deal with complex geometry
- High-order meshes resolving the geometry and viscous boundary layers
  - Coarse meshes (because internal degrees of freedom are added)
- Quality of SGS models
- Wall models to decrease the number of cells in the boundary layer

High order methods

High-Order CFD Methods Needed

- All of the challenges demand more accurate, efficient and scalable design tools in CFD
  - Better engine simulation tools
  - Better design tools for high-lift configurations

$$Error \propto h^{p>2}$$



2nd order

4th order

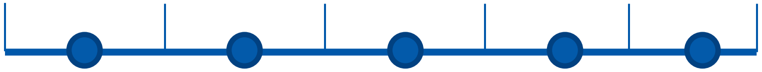
Popular High-Order Methods

- Compact difference method
- Optimized difference method
- ENO/WENO methods
- MUSCL, PPM and K-exact FV
- Residual distribution methods
- Discontinuous Galerkin (DG)
- Spectral volume (SV)/spectral difference (SD)
- Flux reconstruction/Correction procedure via reconstruction
- …

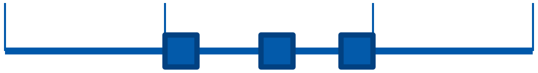
■ Structured grid ■ Unstructured grid

How to Achieve High-Order Accuracy

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



- Add more internal degrees of freedom
  - Finite element/spectral element, discontinuous Galerkin
  - Spectral volume (SV)/spectral difference (SD), flux reconstruction (FR) or correction procedure via reconstruction (CPR), …
- Hybrid approaches
  - PnPm, rDG, hybrid DG/FV, …



Extending Stencil vs. More Internal DOFs

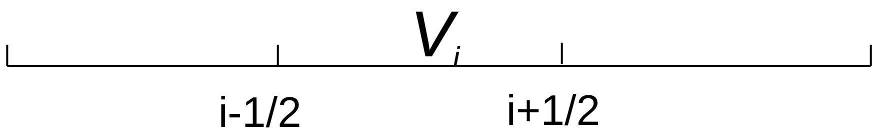
- Simple formulation and easy to understand for structured mesh
- Complicated boundary conditions: high-order one-sided difference on uniform grids may be unstable
- Not compact

- Boundary conditions trivial with uniform accuracy
- Non-uniform and unstructured grids
  - Reconstruction universal
- Scalable
  - Communication through immediate neighbor

Review of the Godunov FV Method

Consider

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



Integrate in V_i

$$\int_{V_i} \left(\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} \right) dx = \frac{\partial \overline{u}_i}{\partial t} \Delta x_i + \int_{i-1/2}^{i+1/2} \frac{\partial f}{\partial x} dx$$

$$= \frac{\partial \overline{u}_i}{\partial t} \Delta x_i + (f_{i+1/2} - f_{i-1/2}) = 0$$

FR/CPR

- Developed by Huynh in 2007 and extended to simplex by Wang & Gao in 2009, …
- It is a differential formulation like "finite difference"

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

- The DOFs are solutions at a set of "solution points"

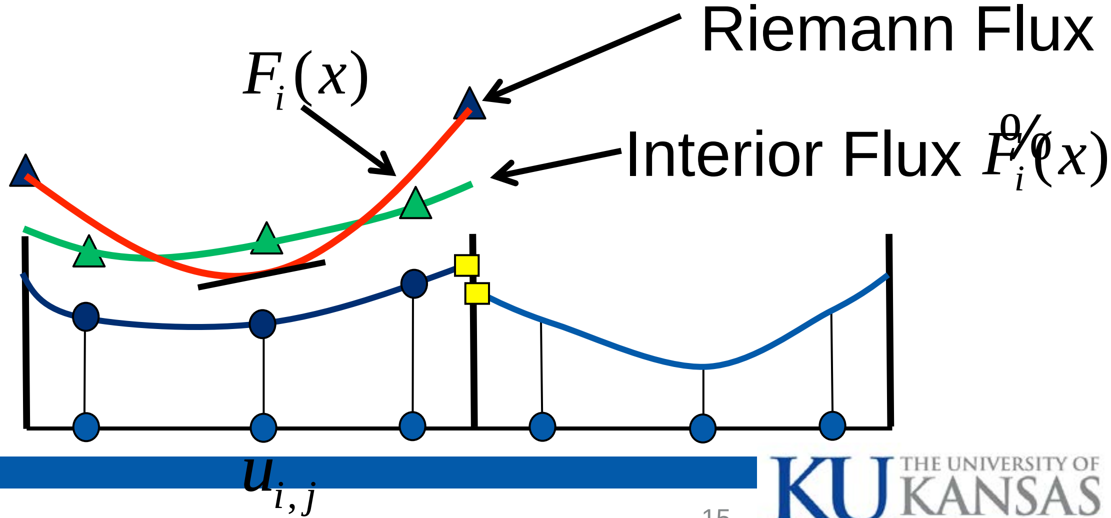
CPR (cont.)

- 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

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



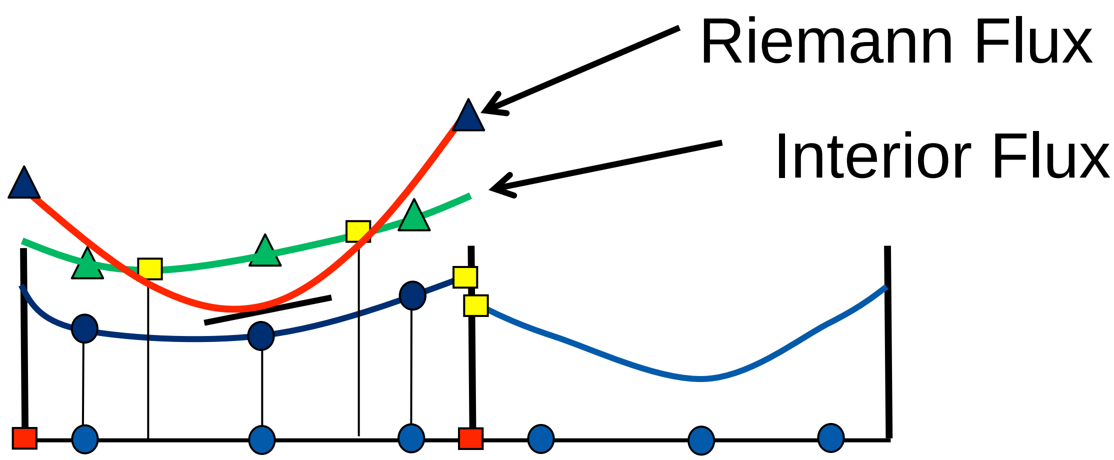
CPR – DG

- If the following equations are satisfied

$$\int_{V_i}\left[\tilde{F}_i(x)-F_i(x)\right]dx=0$$

$$\int_{V_i}\left[\tilde{F}_i(x)-F_i(x)\right]x\,dx=0$$

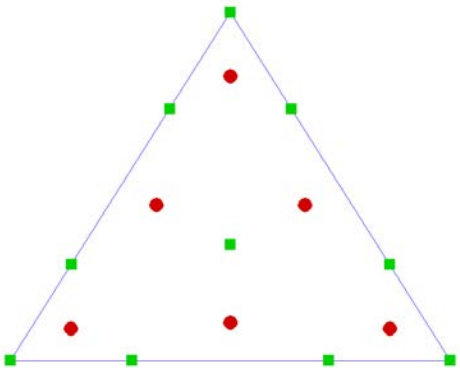
- The scheme is DG!



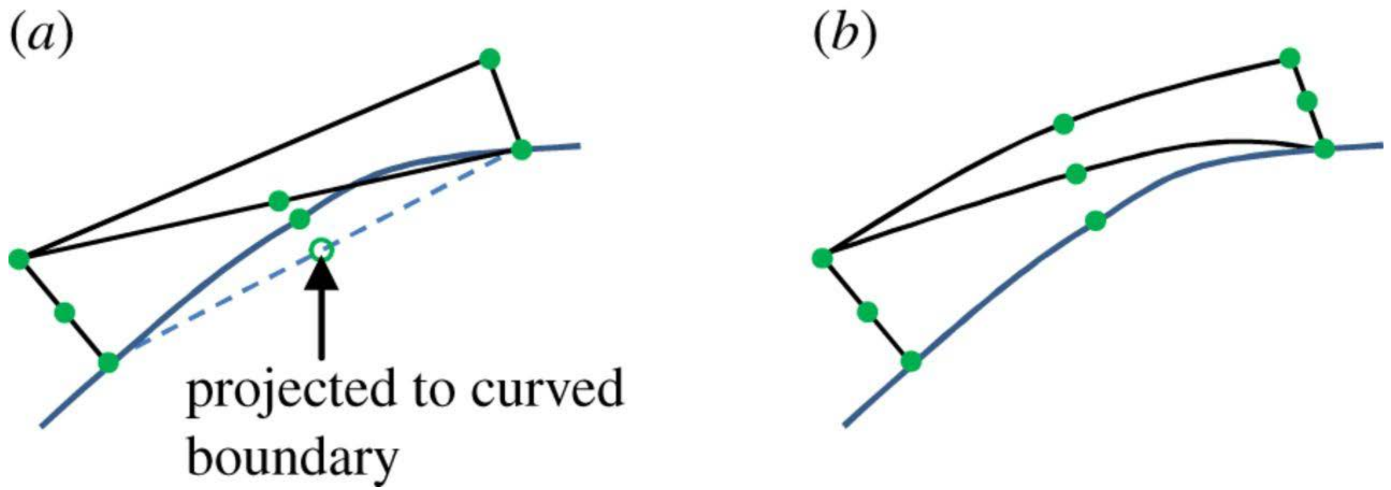
High order mesh generation

The Need for Coarse, High-Order Meshes

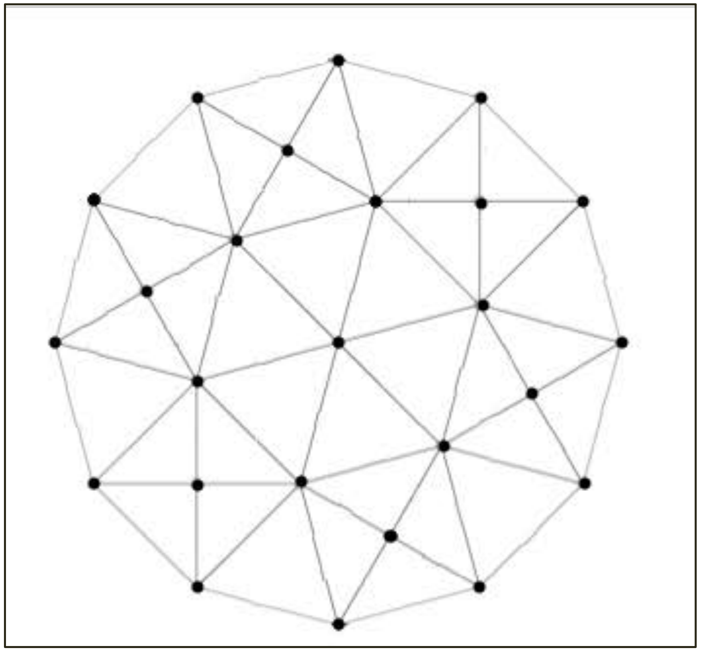
- Internal degrees of freedom are added such that meshes with ~100,000 elements may be sufficient to achieve engineering accuracy



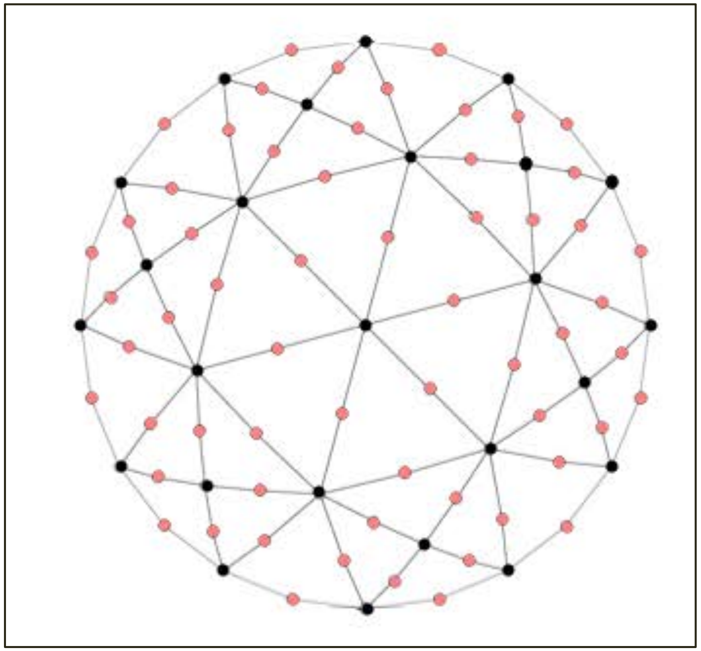
- If boundaries are still represented by linear facets, large errors are generated



Low versus High-Order Meshes:
An Example in 2D



low-order



high-order

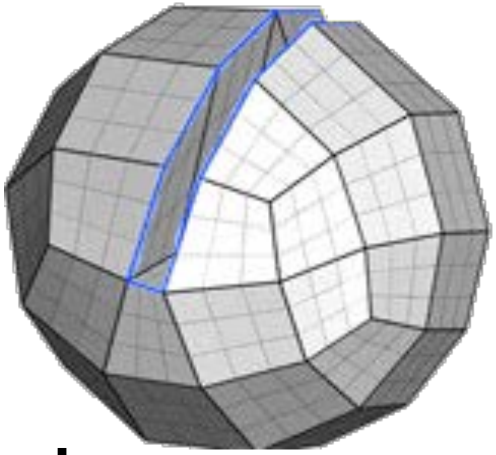
MESHCURVE

CAD Free, Low to High-Order Mesh Conversion

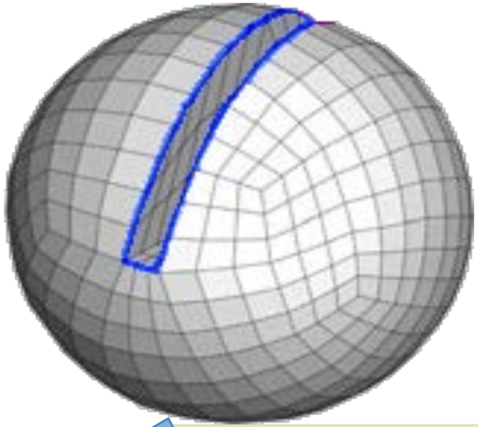
(released free of charge, just google meshCurve)

The Mission

For high-order CFD simulations, we need to



change this



to this

without smoothing away edges.

Main Features

- CGNS meshes : 3D, unstructured, multi-zone, multi-patch
- CAD-free operation
- Feature-curve preservation
- Easy-to-use, cross-platform graphical user interface interface
- Interactive 3D graphics
- Solid code base with minimal reliance on outside software libraries.
- Reasonably low memory footprint and fast operation on a desktop computer.
- Available for: Linux, MS Windows and Mac platforms

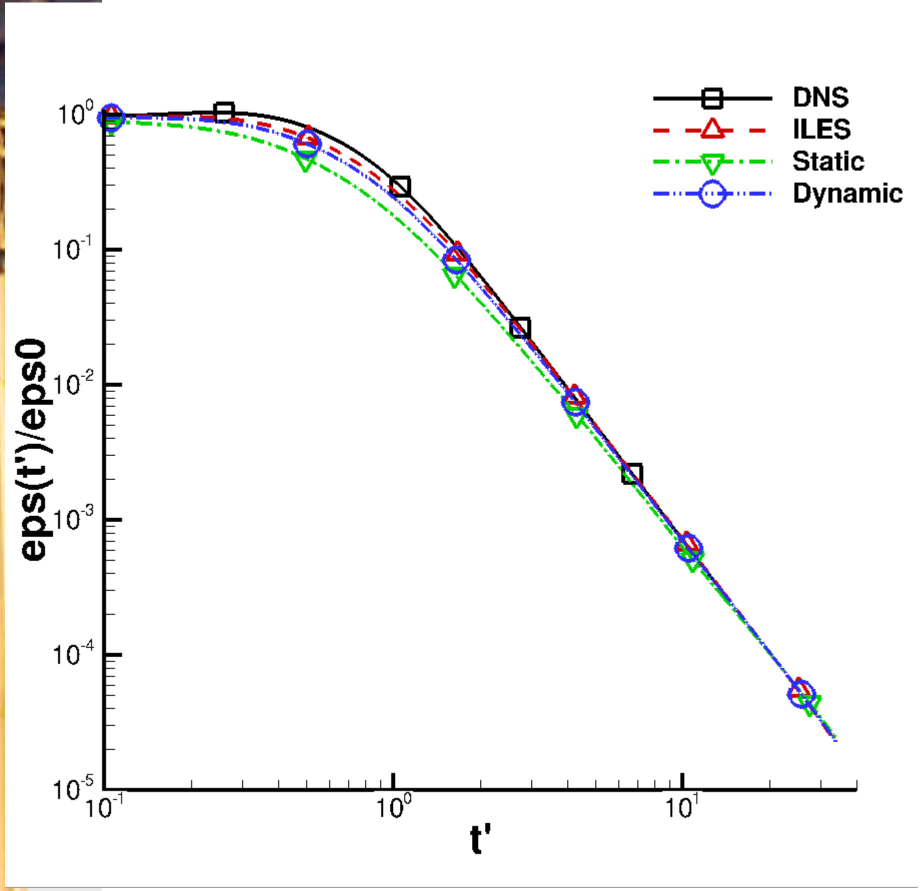
Demo Video

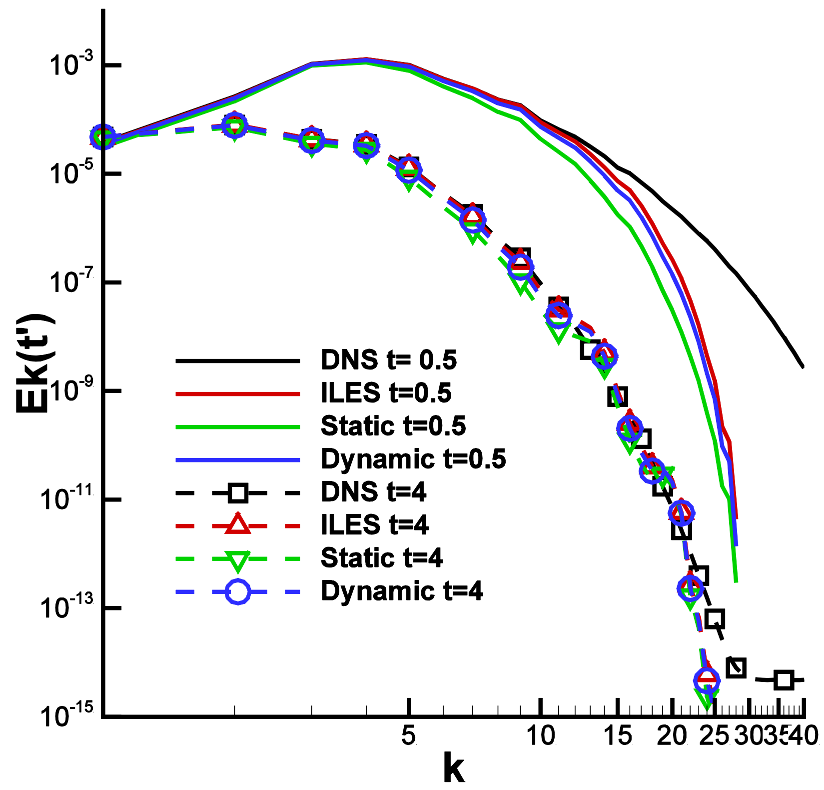
SGS Models with the Burgers' Equation

Our Venture into LES

- Solve the filtered LES equations using
  - FR/CPR scheme
  - 3 stage SSP Runge-Kutta scheme for time marching
- Implemented 3 SGS models
  - Static Smagorinsky (SS) model
  - Dynamic Smagorinsky (DS) model
  - ILES (no model)
- Attempted several benchmark problems
  - Flow over a Cylinder (ILES)
  - Isotropic turbulence decay (SS, DS, ILES)
  - Channel flow (SS, DS, ILES)

LES Results – Isotropic Turbulence Decay





Why ILES Performs Better Consistently

- No good explanation!
- So we decided to evaluate SGS models using the 1D Burgers' equation
  - High resolution DNS can be easily carried out
  - True stress can be computed based on DNS data
  - Both a priori and a posteriori studies can be performed
  - Yes, the physics of 1D Burger's equation is vastly simpler than the Navier-Stokes equations, but if a SGS model has any chance for 3D Navier-Stokes equations, it must perform well for the 1D Burger's equation

Filtered Burgers' Equation

1D Burgers' equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

Filter the equation with a box filter

$$\frac{\partial \hat{u}}{\partial t} + \hat{u}\frac{\partial \hat{u}}{\partial x} = \nu\frac{\partial^2 \hat{u}}{\partial x^2} - \frac{\partial \tau}{\partial x}.$$

where

$$\boldsymbol{\tau} = \frac{1}{2}\widehat{uu} - \frac{1}{2}\hat{u}\hat{u}.$$

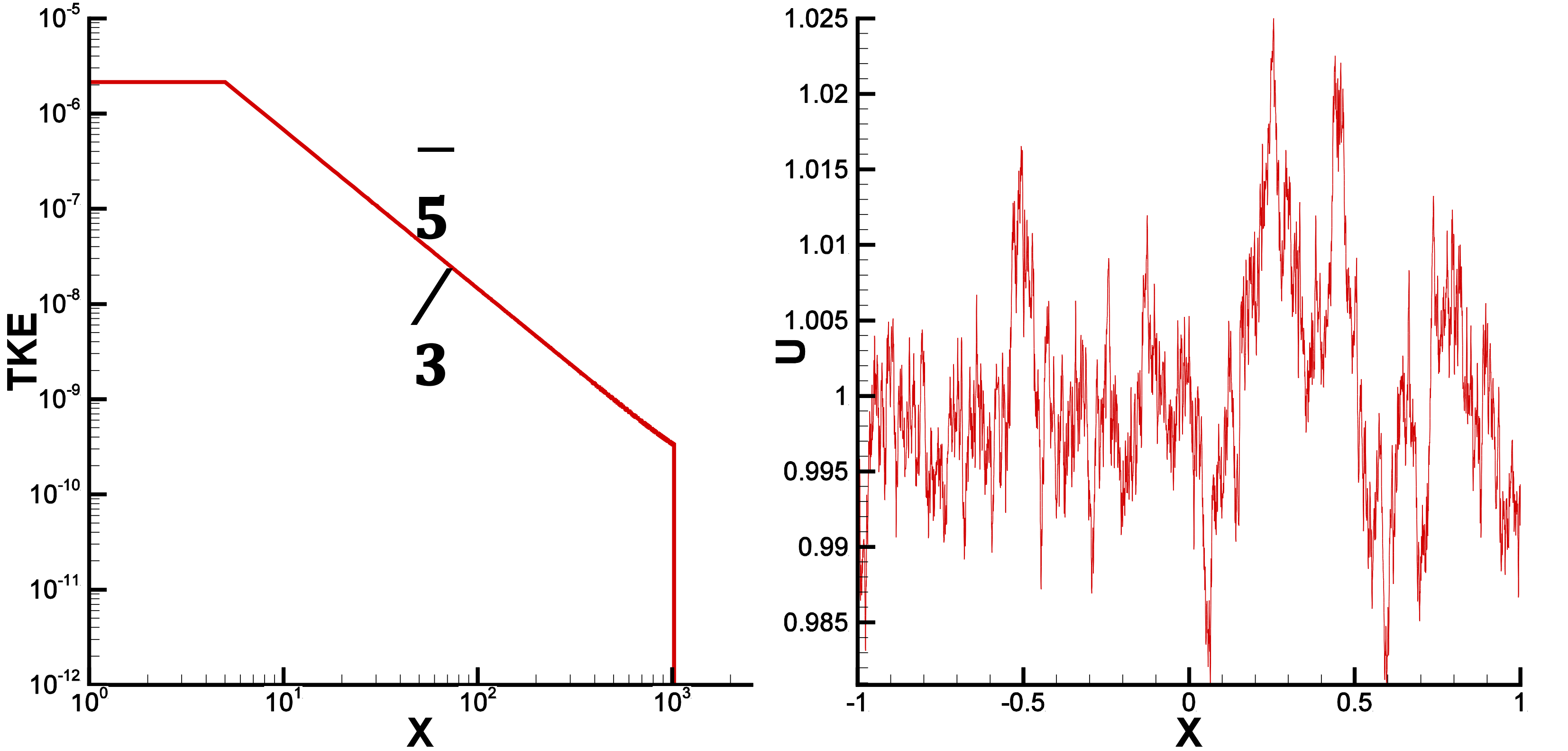
SGS Models Evaluated

- Static Smagorinsky model (SS)
- Dynamic Smagorinsky model (DS)
- Scale similarity model (SSM)
- Mixed model (MM) of SSM and DS
- Linear unified RANS-LES model (LUM)
- ILES (no model)

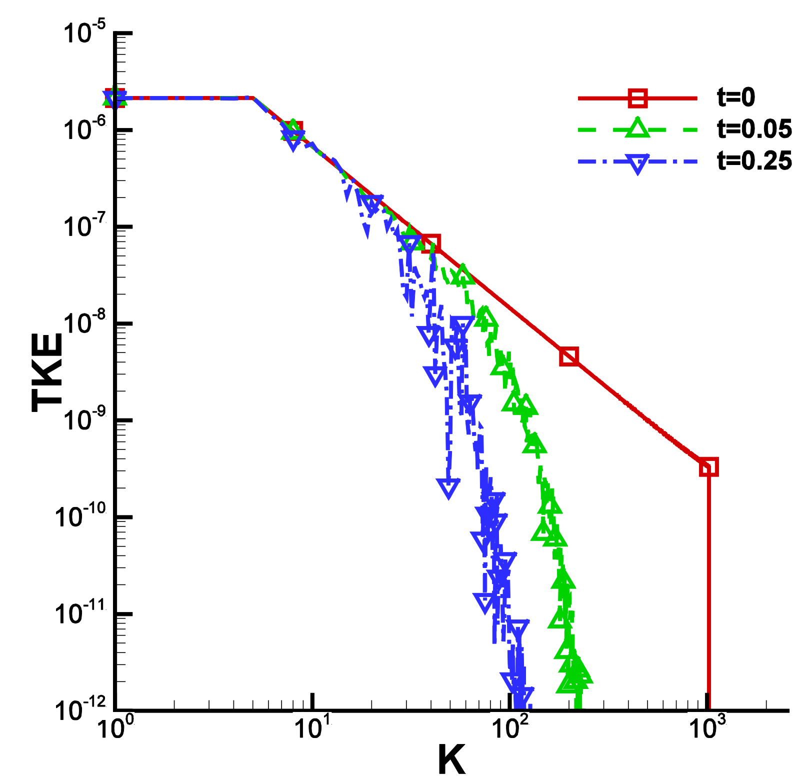
Numerical Method and Problem Setup

- Numerical method
  - 3rd order FR/CPR scheme
  - Viscous flux is discretized with BR2
  - Explicit SSP 3 stage Runge-Kutta scheme
- Problem setup
  - Domain [-1, 1] with periodic boundary condition
  - The initial solution contains 1,280 Fourier modes satisfying a prescribed energy spectrum with random phases
  - The DNS needs 2,560 cells to resolve all the scales
  - The filter width: $\Delta = 32\ \Delta x_{DNS}$
  - Various mesh resolutions for LES $\Delta x_{LES}/\Delta = 1, 1/2, 1/4, 1/8$

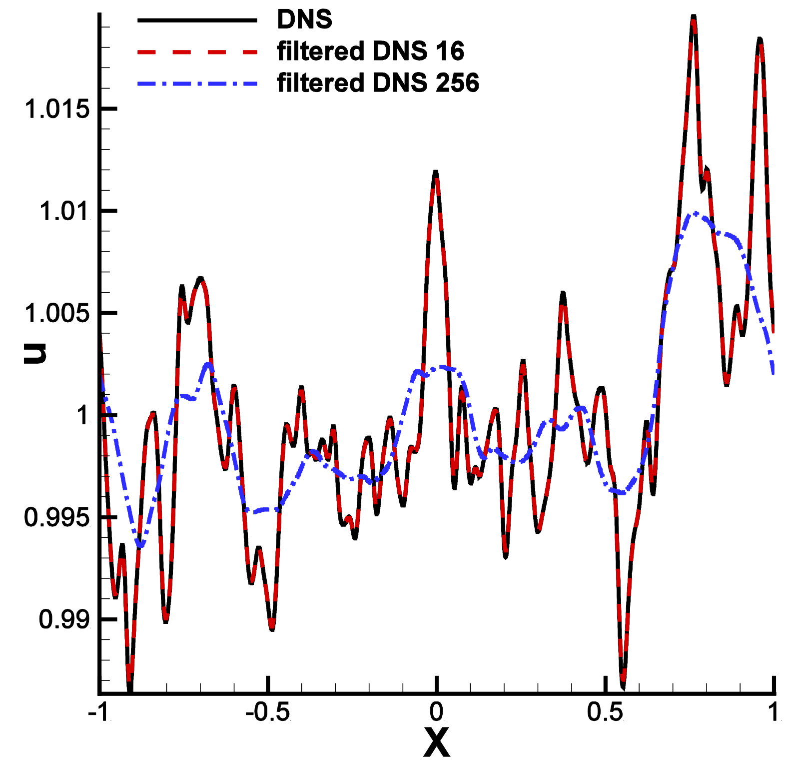
Initial Condition



The DNS Results



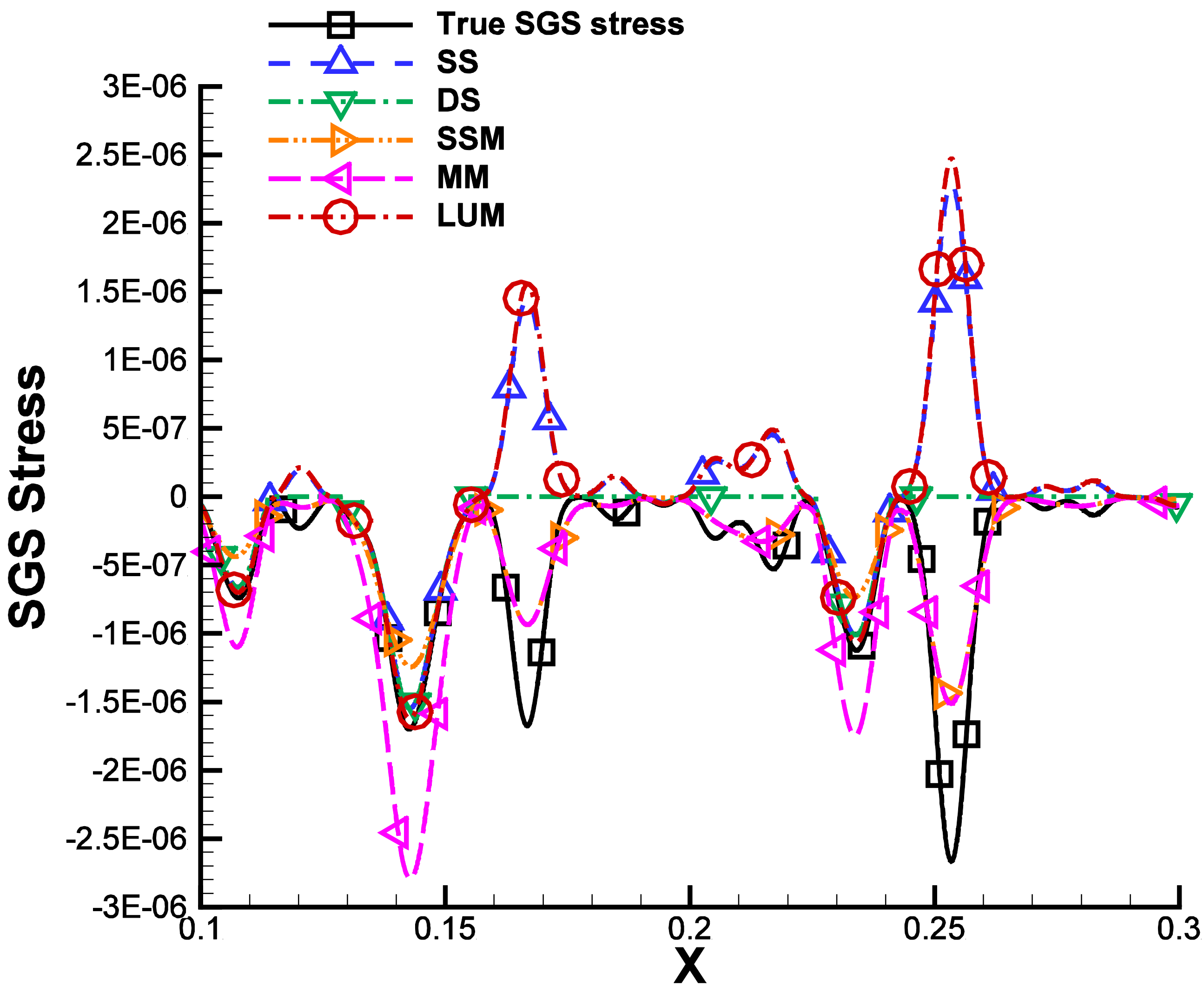
Energy spectrum



Solution at $t\downarrow 2$

Filtered DNS result used as “truth solution” for LES

Comparison of SGS Stresses (A Priori)



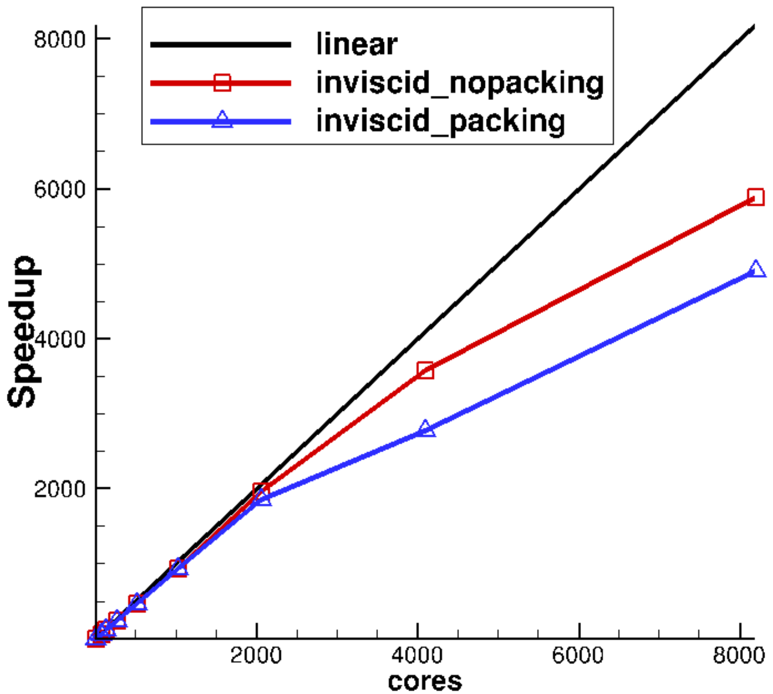
Lessons Learned about SGS Models

- In both a priori and a posteriori tests with the 1D Burgers' equation
  - SGS stresses generated by static, dynamic Smagorisky and LUM models show no correlation with the true stress
  - SSM (and Mixed model) consistently produces stresses with the best correlation with the true stresses
- When the modeling error is dominant, SSM and MM perform the best. When the truncation error is dominant, no model shows any advantage. ILES is preferred
- For methods with dissipation, DO NOT use SGS models. For almost all LES simulations, truncation errors are dominant (Δ = h), the best choice is ILES.

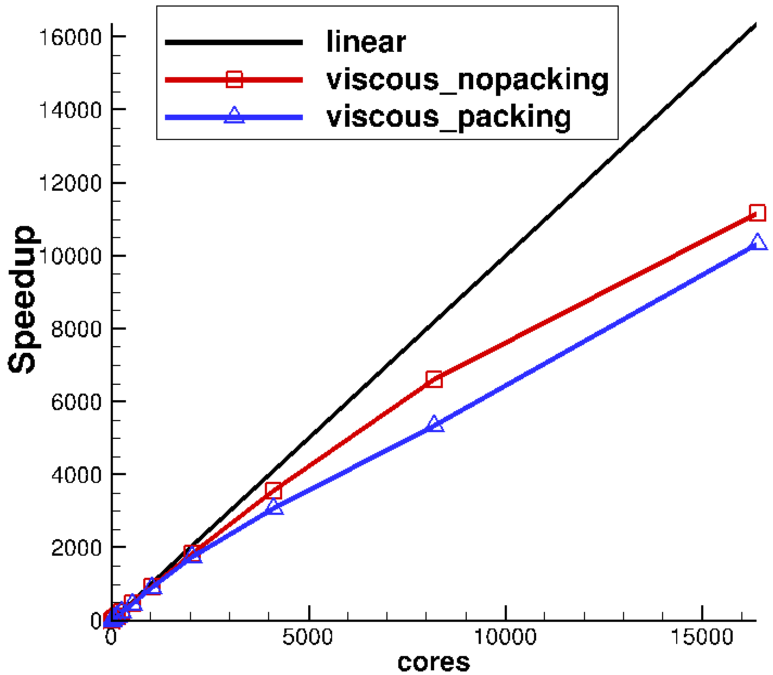
Example Applications

Parallel Efficiency: Strong Scalability Test

- Compare packing/unpacking vs direct data exchange
- P3 100 RK3 iterations on BlueWater; 125,000 Hex elements
- 3D inviscid vortex propagation: 72% at 8192 cores (15 elements/core)
- 3D viscous Couette Flow: 68% at 16384 cores (8 elements/core)



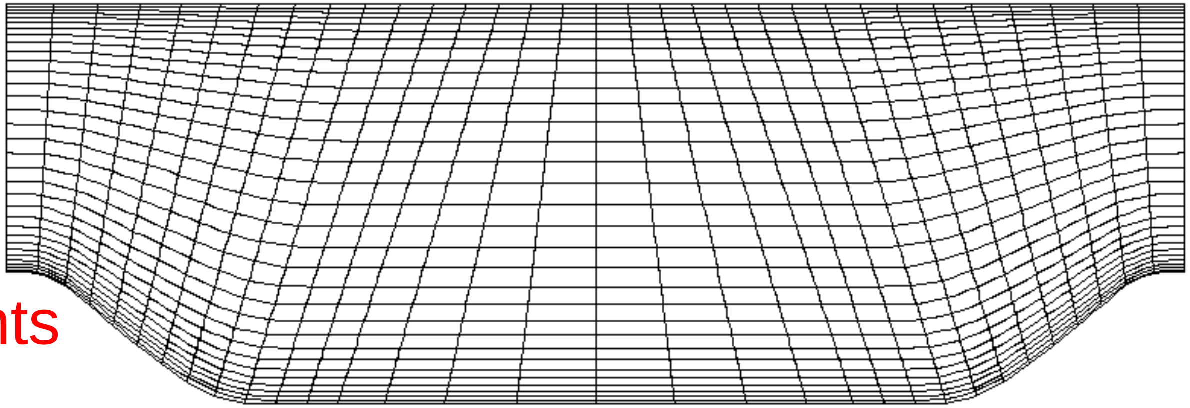
3D inviscid vortex propagation



3D viscous Couette flow

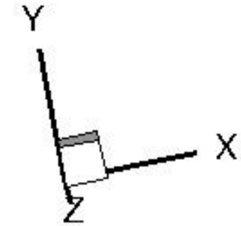
Periodic Hill

- Benchmark problem adopted by the international workshops for high-order CFD methods
- Re = 2,800 and 10,595
- Accurate prediction of separation and reattachment points is a key challenge
- P3 FR/CPR+3rd order SSP Runge-Kutta

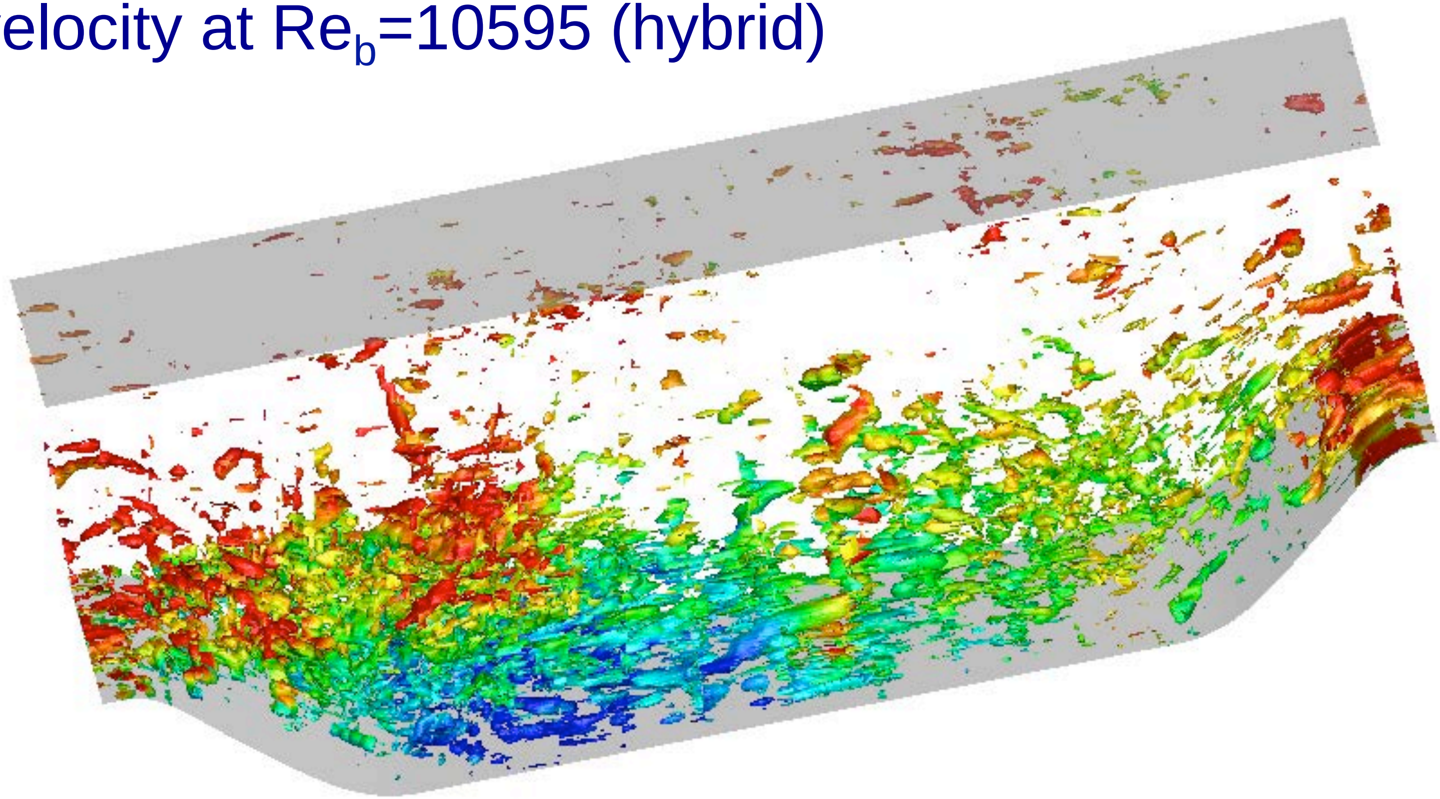


16,384 P3 elements

Periodic Hill

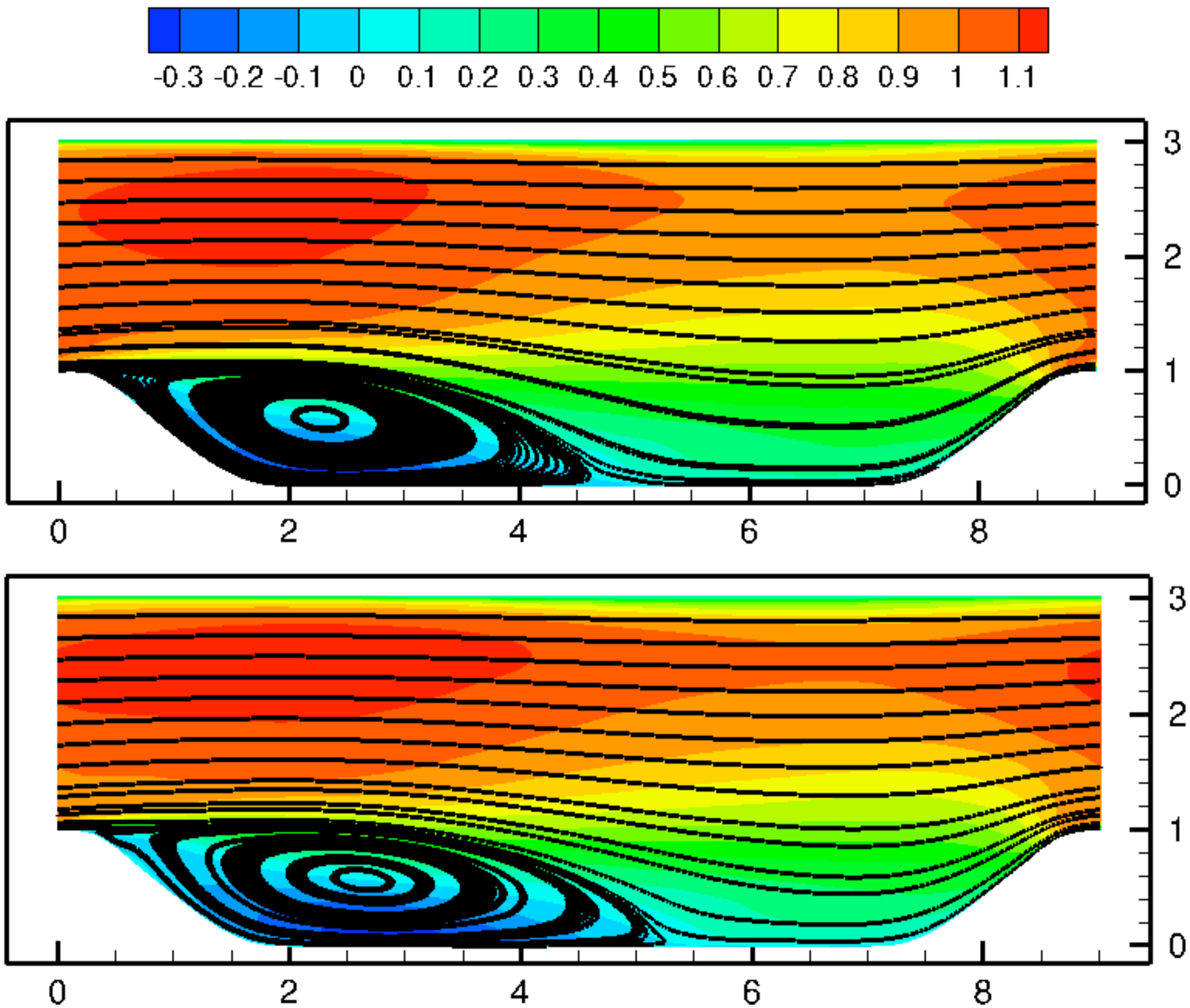


Iso-surface of Q colored by streamwise velocity at Re_b=10595 (hybrid)



Periodic Hill (Re = 2,900)

- Mean streamline

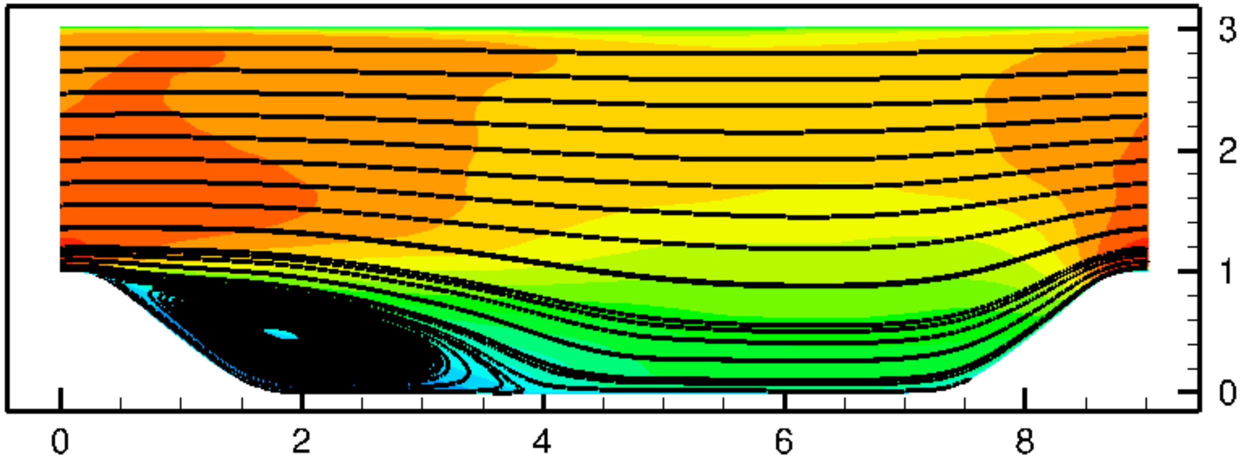


ILES

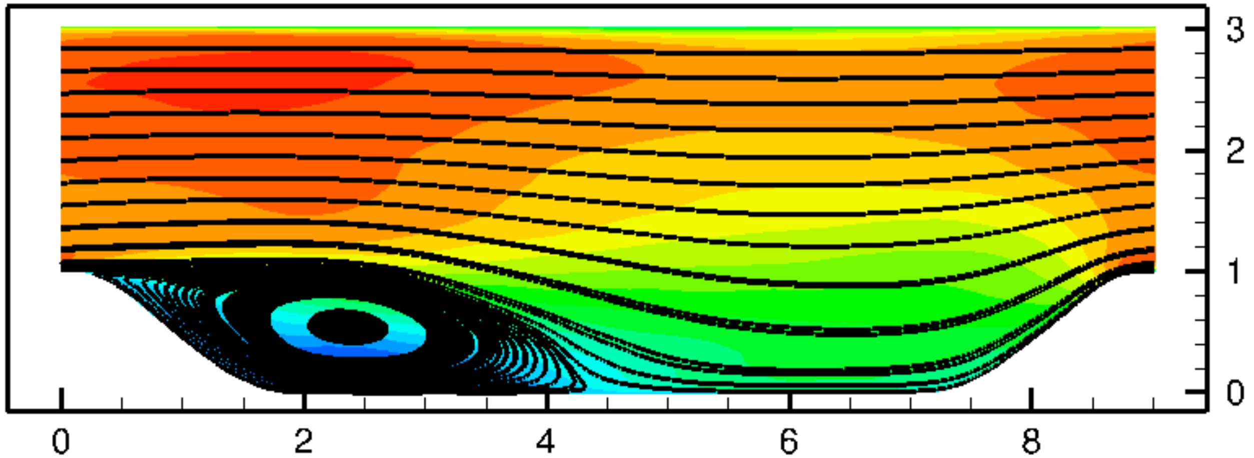
Hybrid

Periodic Hill (Re = 10,595)

- Mean streamline



ILES



Hybrid

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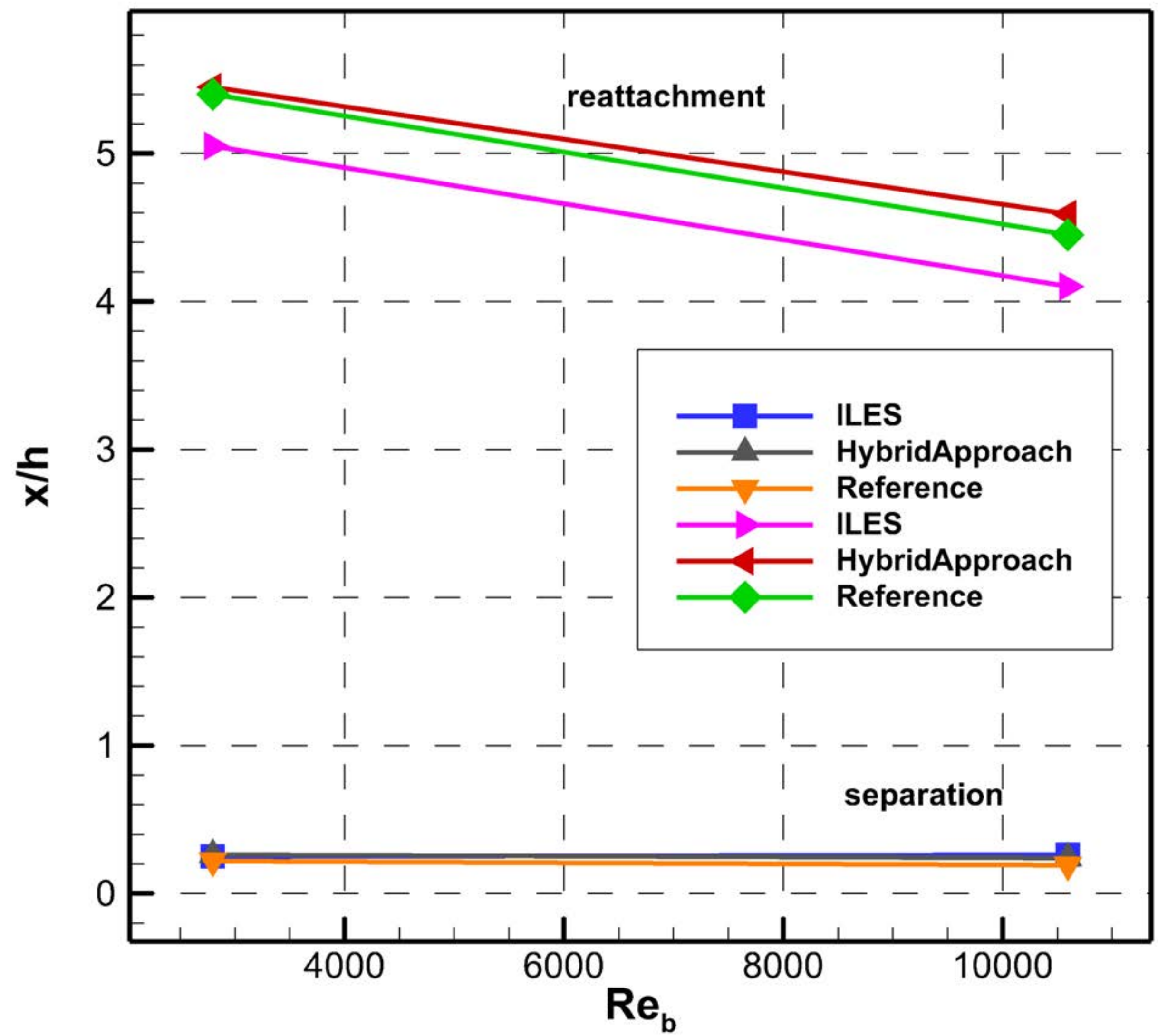
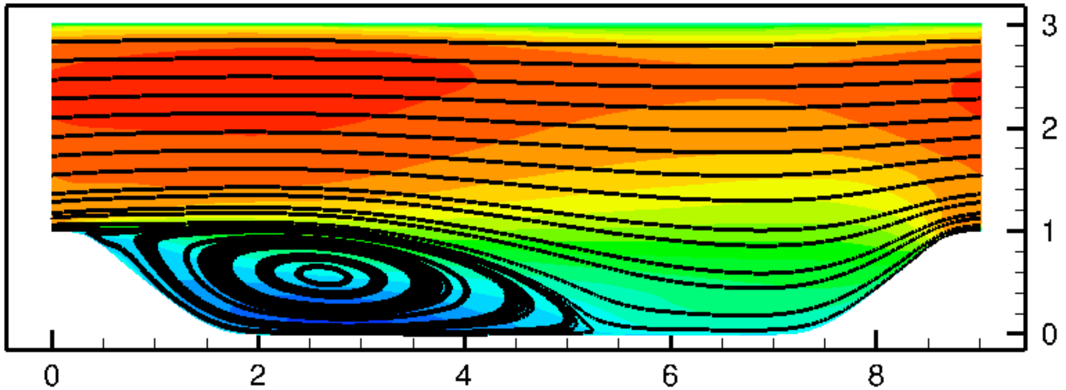
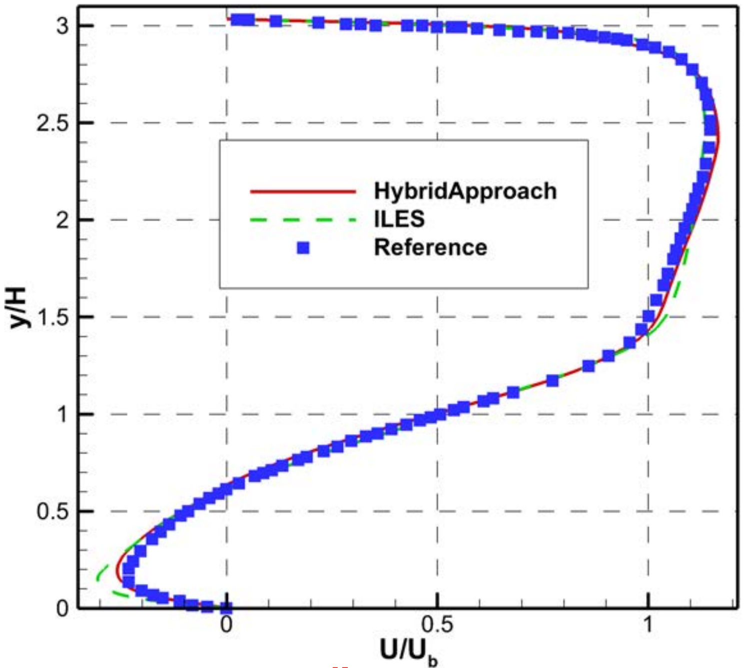
Separation and Reattachment Points

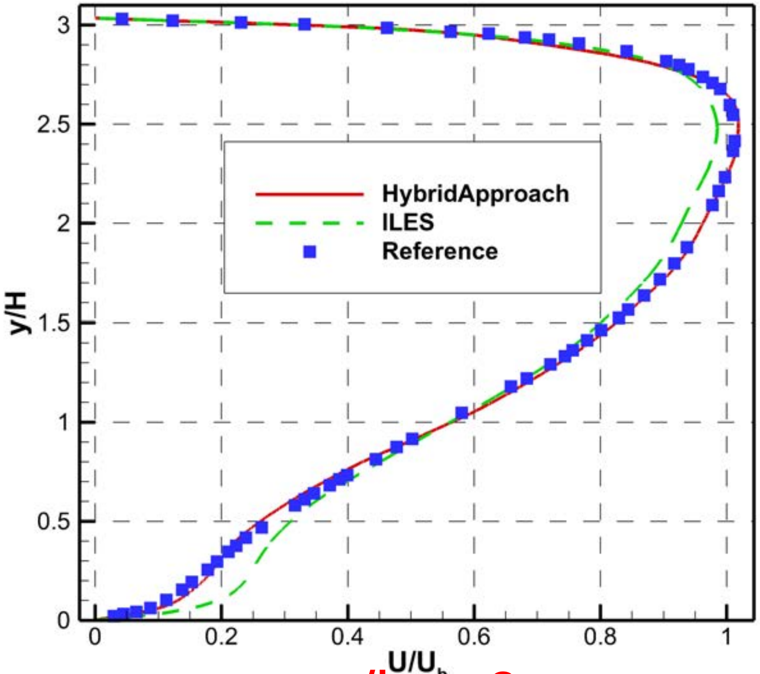


Velocity Profiles, Re = 2,800





x/h = 2



x/h = 6

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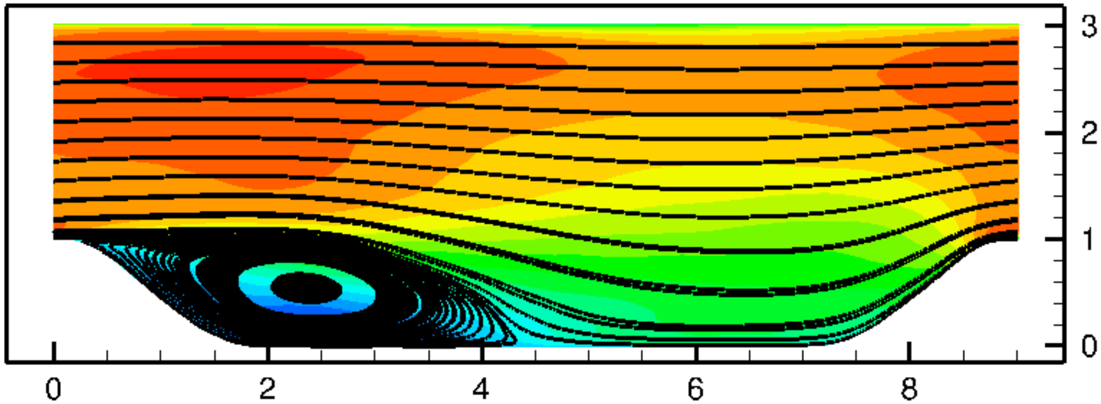
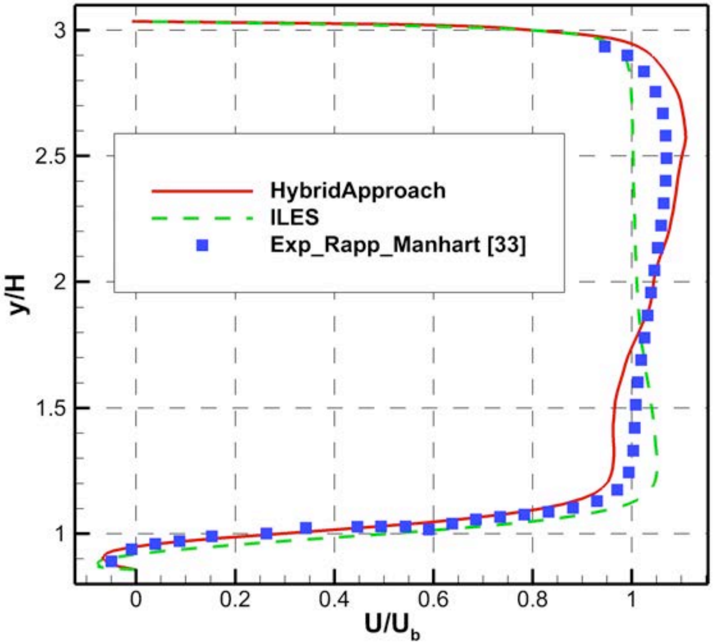
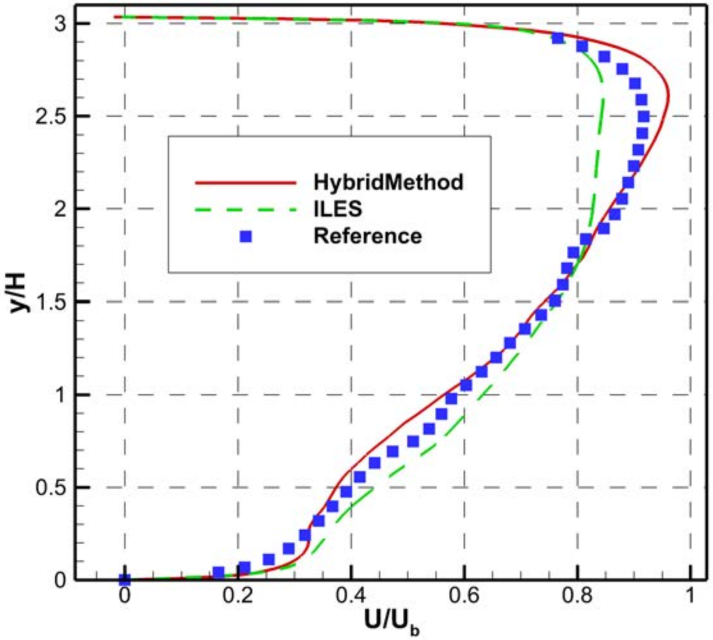
Velocity Profiles, Re = 10,595







x/h = 0.5

x/h = 6

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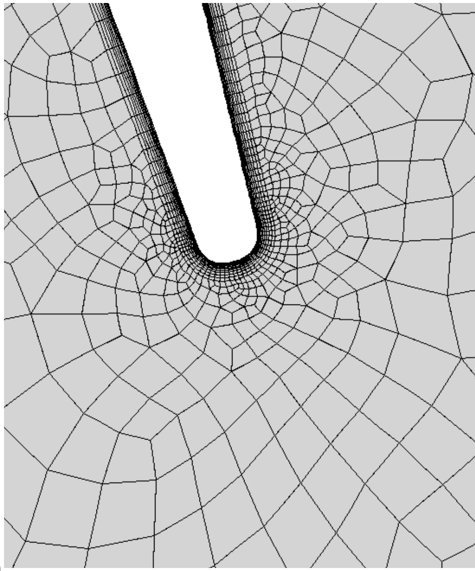
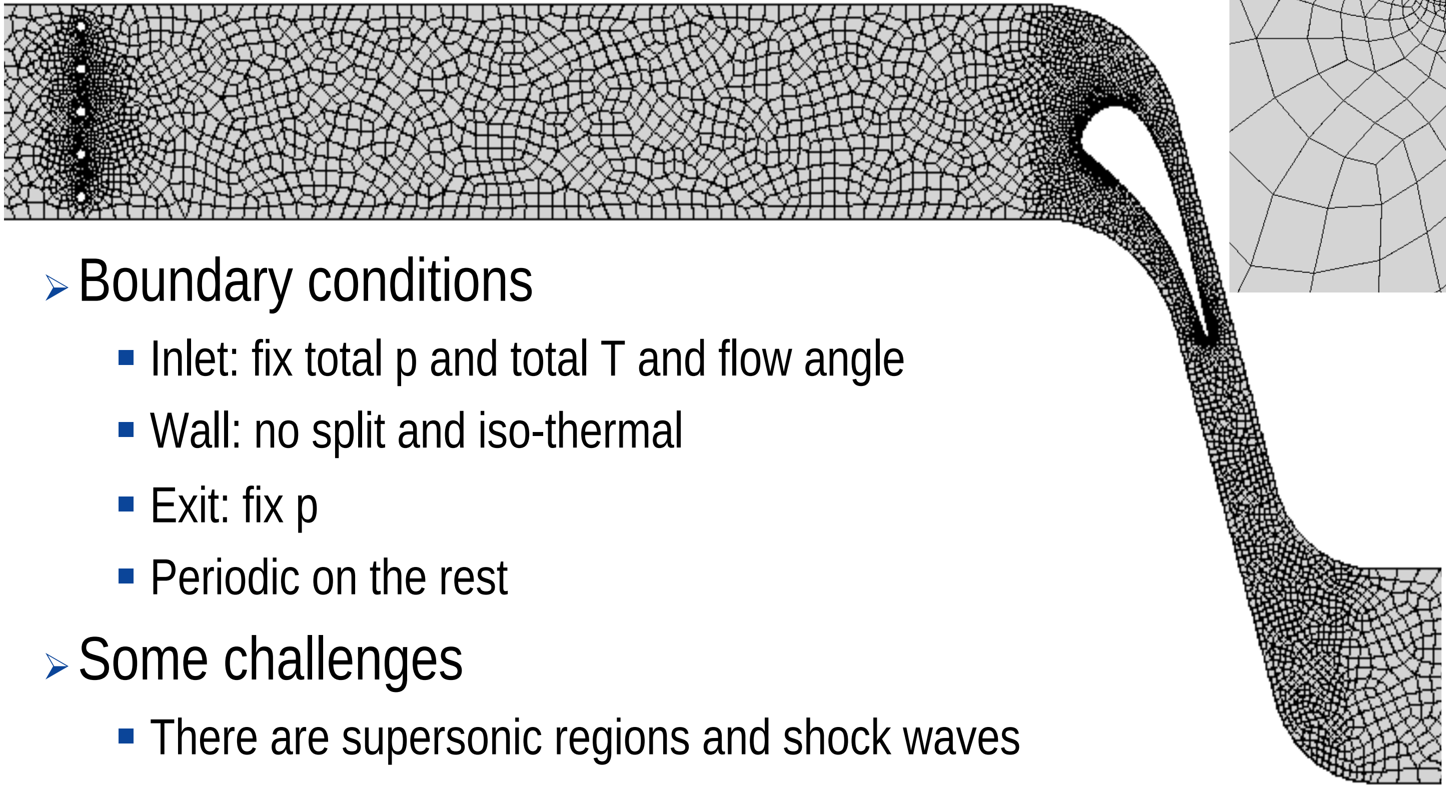
Uncooled VKI Vane Case - Benchmark

- Reynolds number: 584,000, Mach exit: 0.94
- No. of hexahedral elements: 511,744
- nDOFs/equ at p5 (6^{th} order): 110.5M





- Boundary conditions
  - Inlet: fix total p and total T and flow angle
  - Wall: no split and iso-thermal
  - Exit: fix p
  - Periodic on the rest
- Some challenges
  - There are supersonic regions and shock waves
  - Heat transfer is difficult to predict

Simulation Process

- Start the simulation from p0 (1st order), and then restart at higher orders. This is much more robust than directly starting at high order
- Monitor the Cl and Cd histories on the main blades to determine the start time for averaging
- P-refinement studies used to assess the accuracy and mesh and order independence

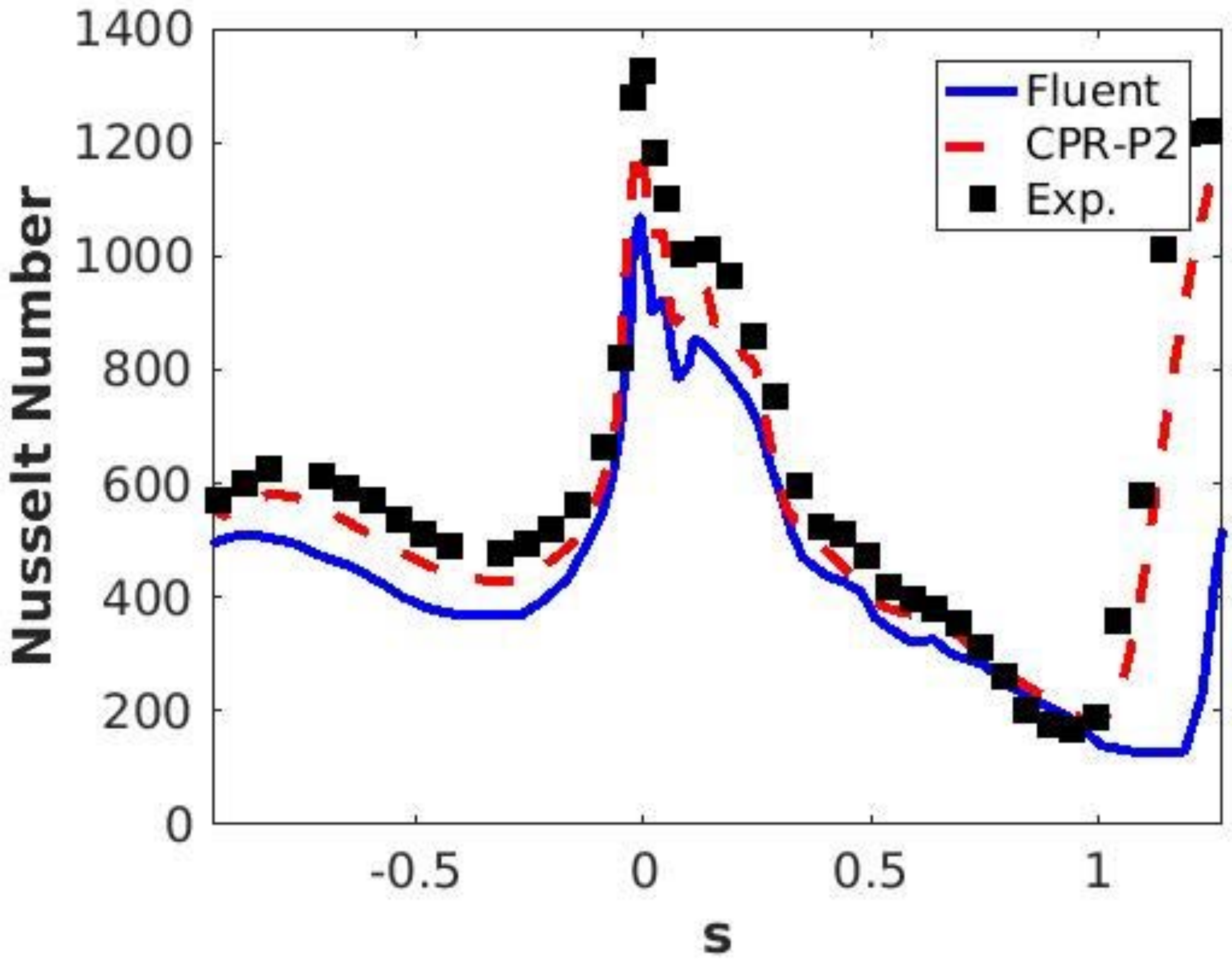
Q-Criterion and Computational Schlierens

Computational Schlierens

FDL3DI – sixth order compact scheme

FR/CPR - sixth order

Comparison of Heat Transfer



Summaries

- Outlined the challenges in LES
- Focused on several pacing items for LES
  - High order methods
  - High-order mesh generation
  - SGS models
- Presented several demonstration cases to show the capability
- Future work includes better wall models and efficient time integration schemes for extreme scale computers

Acknowledgements

- We are grateful to AFOSR, NASA, ARO and GE Global Research for supporting the present work.