Higher-order SU2: DG-FEM and WENO-FV solvers with LES/ILES/WMLES applications

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Pointwise

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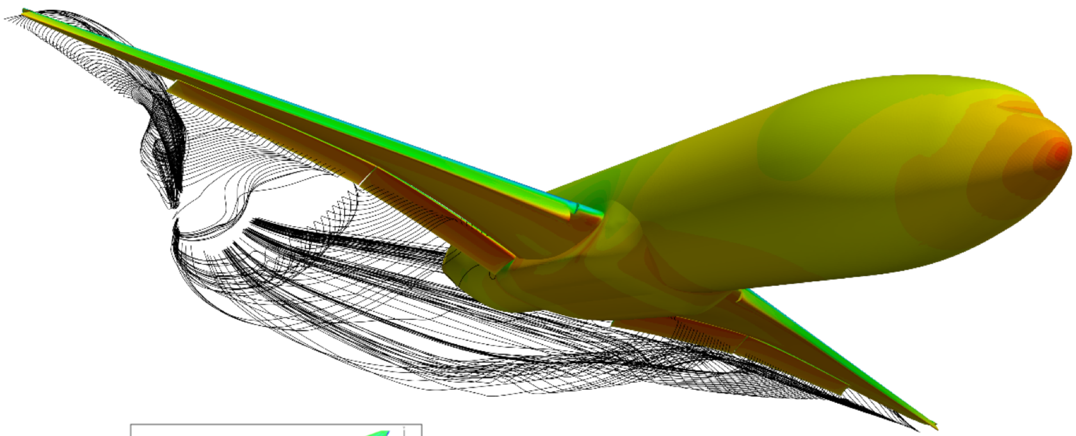
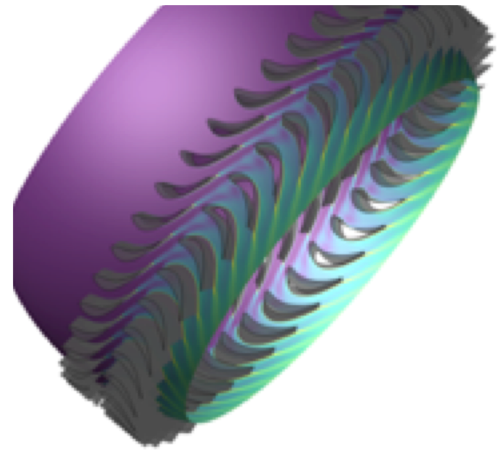
Outline

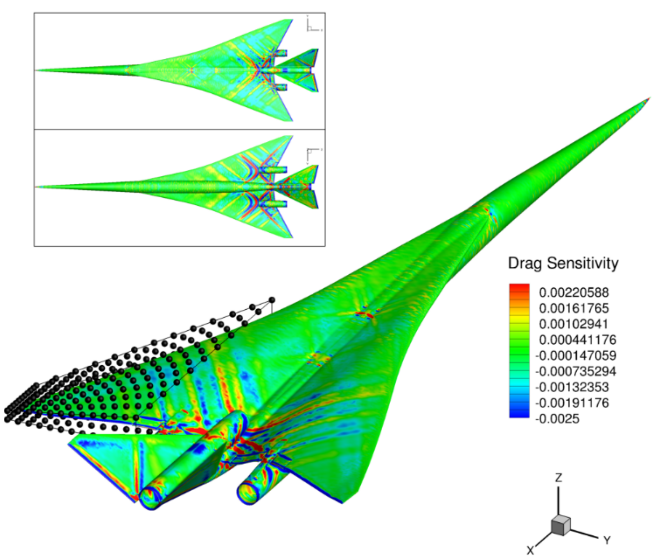
- Motivation for high-order schemes
- WENO solver
- DG solver
    - Shock capturing
    - LES models
    - Performance optimization
- Grid generation
- Access the code
- Future work

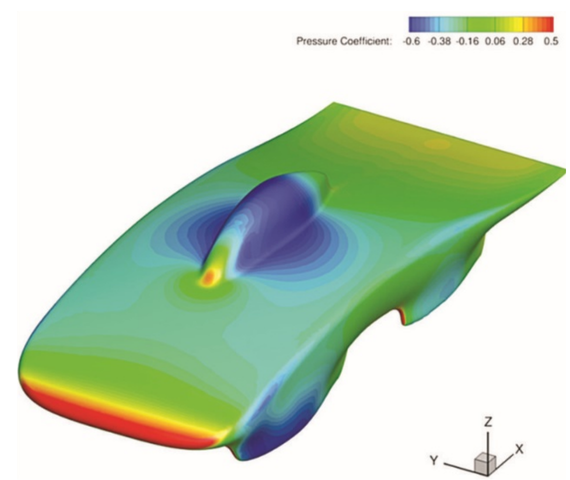
Why do we need high-order schemes?

2nd order schemes have been extremely successful, certainly for RANS. SU2 FV is used for many applications…





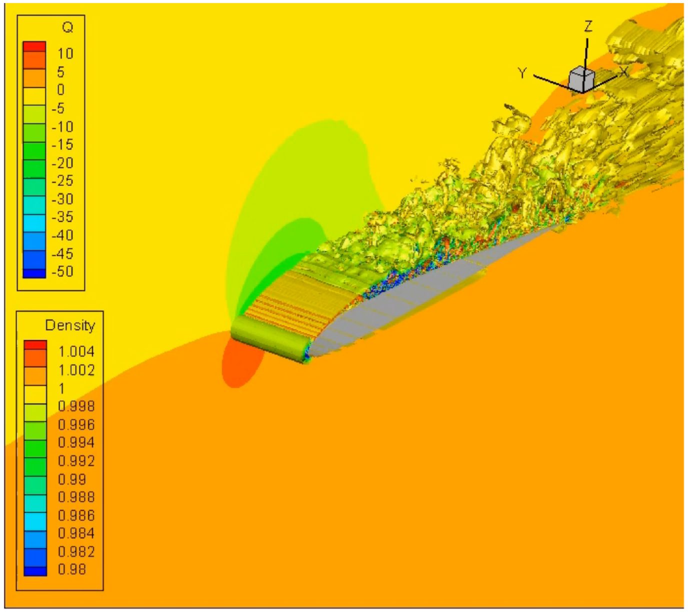




But…

For some applications 2nd order accuracy may not be sufficient

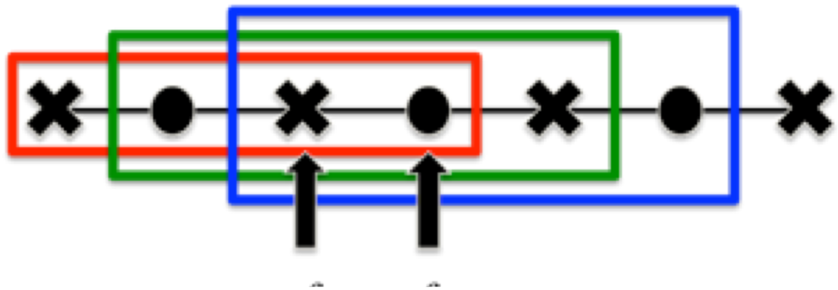
Examples
- Wake and vortex flows
- Noise prediction
- LES/DNS



High-order solver is intended for high-fidelity modeling of the turbulence, i.e. LES (wall resolved and wall modeled) and DNS

Options to increase the order of accuracy

1: Increase the stencil combined with smoothness indicators => WENO-FV



2: Increase the polynomial degree inside the element => DG-FEM

$$\text{Element } k: \; U(x_i) = \sum_{j=1}^{N_p} U_j^k \varphi_j^k(x_i)$$

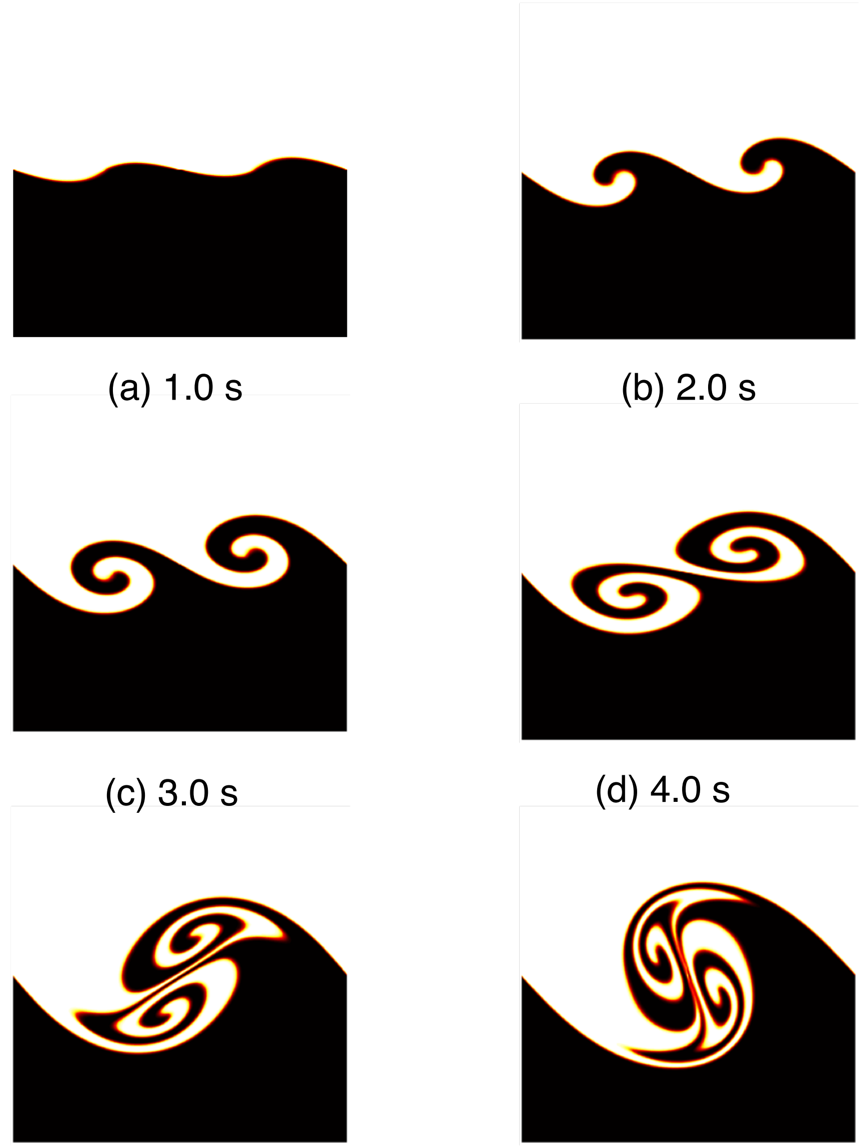
High-Order: SU2 Finite Volume

- Aim: Implementation of high-order schemes within the finite volume solver of SU2

- Objectives
  - 3rd order MUSCL limiters
    - Drikakis-Zoltak
    - Michalak & Ollivier-Gooch
  - Framework for Weighted Essentially Non-Oscillatory Schemes (WENO)
  - Use the Double Vortex Pairing Problem to assess the relative performance of these schemes

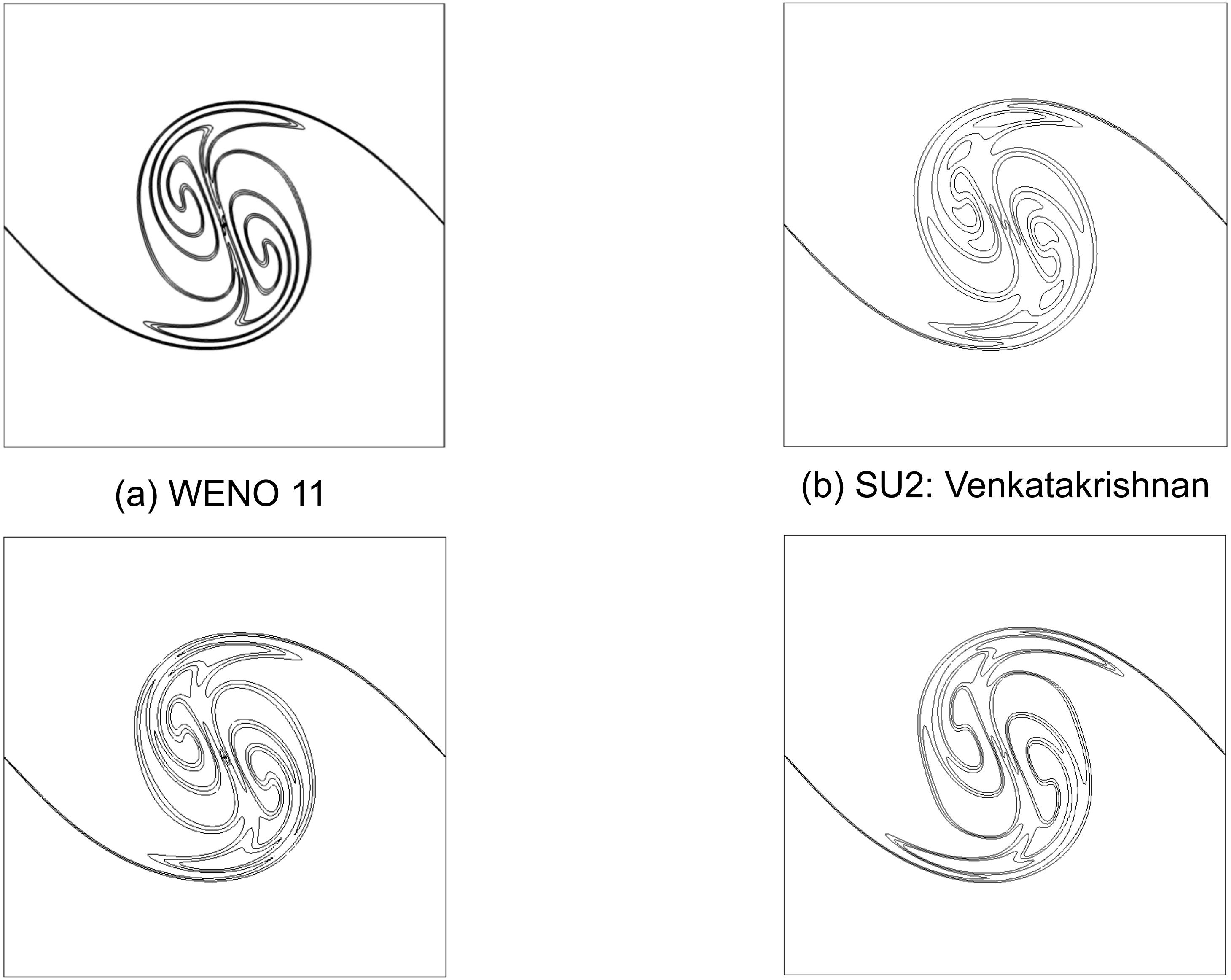
Description of Problem: Double Vortex Pairing

- Mixing layer formed by two co-flowing streams of water
- Initial velocity perturbations inflate forming two distinct vortices
- Vortices roll around each other eventually merging to form one vortical structure
- Chosen as test problem due to presence of fine structures and discontinuities



(a) 1.0 s (b) 2.0 s (c) 3.0 s (d) 4.0 s (e) 5.0 s (f) 6.0 s

Double Vortex Pairing 256x256, M=0.2: Passive Scalar



(a) WENO 11

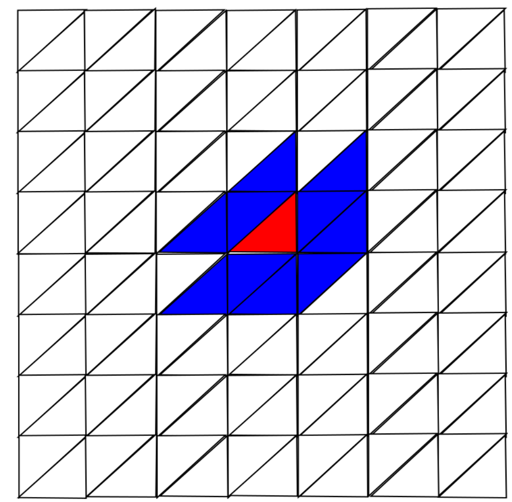
(b) SU2: Venkatakrishnan

(c) SU2: Michalak-Ollivier Gooch

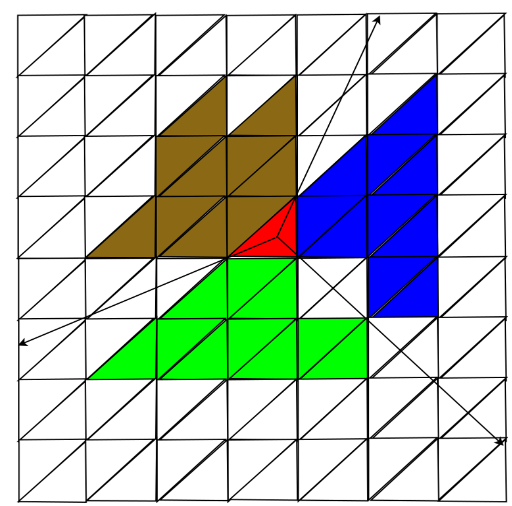
(d) SU2: Drikakis-Zoltak

WENO Outline

- Difficult to achieve orders of accuracy above 3rd order using MUSCL based approach on unstructured grids
- Aim: To create a high-order polynomial for target cell E_0 which has the same cell averaged value as the reconstructed function u
- Reconstruction uses cell averaged value from target cell E_0 as well as cell averaged values from multiple stencils consisting of neighboring cells
- Two types of stencils
  - Central
  - Directional
- Number of cells in the stencil scales with desired order of accuracy
  - $K = \frac{1}{2}(r+1)(r+2) - 1$
  - $M = 2K$



(a) Central Stencil



(b) Directional Stencil

WENO Outline

$$p_{weno} = \overline{u_0} + \sum_{k=1}^{K} \widetilde{a_k}\, \phi_k(\xi, \eta)$$

- Polynomials are constructed using data from each stencil

- "Essentially Non-Oscillatory" part stems from non-linear weights which are used to determine the smoothness of the solution in each stencil

- Central stencil given the largest bias since for smooth solutions the central stencil generally is the most accurate

Current Status

- Geometrical Preprocessing (Commom/src/geometry_structure.cpp)
  - Check the mesh to determine which elements can have WENO reconstruction
  - Central + Directional stencil assembly for triangular elements
  - Obtain unique nodes (solution points) from stencil
  - Functions to handle assembly of mesh dependant parameters
  - LAPACK functions used to carry out matrix operations
  - Function to determine which two elements share a common edge

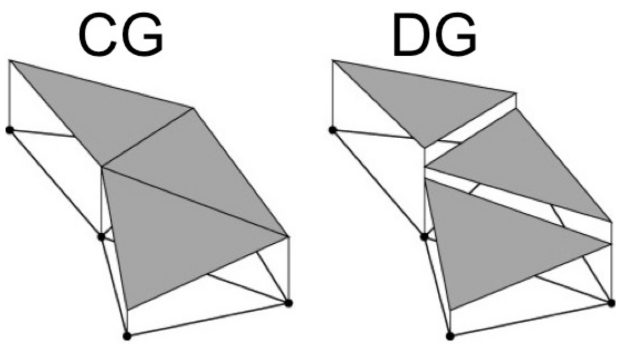
- Solution Reconstruction (SU2_CFD/src/solver_direct_mean.cpp)
  - MUSCL reconstruction used in region of the grid which cannot have WENO reconstruction
  - 3rd order WENO reconstruction done for remainder of domain

- Some Issues
  - Oscillations present at discontinuities
  - ~ 10 - 100 times slower than MUSCL scheme (depending on grid resolution)

Future Work

- Fully Functional in 2D
  - Quadrilateral elements
  - Hybrid grids
- Extension to higher-orders (4^{th} , 5^{th} etc)
- Full functionality in 3D
  - Requires additional steps in the geometrical preprocessing
  - Data structures require extension to handle the extra necessary information
- Add tunable parameters as options to be read from config file
- Parallel implementation
- Performance optimizations!

DG-FEM: the basic principles



$$\text{Element } k: \; U(x_i) = \sum_{j=1}^{N_p} U_j^k \varphi_j^k(x_i)$$

System of PDE's: Weak formulation

$$\frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} = 0 \quad \Rightarrow$$

$$\iint_{V_k} \frac{\partial U}{\partial t} \varphi_m^k \, dV - \iint_{V_k} F_i \frac{\partial \varphi_m^k}{\partial x_i} \, dV + \oint_{\partial V_k} F_i n_i \varphi_m^k \, d\Omega_k = 0, \quad m = 1, \ldots, N_p$$

Integrals are computed with high enough accuracy to prevent instabilities due to aliasing errors. Computationally intensive!!

However: DG solver can be run very efficiently on modern hardware. Also hybridized DG techniques to reduce CPU requirements.

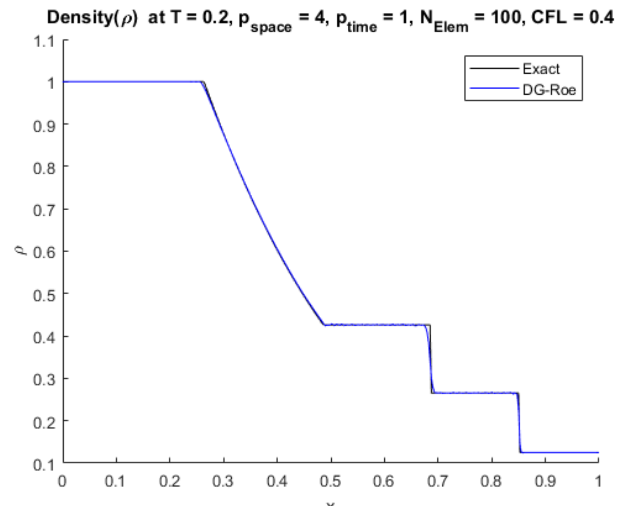
Current Capabilities

- Both 2D and 3D, just like SU2-FV
- All standard elements (tri, quad, tet, pyra, prism, hex)
- Curved elements of arbitrary order
- Polynomial order can differ in individual elements
- Symmetric Interior Penalty method for viscous fluxes
- Explicit time integration schemes (Runge-Kutta type)
- Time-accurate local time stepping via ADER-DG
- Preliminary implementation of LES models and shock capturing

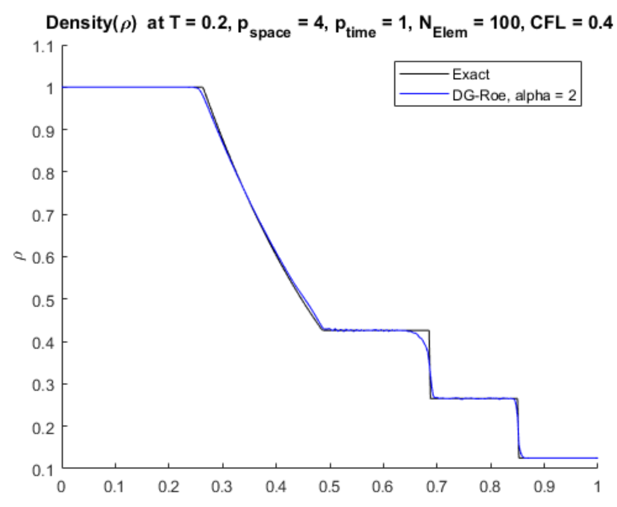
Shock capturing

- Shock capturing relies on two components:
  - Sensing the discontinuity
  - Resolving the discontinuity
- Sensing the discontinuity:
  - Persson and Peraire : Modal decay
  - Clain, Diot and Loubere : MOOD
- Resolving the discontinuity
  - Limiter
  - Artificial viscosity / filtering
  - Sub-cell limiting

<Sod's shock tube problem>



MOOD sensor / Subcell limiting



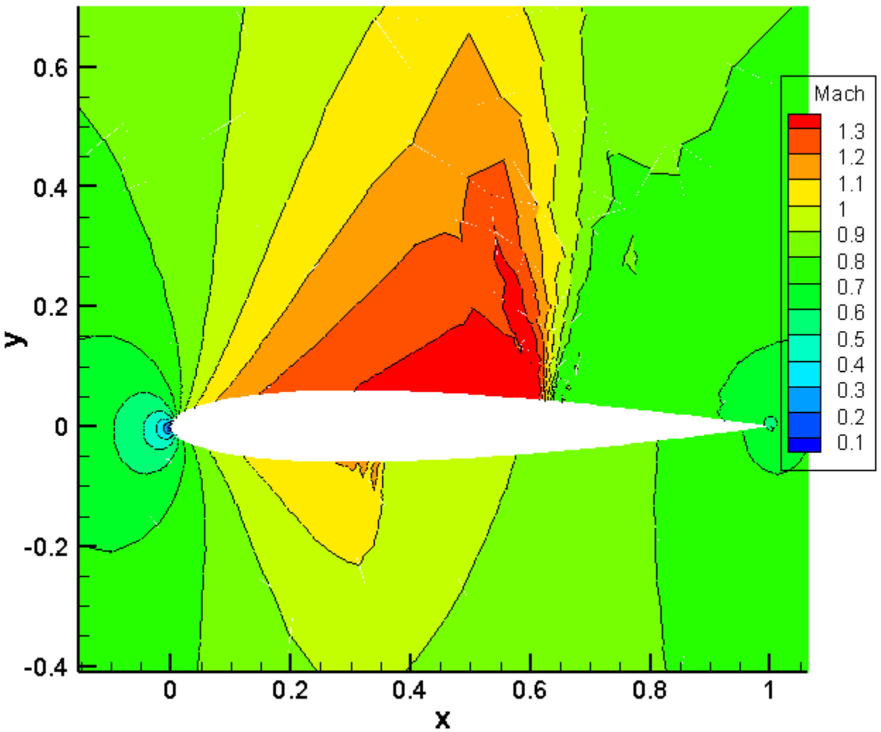
MOOD sensor / Filtering

Shock capturing

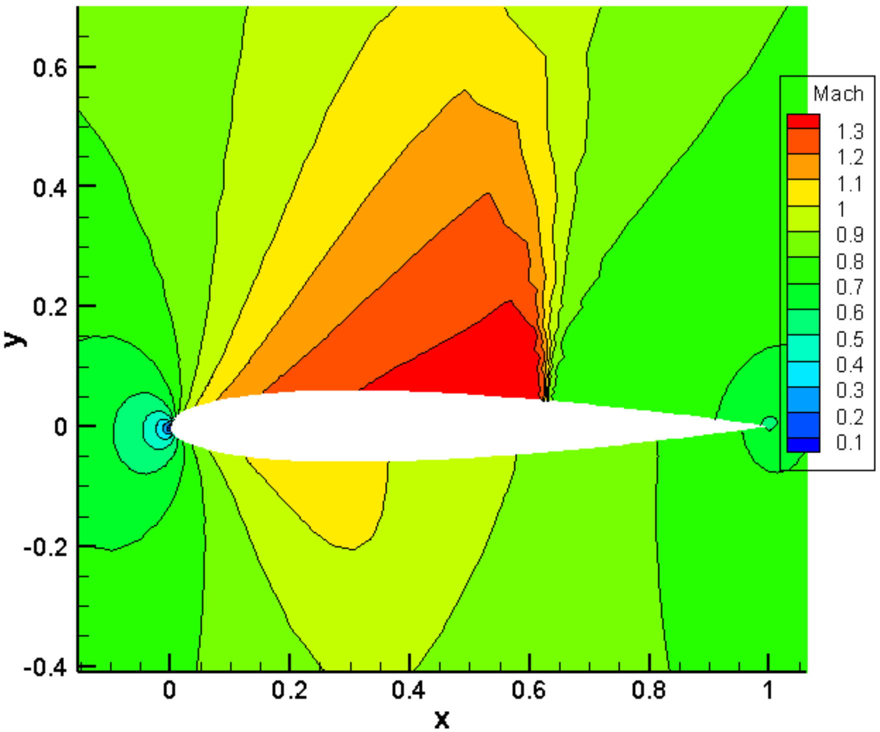
- Shock capturing method in DG-FEM
  - Discontinuity sensor : Use the ratio of the norms of the highest and the lowest modal coefficients. (Extension of Persson's shock sensor)
  - Resolving method : Use filtering method where the filtering strength is determined by sensor value.
- Current status
  - 2D triangular elements up to p = 3
  - Filtering strength can be modified with one input parameter

Shock capturing

- Transonic flow over NACA0012 airfoil
  - p = 1 | 7,990 triangles | 119 elements on each surface | 238 DOFs on each surface



Lax-Friedrich, DG



Roe, FVM, Venkatakrishnan Slope Limiter

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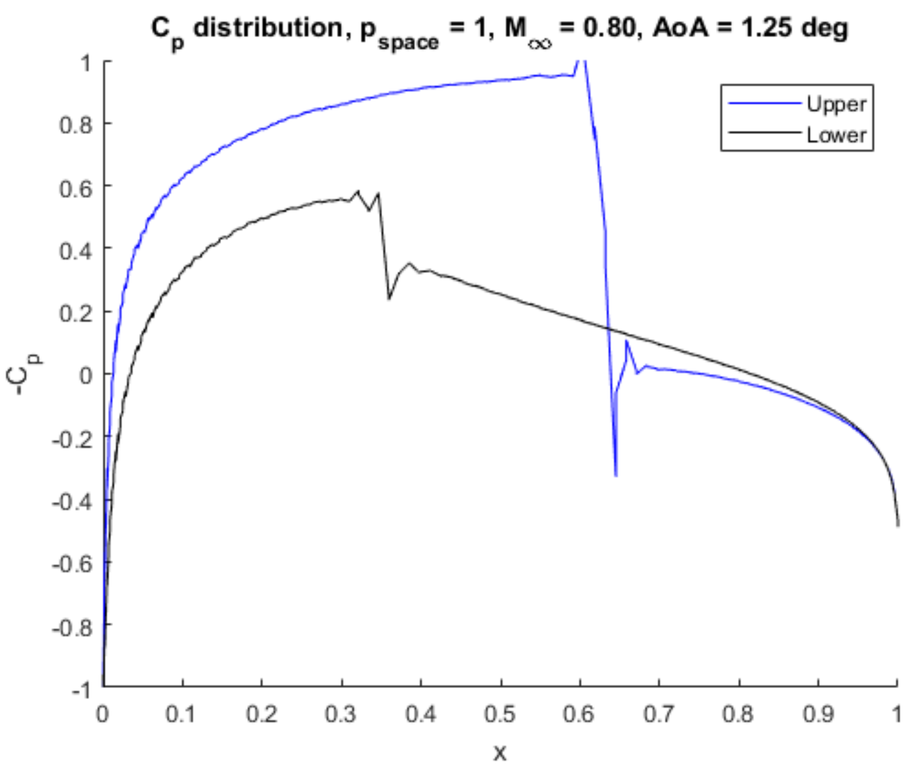
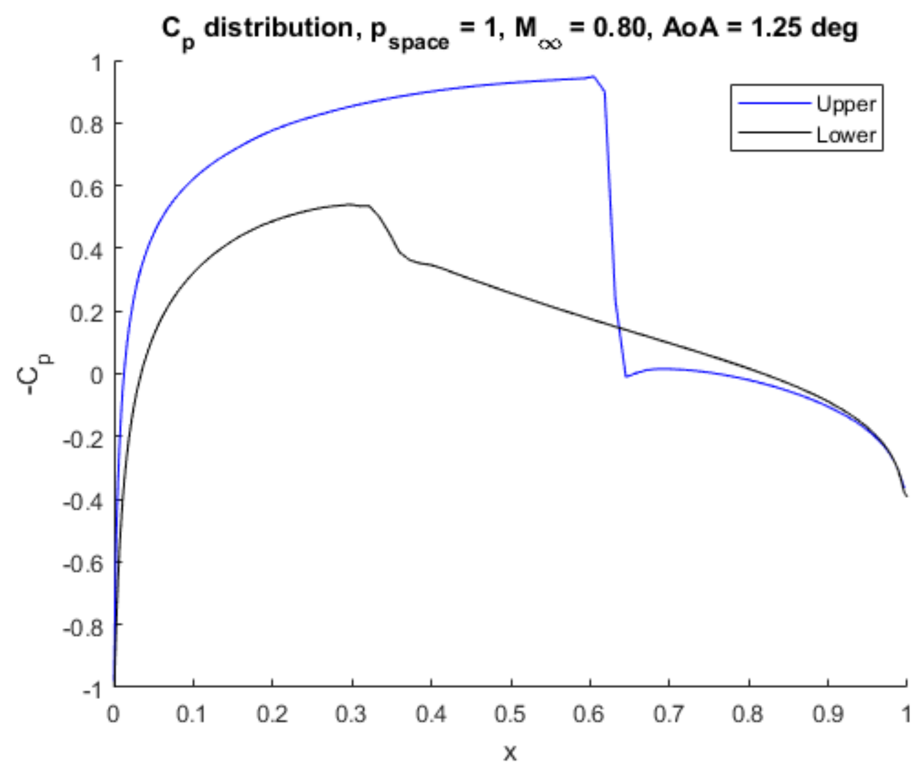


Lax-Friedrich, DG



Roe, FVM, Venkatakrishnan Slope Limiter

LES Models

- SGS Models
  - Constant Smagorinsky

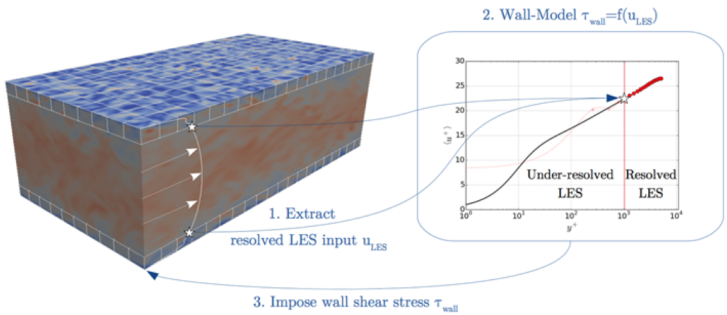
    $$\nu_{sgs} = C_s^2 \Delta^2 |\tilde{S}|$$

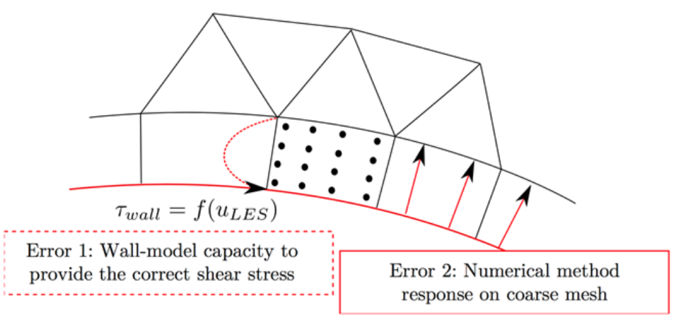
  - Wall-Adapting Local Eddy Viscosity (WALE)

    $$\nu_{sgs} = (C_w \Delta)^2 \frac{\left(S_{ij}^d S_{ij}^d\right)^{(3/2)}}{\left(\widetilde{S_{ij}}\widetilde{S_{ij}}\right)^{(5/2)} + \left(S_{ij}^d S_{ij}^d\right)^{(5/4)}}$$

  - More sophisticated models to be implemented in future
    - Dynamic Smagorinsky, etc.

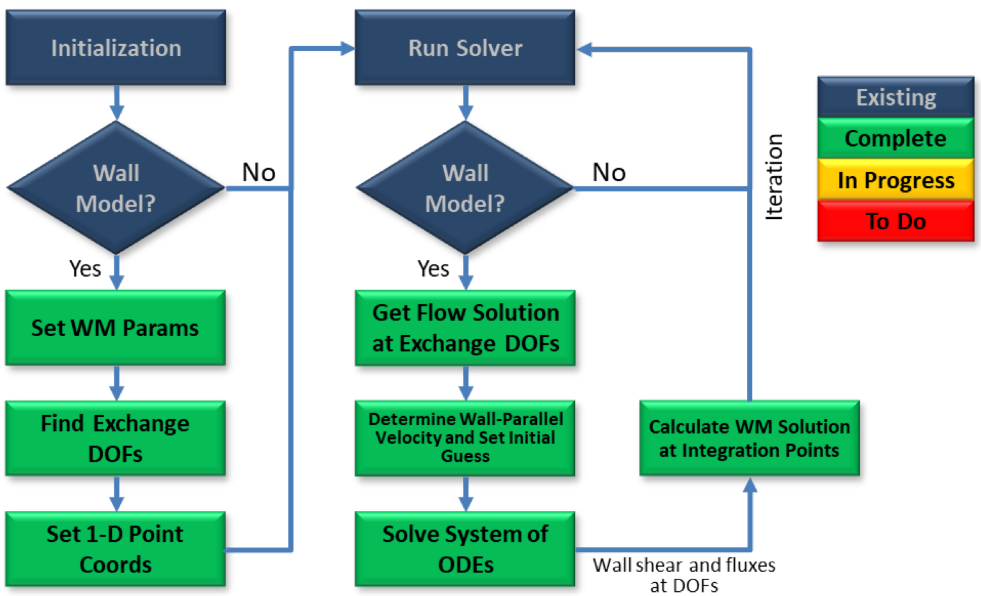
- Wall Models
  - One-dimensional Equilibrium BL Equations





Implementation of wall models within the context of DG-FEM solvers. A. Frére, C. de Wiart, K. Hillewaert, P. Chatelain, G. Winckelmans, Phys of Fluids, Jul 2017

Development of Wall-Models

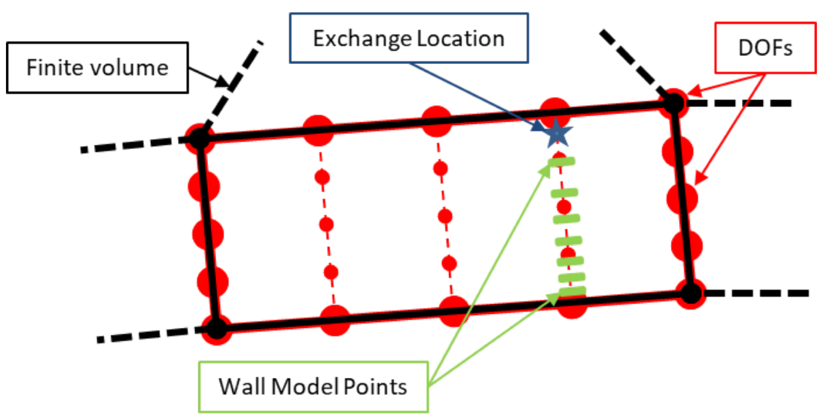


- One-Dimensional Equilibrium Model (1DEQM) of Larsson / Kawai / Bodart
  - Mixing length model with wall-damping used for turbulent viscosity

$$\frac{d}{dy}\left[(\mu - \mu_t)\frac{d\tilde{u}_{\parallel}}{dy}\right] = 0$$

$$\frac{d}{dy}(\bar{p}) = 0$$

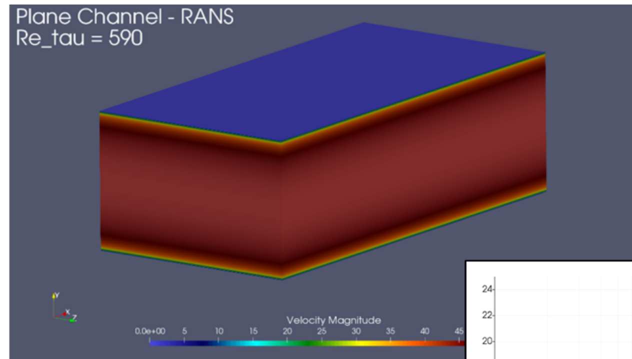
$$\frac{d}{dy}\left[\tilde{u}_{\parallel}(\mu + \mu_t)\frac{d\tilde{u}_{\parallel}}{dy} + \left(\frac{\mu c_p}{Pr} + \frac{\mu_t c_p}{Pr_t}\right)\frac{d\tilde{T}}{dy}\right] = 0$$



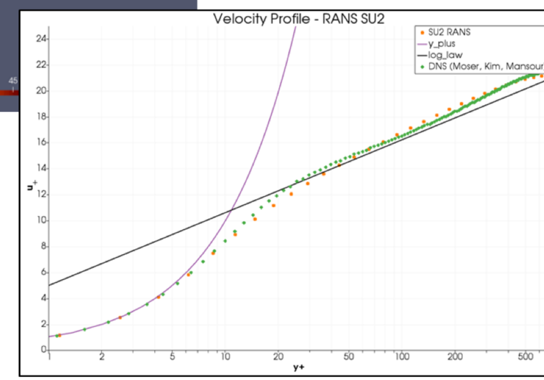
- Exchange location permitted in large-scale parallel computations:
  - On any element type on the surface (hexa, tetra, pyramid, prism)
  - Not necessarily on first element on the surface
- Full parallel search capability (ADT based), all necessary communication, and implementation of equilibrium WM have now been completed and being tested
- ADER-DG time-step requirements respected in partitioning / search

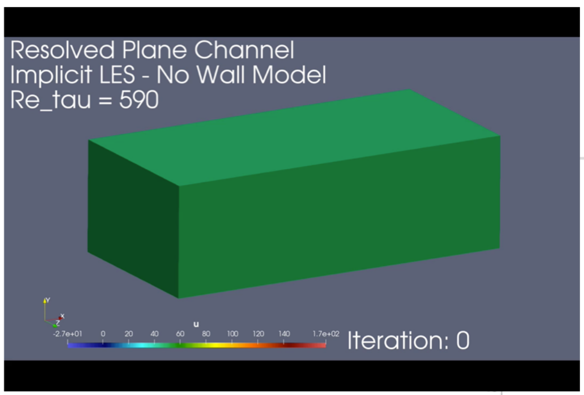
Wall-Model Validation: Plane Channel Flow

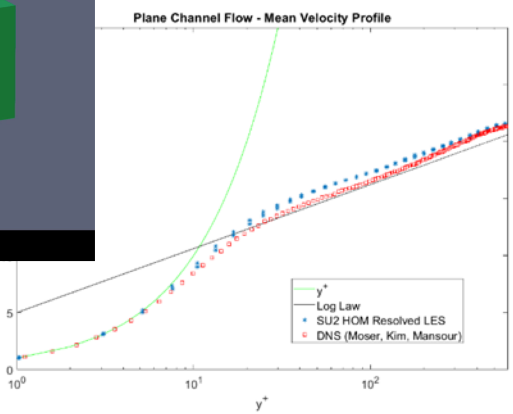
- Plane Channel simulations conducted with RANS and with *resolved* LES for comparison with WMLES
  - Flow Re_τ=590
  - Friction length l_τ=1.7x10^{-10} m
  - Friction velocity u_τ=2.53 m/s
  - Channel half-height δ=0.1 m
  - Domain size = 2πδ x 2δ x πδ



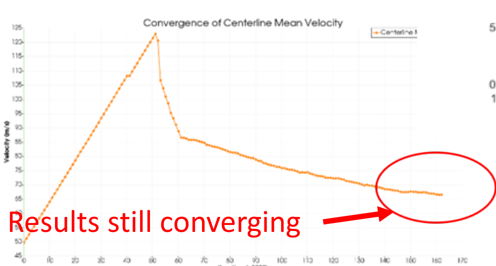
RANS Simulation
Mesh: 30x60x30







Resolved LES Simulation
Mesh: 22x22x22
P = 3

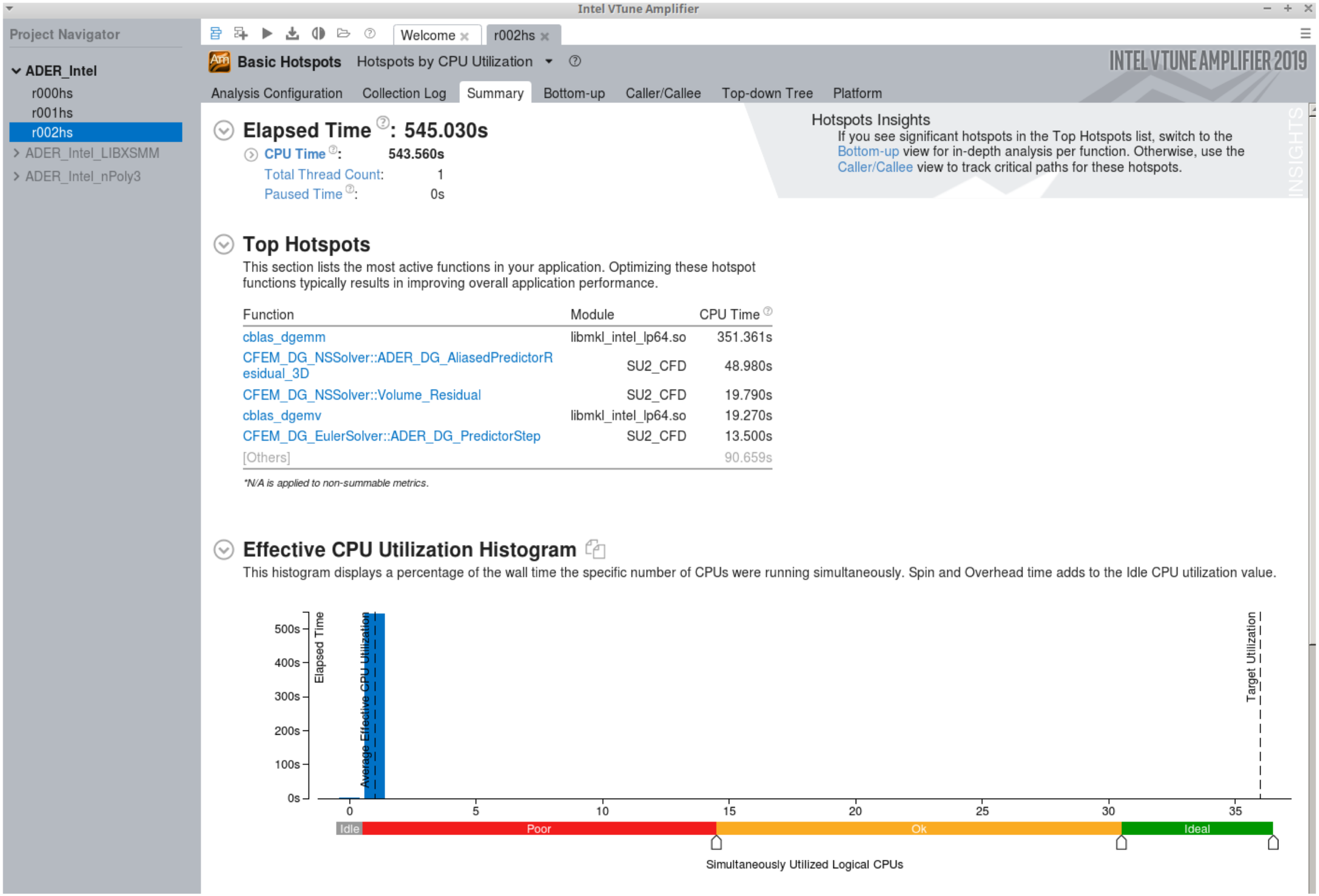


- Debugging/testing of plane channel flow with SU2 DG-FEM wall-modeled LES underway

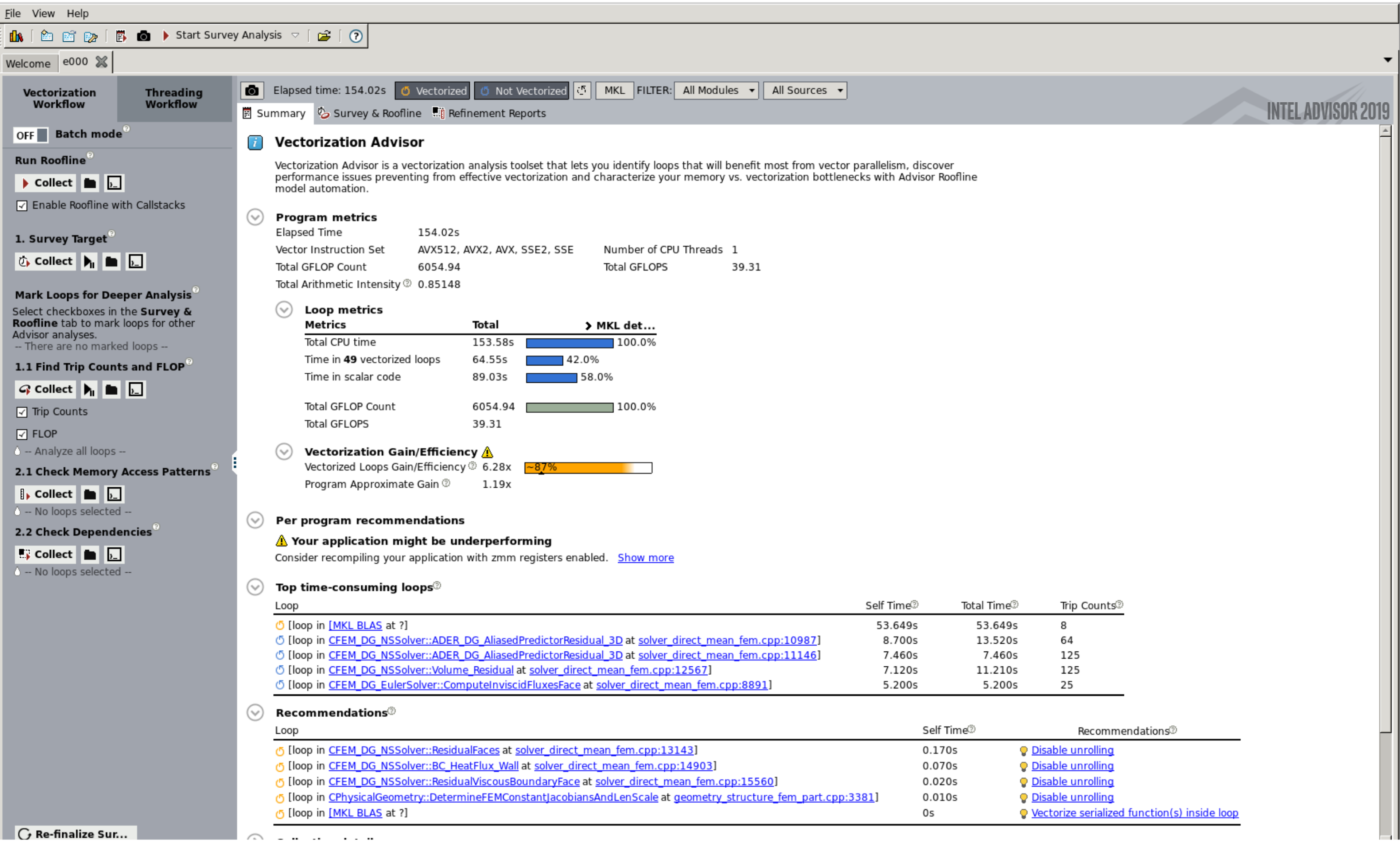
Performance optimization (with Intel)

- First implementation was very inefficient (< 5% peak on Xeon)
- Collaboration with Intel to improve efficiency
  - Specialized matrix multiplication software (MKL, LIBXSMM)
  - Explicit unrolling of small loops (specialized 2D, 3D code)
  - Vectorization direction matrix multiplication: 128 byte aligned
  - Element-wise operation fusion for vectorization
  - Gemm calls: $\approx$ 60% peak on Xeon
- Performance entire code: $\approx$ 35-40% peak on Xeon (single core)
- Hybrid MPI-OpenMP to increase flexibility (about to start)

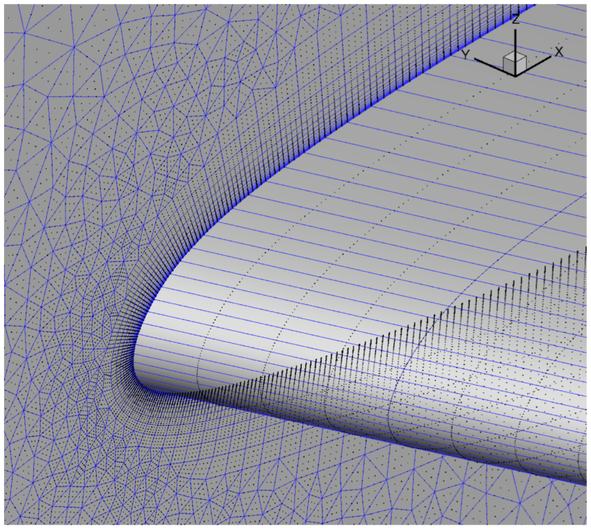
Performance analysis tools (Intel)

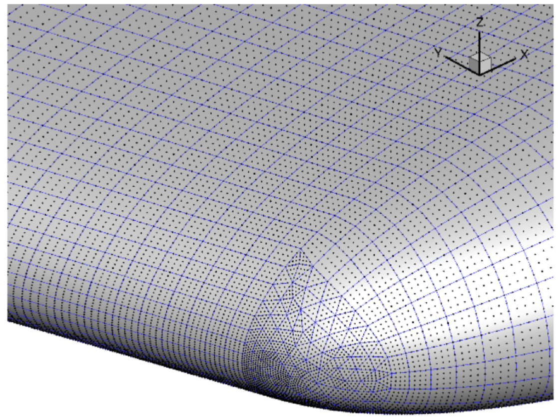


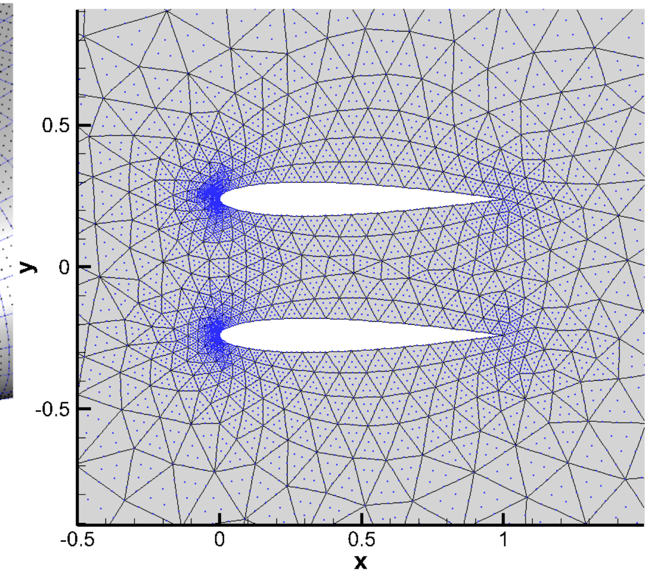
Performance analysis tools (Intel)



Higher-order Grids with Curved Elements (with Pointwise, work of Steve Karman)





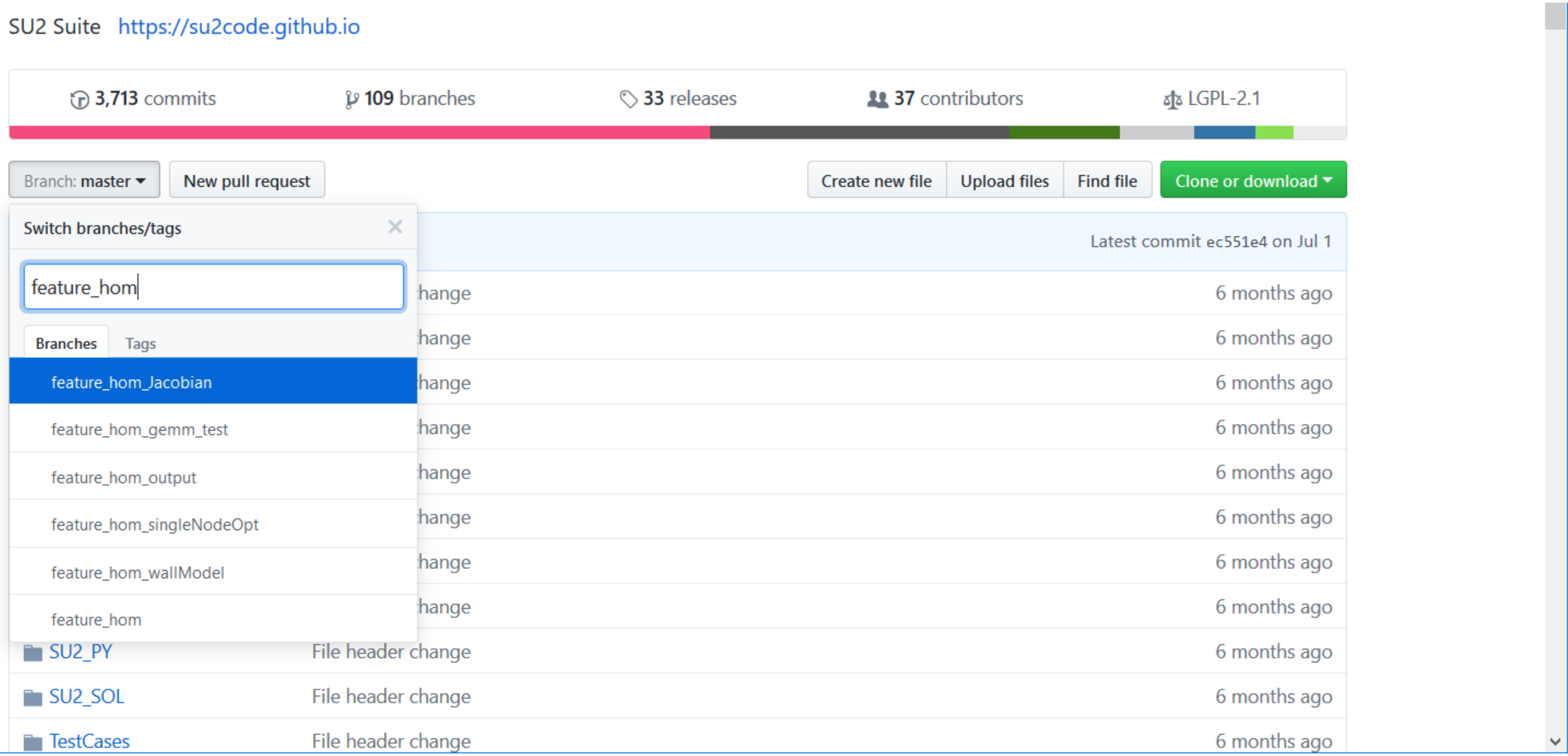


In-house capability to generate higher-order grids for simple cases.

Pointwise V18.2 will have degree elevation and mesh curving capabilities. Available end of September 2018.

Access the code

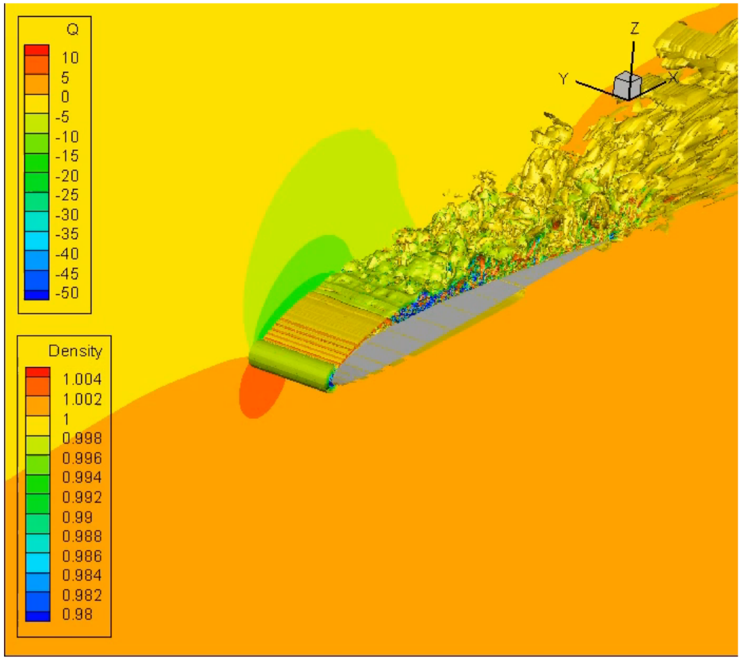
- *feature_hom* branch on GitHub is the main branch for the DG solver. It is about to be merged with develop.
- Several other development branches exist

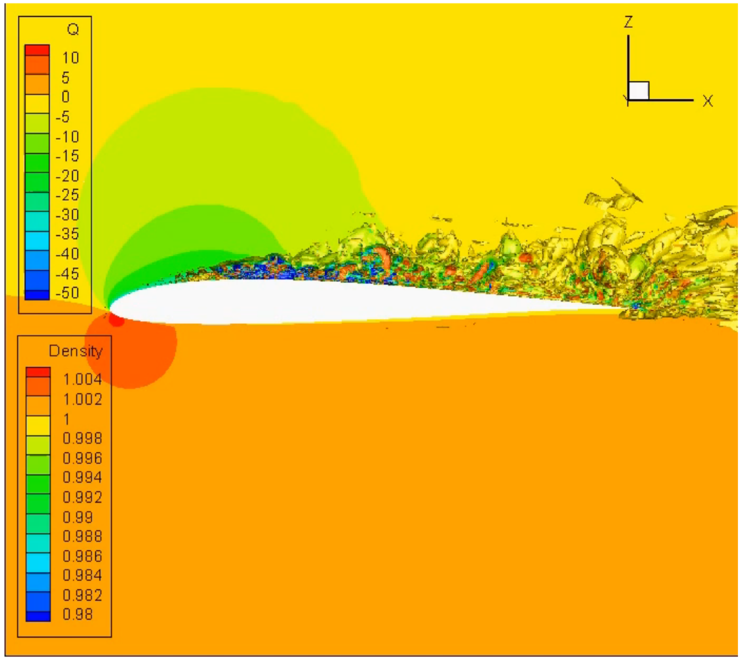


Future Work DG-FEM

- Finish Shock Capturing and LES wall models
- LES statistics (common to DDES and URANS)
- Improve boundary conditions (non-reflective)
- Improve time step estimates by eigenvalue analysis of the Jacobian matrix (computed with CodiPack)
- Parallel performance optimization, including OpenMP
- Entropy variables
- Hybridized techniques, e.g. Embedded Discontinuous Galerkin (EDG), to reduce computational requirements
- Implicit algorithms
- Discrete adjoint version
- Verification and Validation (Manufactured solutions)

Results, viscous
Implicit LES, SD 7003 (Reynolds = 60,000)





p = 4, hexahedra