Numerical Simulations of General Conservation Laws Using the Space-Time Conservative CESE Method

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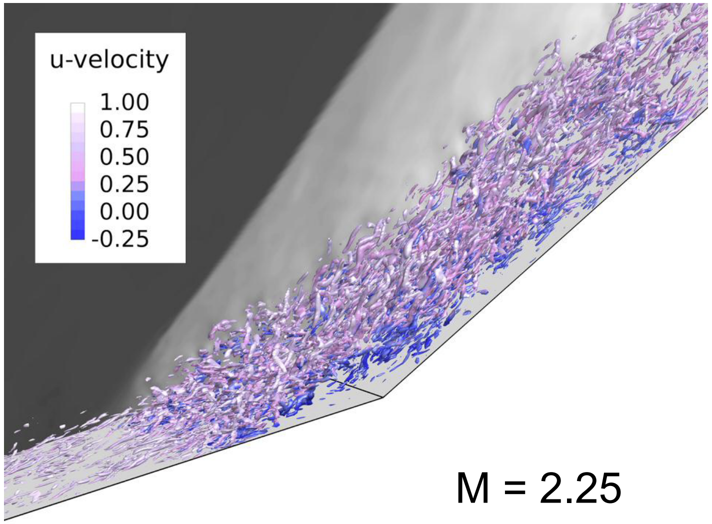
To Dr. I-Shih Chang of Aerospace Corporation (1945-2014)

- For his passion, love and contribution to his motherland, in rocket propulsion and to the CESE method

Outline

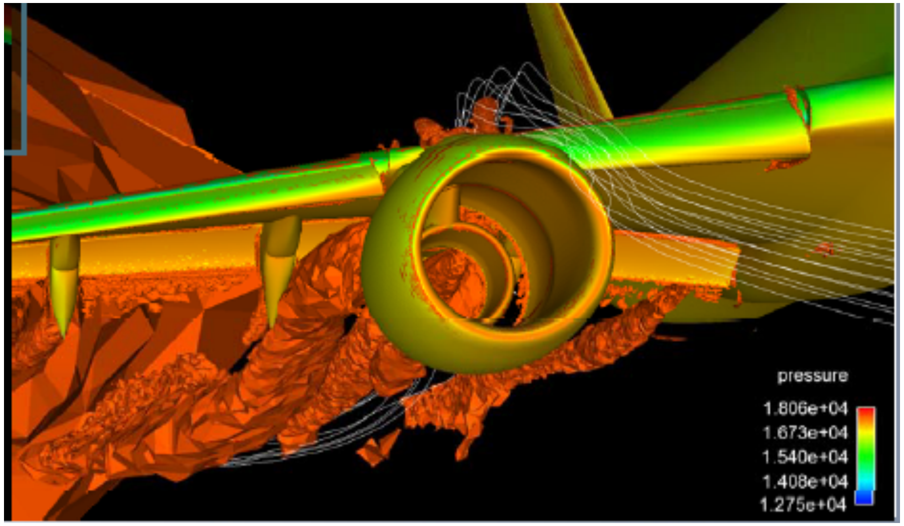
- Background
- The space-time CESE method
- Current applications in fluid dynamics
- Applications to other disciplines
- Concluding remarks

Examples of critical complex flow physics



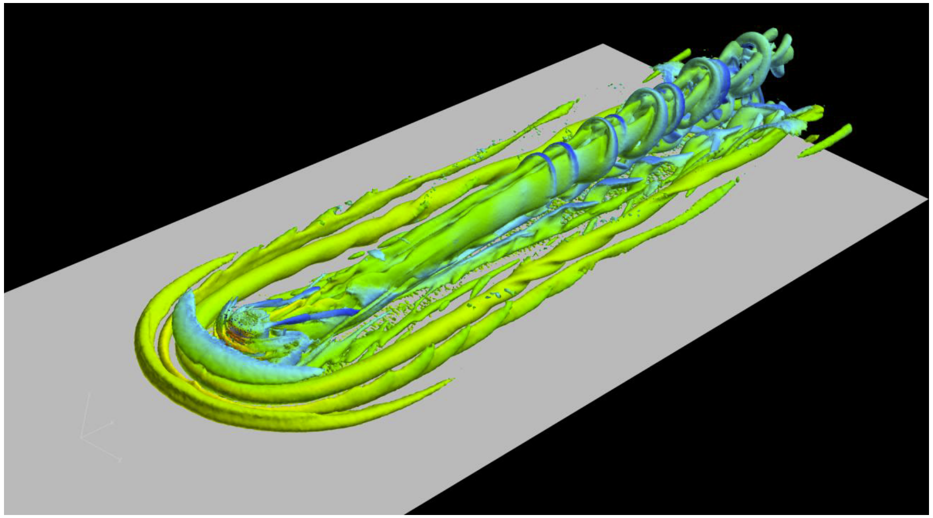
M = 2.25

Bisek, N and Poggie J., "Large Eddy Simulations of Separated Supersonic Flow with Plasma Control," AFRL presentation, April 23, 2013.



http://www.fzt.haw-hamburg.de/pers/Scholz/dglr/hh/text_2012_01_26_CFD.pdf

Q (second invariant of the velocity gradient tensor) isosurfaces with color shaded by temperature



Supersonic (Mach 6) transition induced by roughness

Future CFD Software

- Complex geometries
- Time-accurate computations routine
- Multi-discipline calculations routine
- Increasing fidelity and accuracy requirements
- (Parallel) efficiency and robustness in massively parallel clusters
- Output and visualize large 3D, unsteady data set

Conservation Laws

- Fundamental physics dictates conservations of
  - Mass
  - Momentum, force
  - Energy
- Other derivable or non-derivable equations
  - Can be cast in conservative forms
  - E.g. wave equations, Schrodinger equations
- Discretized solutions in space-time domain
  - Local/global conservation critical
    - Resolve flow discontinuities and unsteady waves
  - Conservation in time important for unsteady problems
    - Temporal accuracy
    - Easy treatment of boundary conditions

Numerical/Software Framework for Multi-Discipline Simulations

- Mesh handler
  - General unstructured/cartesian meshes
  - Flexibilities in control (integration) volumes
  - Low to high order mesh information
- Pluggable physics in conservation laws
  - Ideally in certain software template forms
- Schemas for different methods of integrations
  - Explicit schemes vary in integration paths and integral equations
  - Implicit schemes require efficient large matrix solvers
- Pluggable boundary/initial conditions
  - In dynamically link library (DLL) or template forms
  - Allowing communications between codes/data
- Multi-core/CPU/GPU parallel computation infrastructures
  - Independent of computational modules
- Output modules
  - Allowing flexible user outputs in DLL or file sharing modules

Core Ideas of the CESE Method (I)

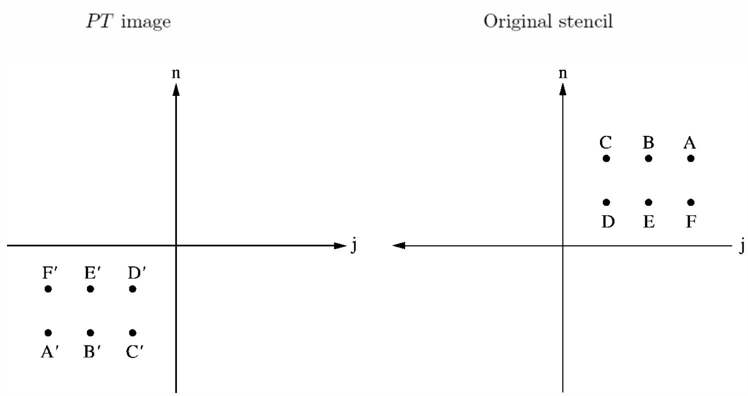
- Construction of non-dissipative schemes
  - By solving derivatives using individual CE
  - Alternatively by solving derivatives using dependent variables at vertices

$$Q(x,y,t) = Q_0 + Q_t(t - t_0) + Q_x(x - x_0) + Q_y(y - y_0)$$

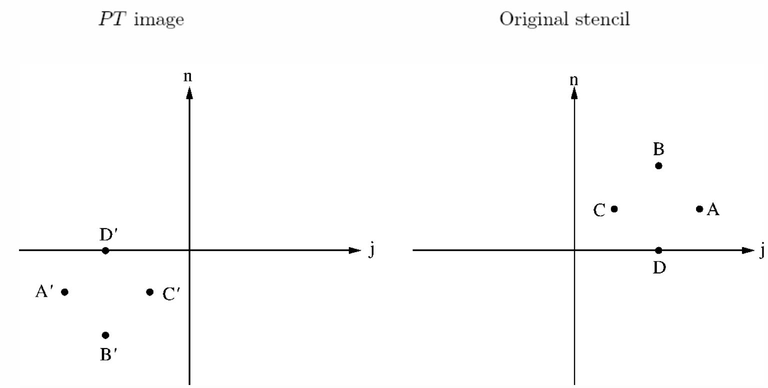
- Add numerical dissipation as desired
  - Via modification of derivatives
- Allows numerical dissipation controls
  - Numerical dissipation scales with smallest grid spacing
  - Alternative form of subgrid scale modeling

PT Invariant, Non-dissipative Core CESE Schemes (S.-C. Chang)

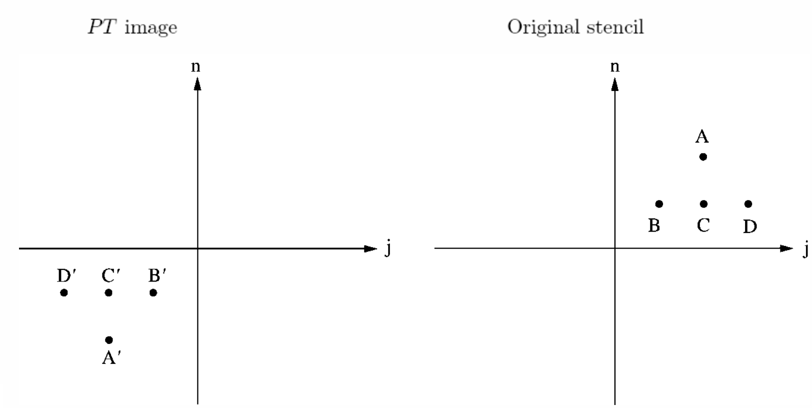
- Parity (spatial-reflection) and time reversal
- Symmetric stencil in space-time



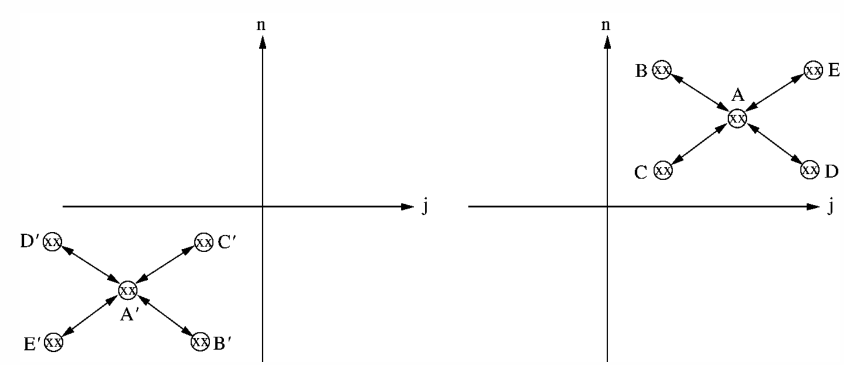
Crank-Nicolson



Leapfrog scheme



Lax-Wendroff



The scheme is two-level, explicit, and PT invariant.

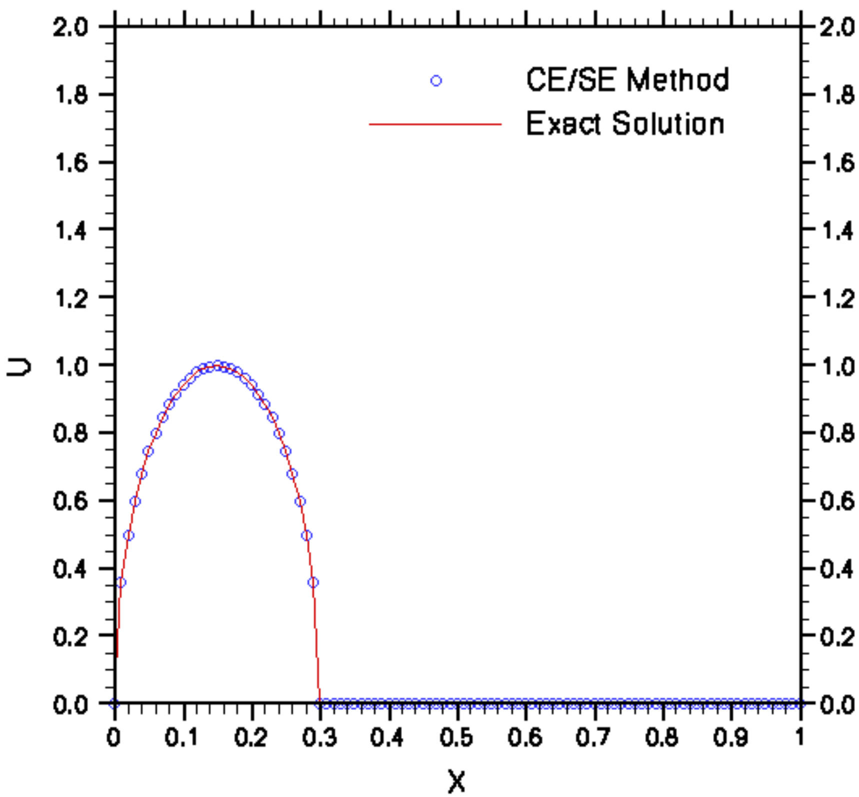
$$(x,t) \leftrightarrow (-x,-t)$$

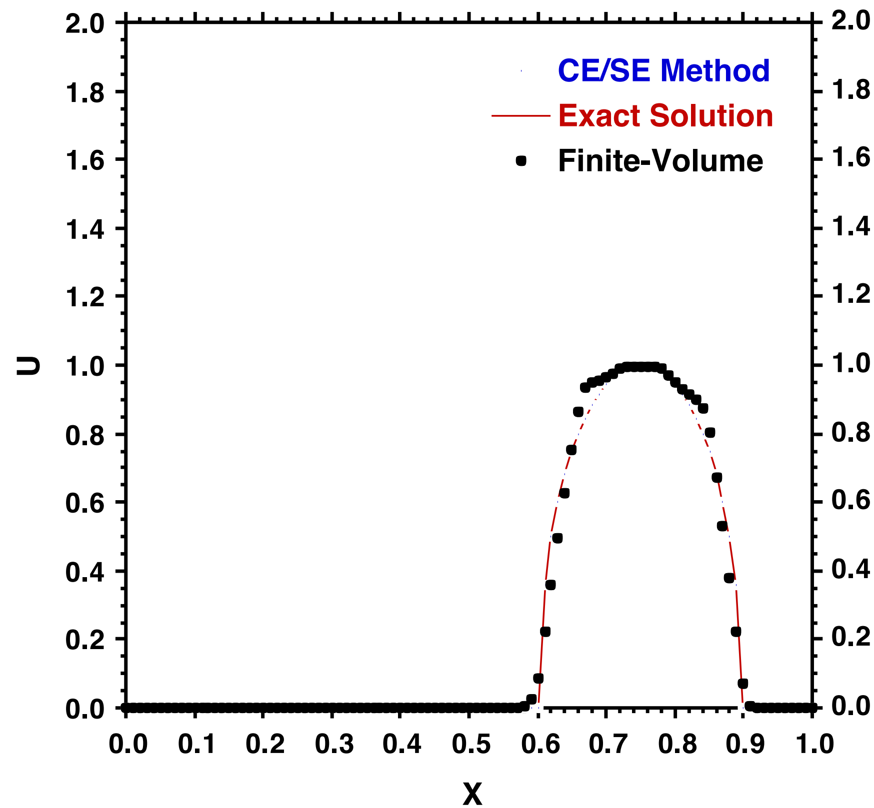
CESE a-scheme

Elliptical Wave Propagation Using the CESE Method

The space-time conservation element, solution element (CESE) method

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$





Courtesy I.-S. Chang, Aerospace Corp.

Zalesak, S. T., “A Preliminary Comparison of Modern Shock-Capturing Schemes: Linear Advection,” Advances In Computer Methods for Partial Differential Equations, Vol. VI, ed. R. Vichnevetsky and R. S. Stepleman, Proceedings of the 6th IMACS Inter’ l Symp., pp.15-22, June 23-25, 1987.

Numerical Formulation

- Conventional schemes

$$\frac{dQ}{dt}V = -\sum_{i=1}^{N}\int_{S_i} F \bullet d\vec{s} + \int_V K dV$$

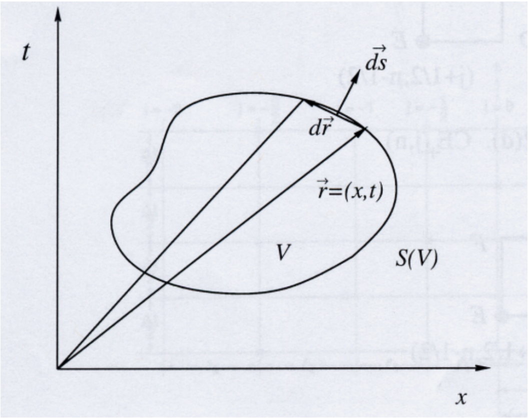
Explicit, implicit time advancement

Spatial integration, FEM or FVM

- In CESE, unified temporal and spatial volume integration
  - In strong form

$$\oint_{CE} \vec{h} \bullet d\vec{s} = 0$$

$$\vec{h} = (Q, E, F, G) \qquad \vec{s} = (t, x, y, z)$$

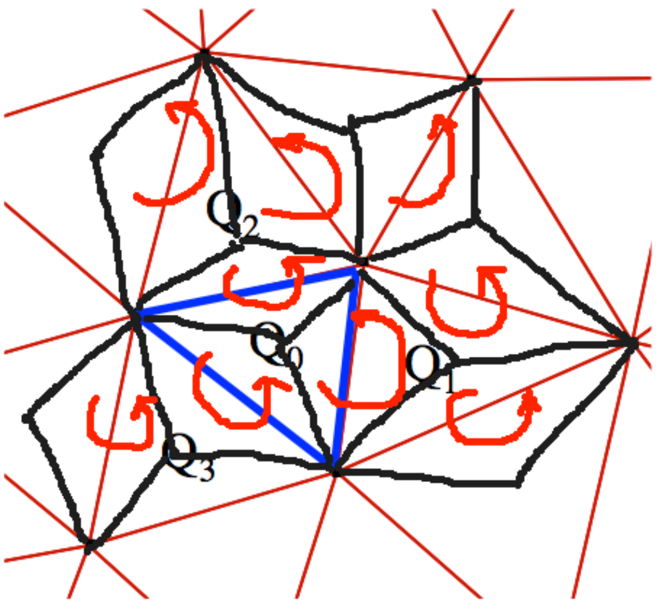


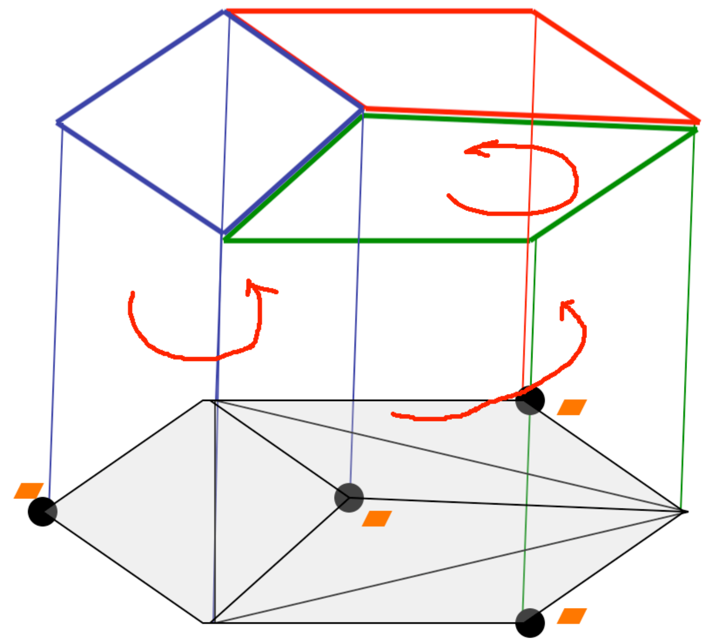
$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = 0$$

Differential form only
Used to compute time derivatives

Core Ideas of the CESE Method (II)

- Local and global *space* and *time* conservation
- Sum of total flux equals to boundary fluxes
- Flux vectors only functions of dependent variables expressed in finite series expansions



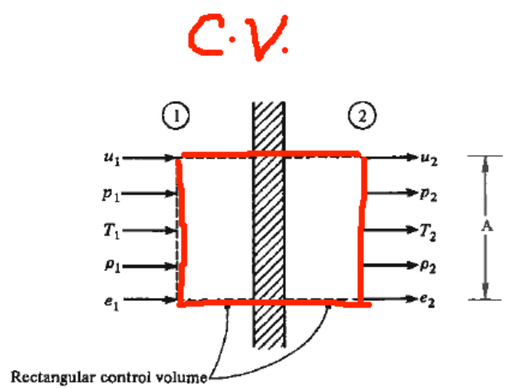


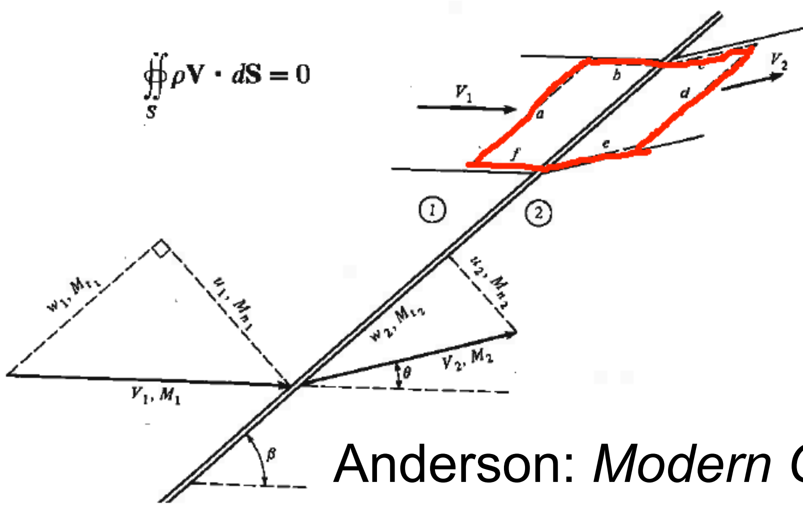
A Note on Entropy and Kinetic Energy Preserving Schemes

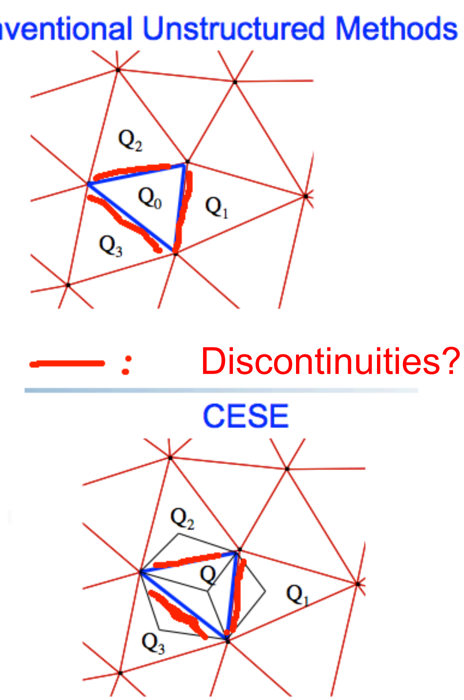
- Global conservation of the CESE framework guarantees that entropy production only comes from the boundaries
  - No production at cell interfaces
- Kinetic energy is formulated using first-order or third-order polynomials of dependent variables, no alternative forms are intrinsic to the formulation
- Flux vectors are functions of the approximation polynomials with no ad-hoc reconstructions required
  - Degree of conservation of fundamental laws depends on polynomial order only

Core Ideas of the CESE Method (III)

- Distinguishing solution elements and conservation elements (control volume)

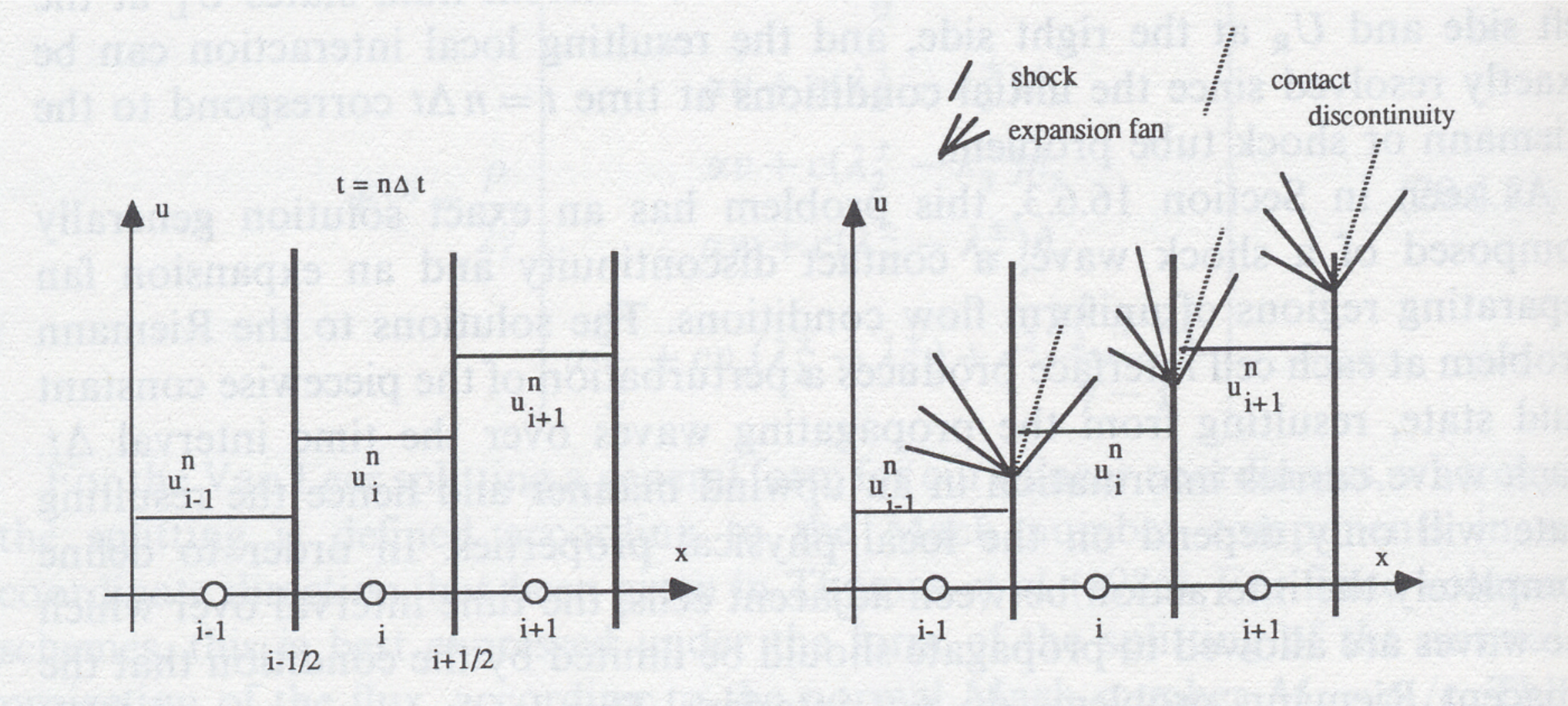






Anderson: *Modern Compressible Flows*

Cell Interfaces and Riemann Solvers

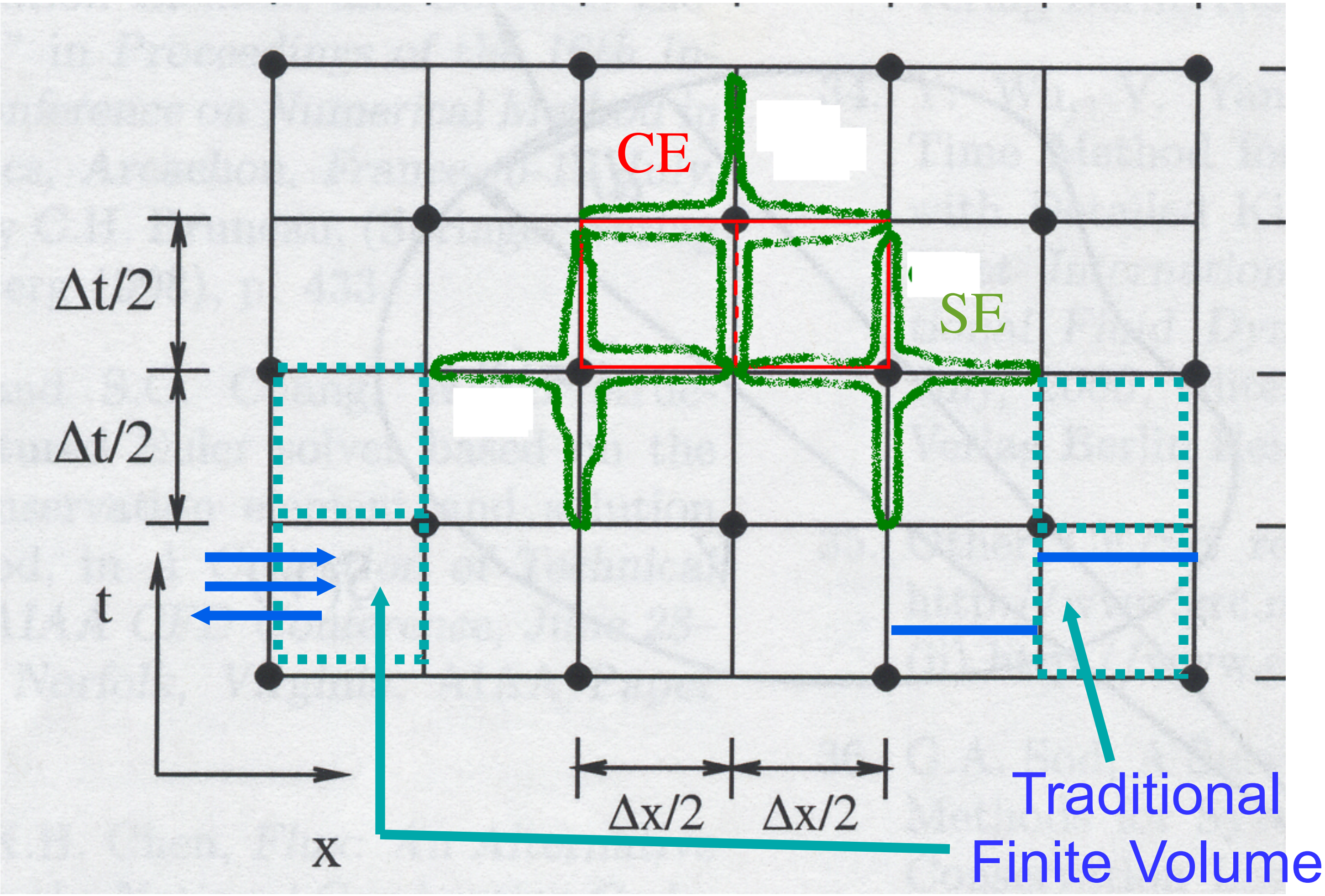


Seeking exact or approximate solution at the discontinuous interfaces

- 1D approximate/exact solution well established
- Dimensional/directional splitting for structured mesh needed
- Multi-dimensional extension for unstructured mesh?

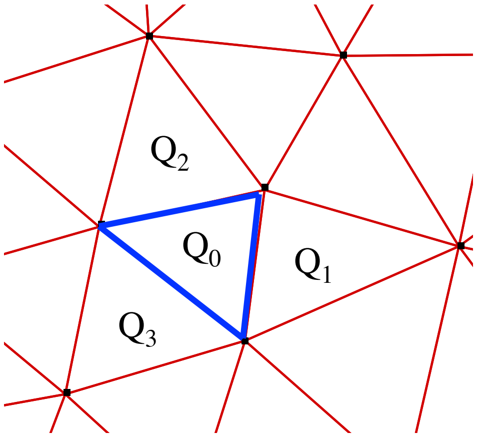
The CESE Method

- Staggered solution element (SE) & conservation element (CE) for flux integration



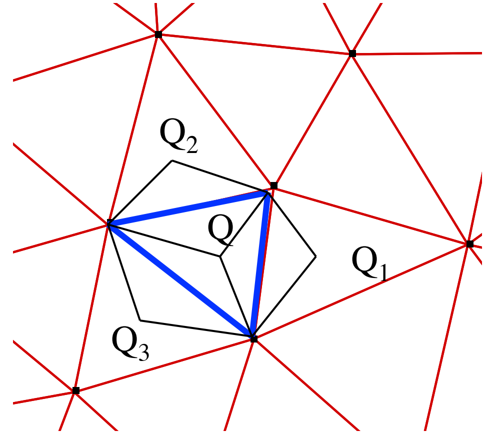
Numerical Flux Integration

Conventional Unstructured Methods



- Solution element : Q_0, blue triangle
- Integration volume : blue triangle
- Three interface integrations:
  - Q_0- Q_1, Q_0 – Q_2 , Q_0- Q_3
  - Three (approximate) Riemann solutions
  - Reconstruct a unique flux vector at the interfaces

CESE



- Solution element (SE) : blue triangle

$$Q(x,y,t)=Q_0+Q_t(t-t_0)+Q_x(x-x_0)+Q_y(y-y_0)$$

- Integration volume : three quads (conservation elements, or CE)
- Six interface integrations:
  - All within an SE
  - No jumps across interfaces
  - No flux reconstruction or Riemann problems needed

Space-Time CESE Method

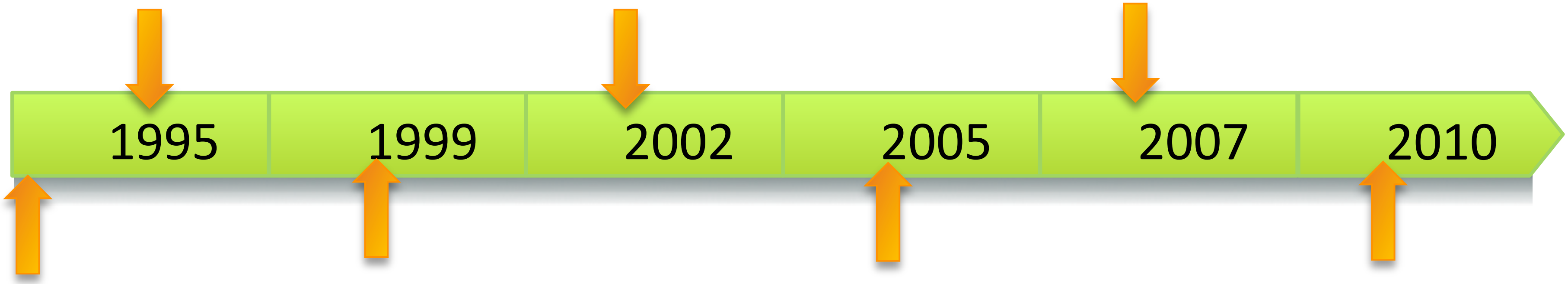
- Flux conservation over discretized space-time domain – not just along spatial coordinates
- Staggered integration volumes (conservation element) and solution volumes (solution element)
  - No cell interface Riemann solution needed
  - No1D approximations at cell interfaces
- Genuine multi-dimensional formulation
  - No dimensional/directional splitting necessary
- Non-dissipative baseline a-scheme
  - Numerical dissipation added when necessary
- Simplicity – geometry & simple integration

Timeline of the CESE Method Development

S.-C. Chang JCP paper:
layout for non-dissipative schemes and space-time formulations

Zhang, Yu & S.-C. Chang: quad. and hex. Meshes
S.-C. Chang: Courant number insensitive schemes

C.-L. Chang: edge-base derivatives approaches, triangular/tetrahedral viscous simulations



S.-C. Chang: NASA TM, 1991, 1993

X. Wang & S.-C. Chang: staggered triangular mesh CESE schemes

S.-C. Chang, Wu, Yang & Wang: time-accurate local stepping for 1D flows

S.-C. Chang: high-order CESE methods for general conservation laws

Time-accurate Computations

- Accuracy
  - High-order temporal and spatial formulations
  - Numerical dissipation control
  - Resolving discontinuities/waves simultaneously
- Efficiency
  - Time step (CFL number) determined by physics, not numerics
  - Local time stepping for multi-scale, multi-physics
  - Scalable parallel computations
- Robustness
  - Numerical stability, minimal attention
  - Complex geometries
    - Unstructured or Cartesian meshes

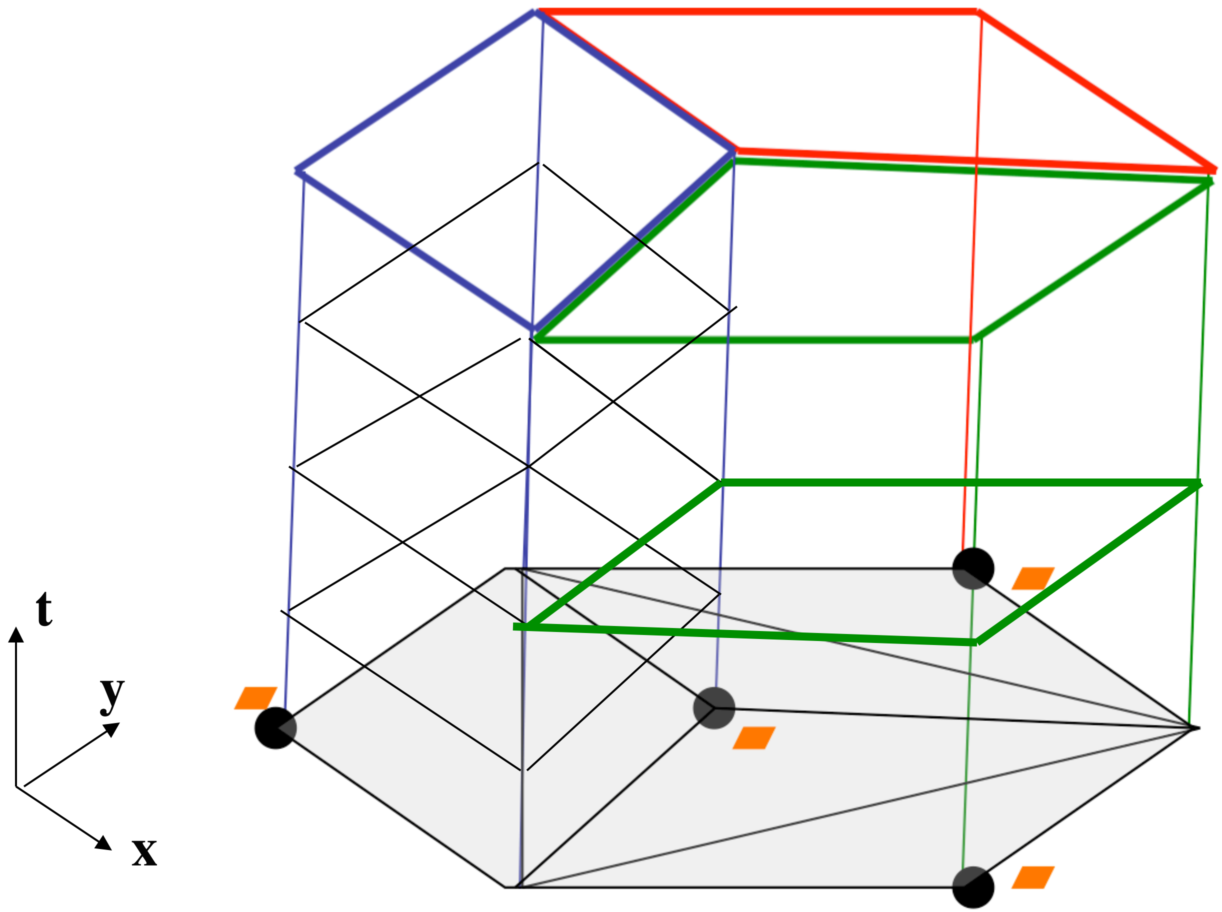
CESE Development Toward Large-Scale Multi-discipline LES Simulations

- Time-accurate local time stepping (TALTS)
  - Unsteady simulations with a large disparity of spatial (thus temporal) scales
  - Improve accuracy/efficiency
- High-order (4^{th} or higher) formulations
  - Explicit schemes, simulating acoustic scales
  - CFL bound < 1, regardless of order of accuracy
- Tetrahedral mesh
  - Free of "orientation", dissipation ideal for small scales
- Moving boundary formulation in the context of space-time conservation

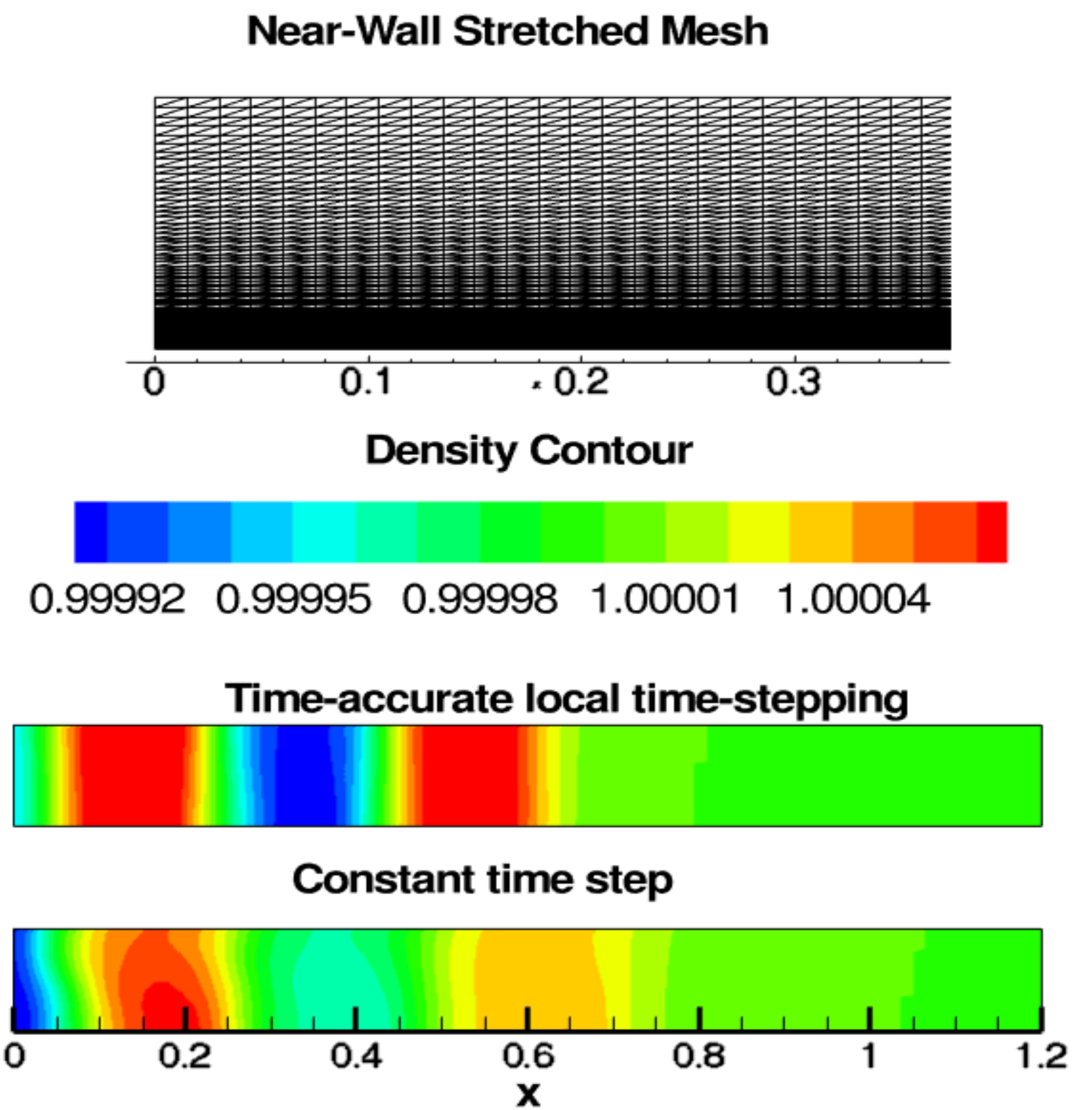
Time-accurate local time-stepping (TALTS) CESE method

- Preserve temporal accuracy
  - Flux conservation enforced in the space-time domain through space-time flux integration
- Accurate solutions for both time-dependent and state-state problems
- Numerical methods
  - Sorting time steps: calculate time steps using a CFL number, let Δt = minimum time step, construct allowable array of time steps by $f(k) = 2^k \Delta t$
  - Determining solution levels
  - Integrating flux in space-time with patches with a physical clock

Topology for time-accurate local time-stepping flux integration

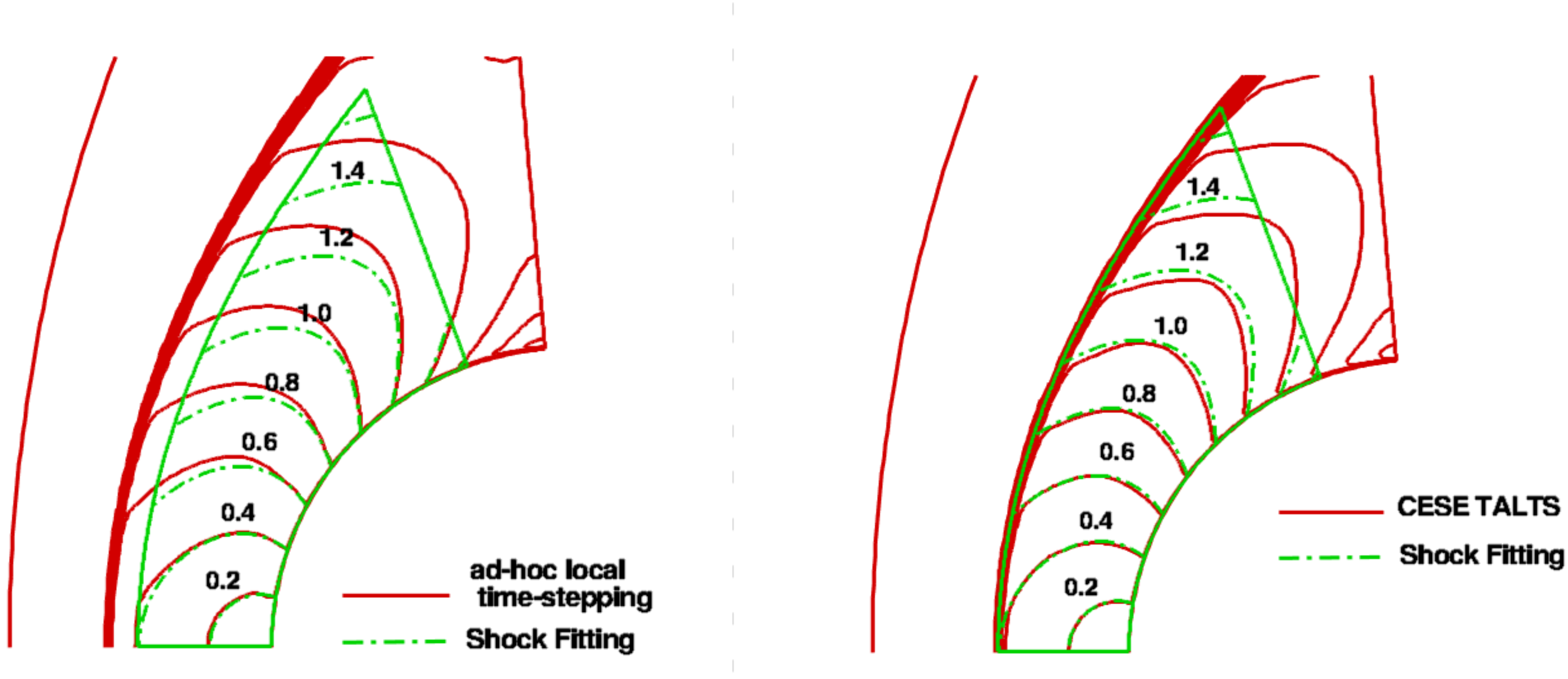


Acoustic Wave Propagation with Non-Uniform Mesh



Mach 6 Flow over a Cylinder

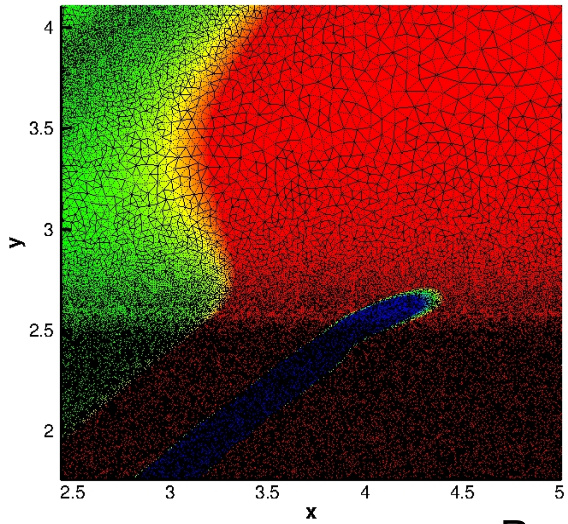
- Navier-Stokes computations with triangular mesh
  - Max. aspect ratio = 10^3 and $\Delta t_{max}/\Delta t_{min} = 2^{10}$

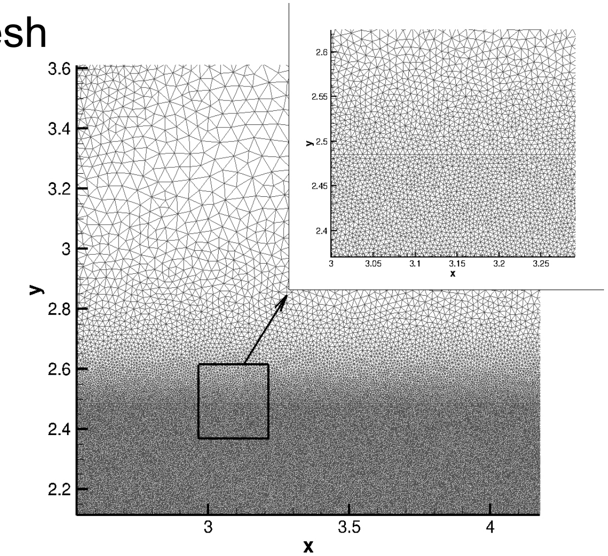


Shock-fitting solutions by: Salas, M. D. and Atkins, H. L., “On Problems Associated with Grid Convergence of Functionals,” *Computers & Fluids*, Vol. 38, Issue 7, pp. 1145-1454, 2009.

Mach 1.6 flow over a Cone with Counterflowing Jet

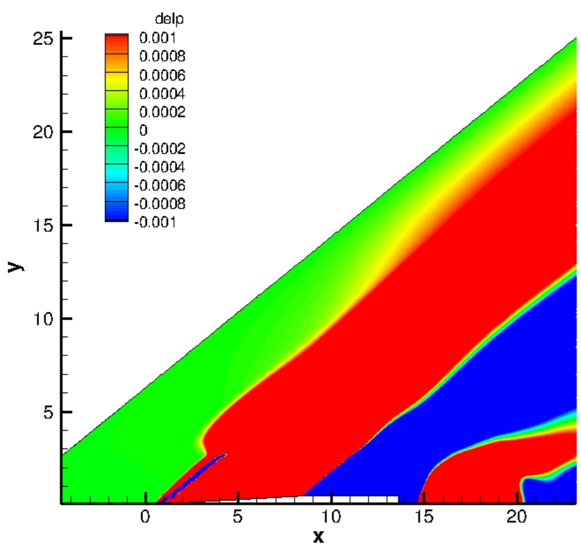
Mesh



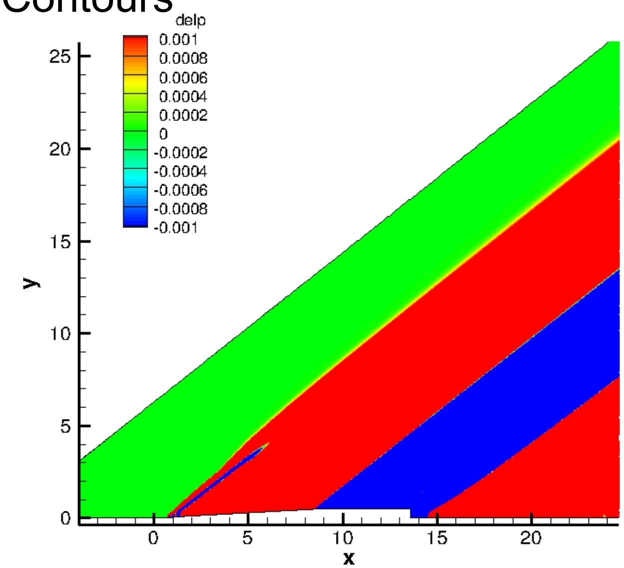


$\Delta t_{max}/\Delta t_{min} = 2^{11}$

Pressure Contours



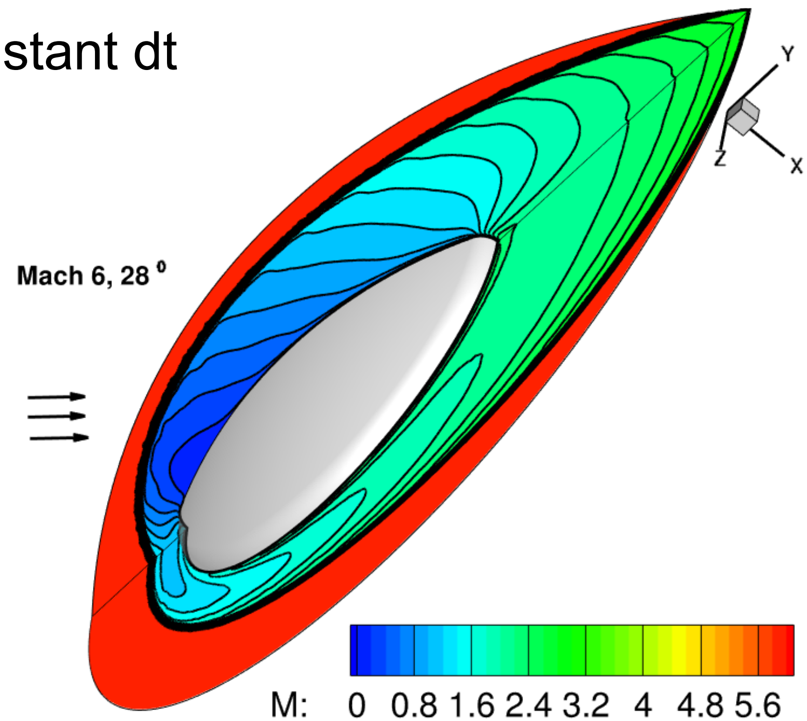
Constant time step



Time-accurate local time-stepping

Mach 6 flow over a large blunt body with 28° angle of attack

- 32 million tetrahedral elements, $\Delta t_{max}/\Delta t_{min} = 2^9$
  - Unknowns are U, U_x, U_y, and U_z
  - Using 120 Sandy Bridge cores
- Computational time (wall clock)
  - 1.38 sec/iteration using TALTS
  - 4.20 sec/iteration using constant dt
  - Non-ideal load balancing



High-Order CESE Methods

- Introduced by S.-C. Chang 2010
- Numerical framework allows constructions of 4^{th}, 6^{th}, 8^{th}, and higher order CESE schemes
  - Odd orders can also be formulated
- With identical compact stencil for quad/triangle or tetrahedral/hexahedral meshes
- Numerically stable for CFL < 1
  - No reduction in CFL limit as order of accuracy increases as in many explicit high-order methods

4^{th}-order CESE Method

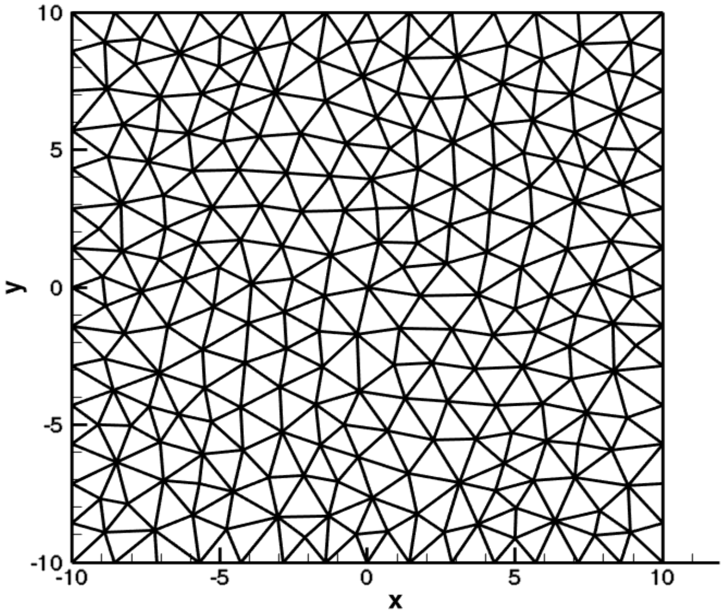
- Solve 2^{nd} derivative equations using 2^{nd}-order schemes
- Calculate 3^{rd} derivatives using finite-differences
- High-order flux integrations over discretized space-time conservation elements, solve for zero-th derivatives
  - High-order moments on top and bottom faces
  - High-order Gaussian quadrature on side faces
    - Alternatively, Jacobian tensors can be derived for flux vectors and used for integration (tedious)
- Solve first derivatives using finite differences, apply numerical dissipation
- Calculate temporal derivatives using governing equations

$$U_{tt} = \frac{\partial F_{xt}}{\partial x} + \frac{\partial F_{yt}}{\partial y} + \frac{\partial F_{zt}}{\partial z}$$

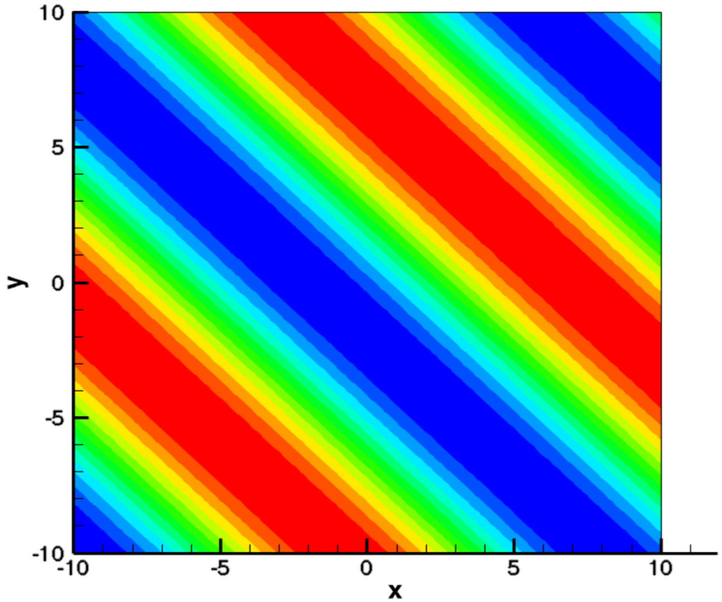
- Computational time (with Mathematica generated expressions, non-optimized) is about 25~32 times the 2^{nd} order code

Verification with Full Euler Equations

- Acoustic wave propagating diagonally through a square domain with isotropic triangular mesh
- Compared with linear acoustic wave solutions



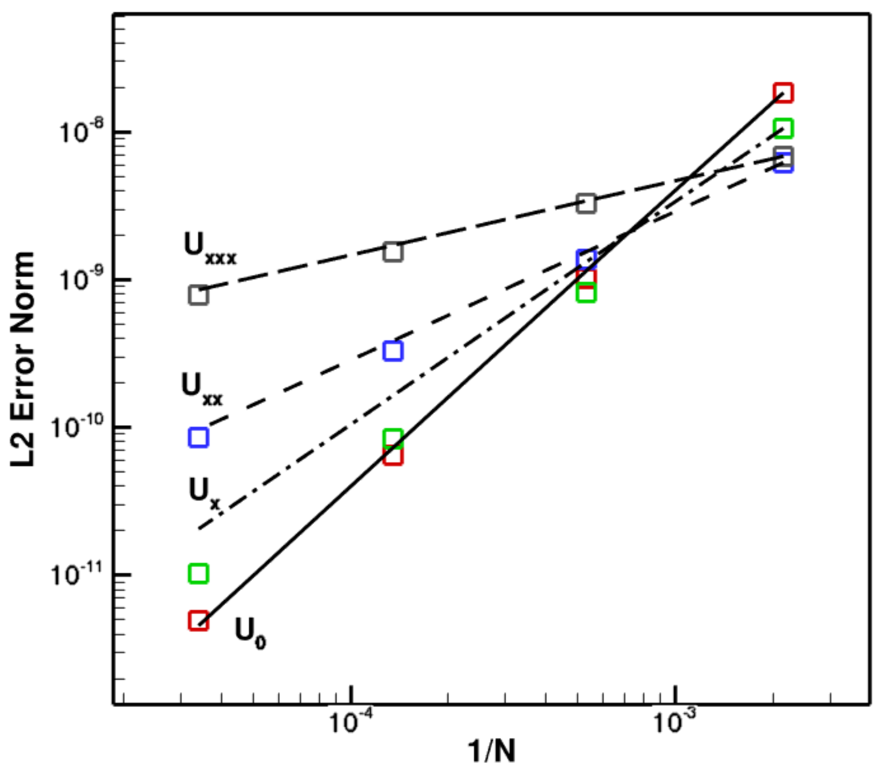
Triangular mesh



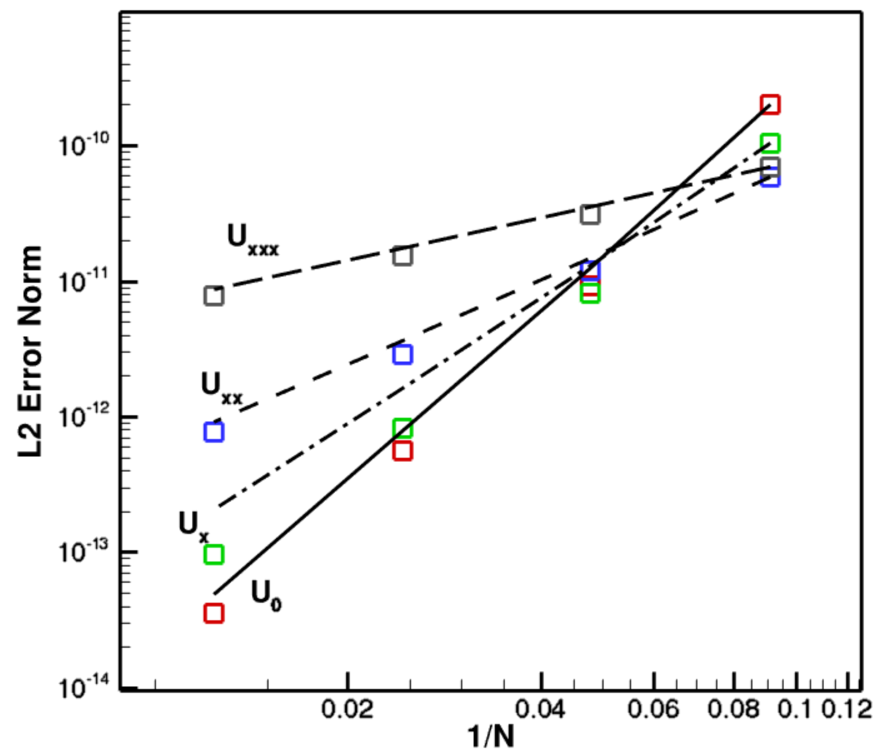
Velocity contours

Verification with Full Euler Equations

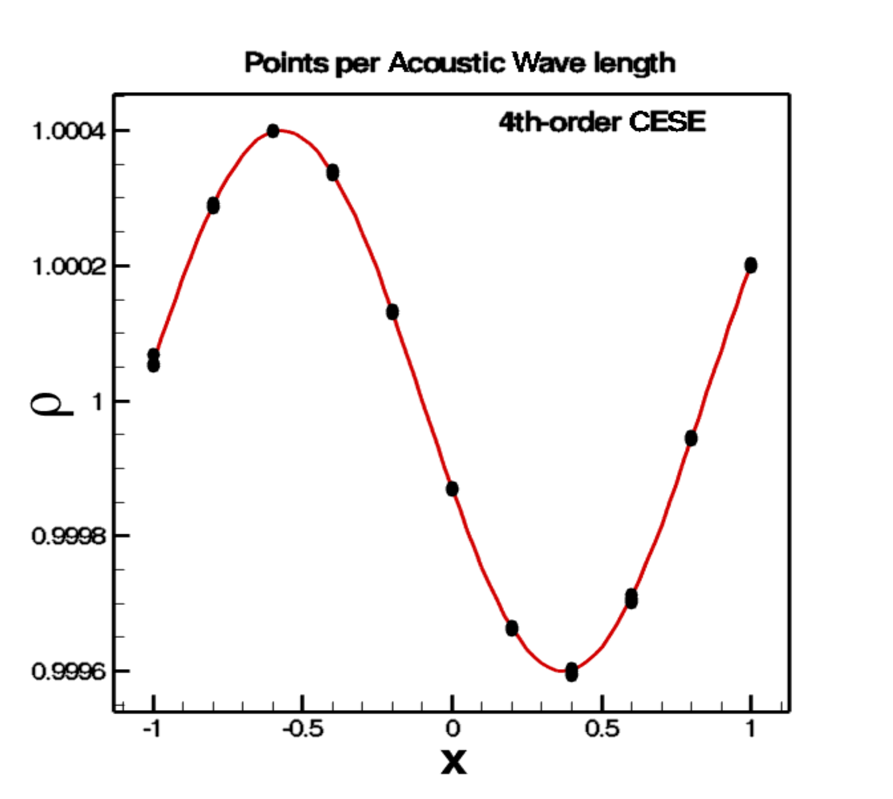
Amplitude = 10^{-6}

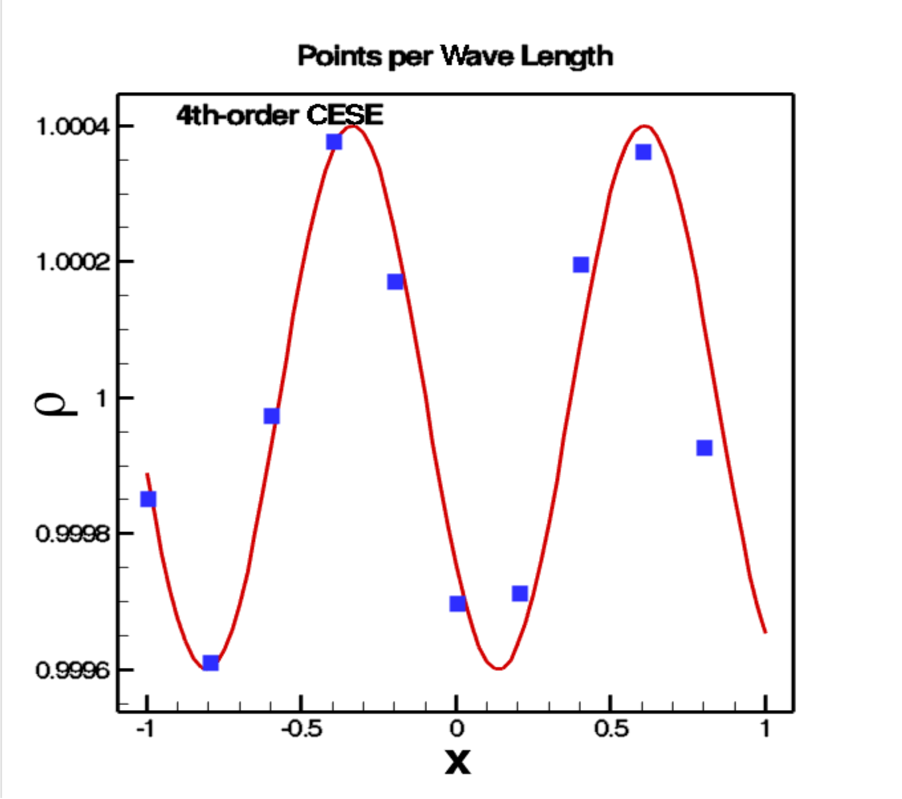


Amplitude = 10^{-8}



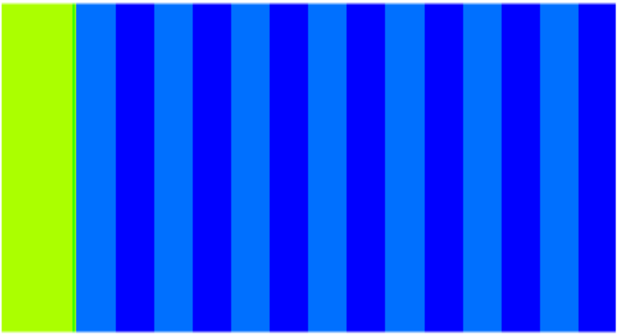
Grid Resolution Required for Waves

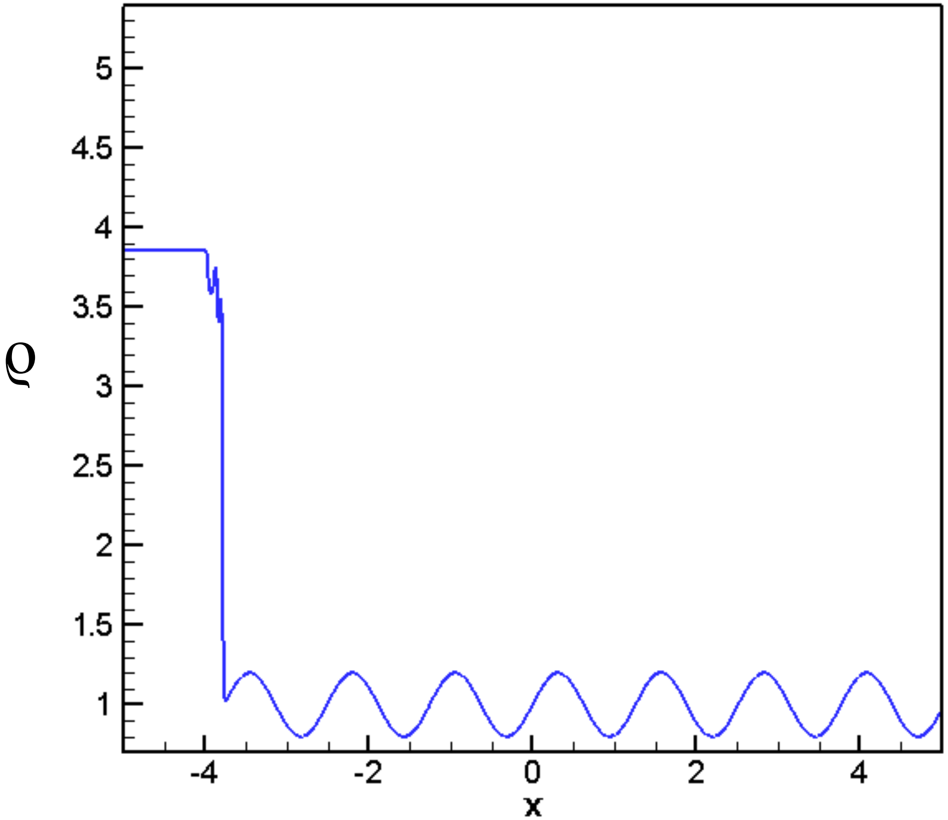




1D Shock-Acoustic Wave Interaction

Used by ENO, WENO, schemes to validate accuracy

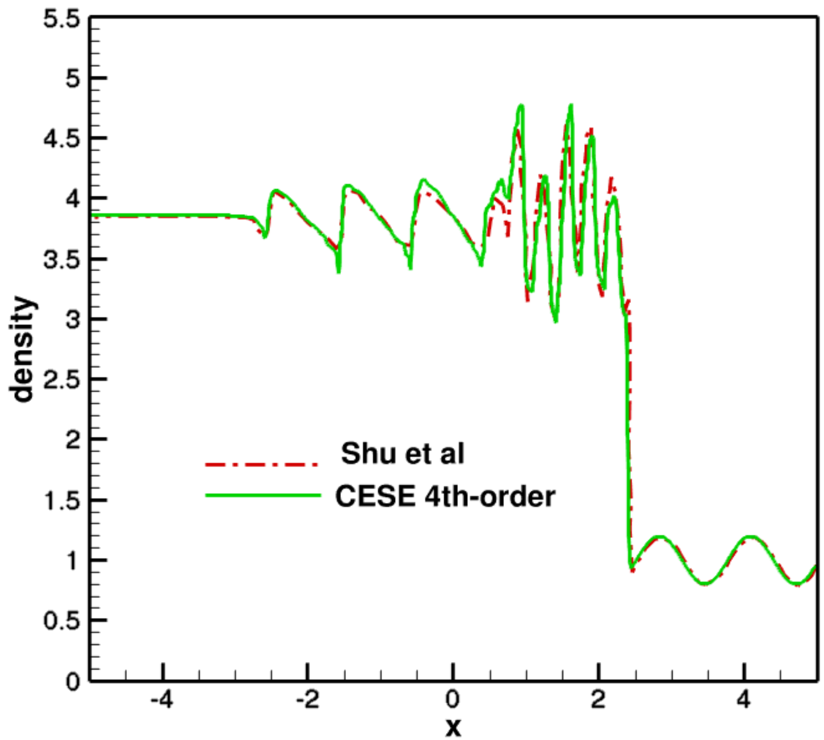


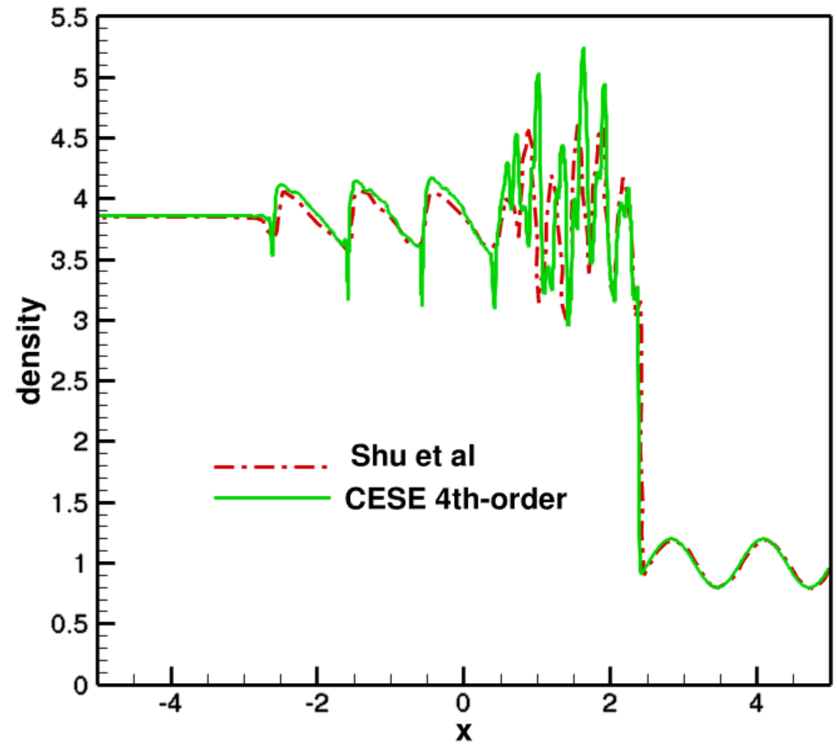


Density Contours and distribution

Shu & Osher Benchmark Problem (Shock/acoustic wave interaction)

1600 points

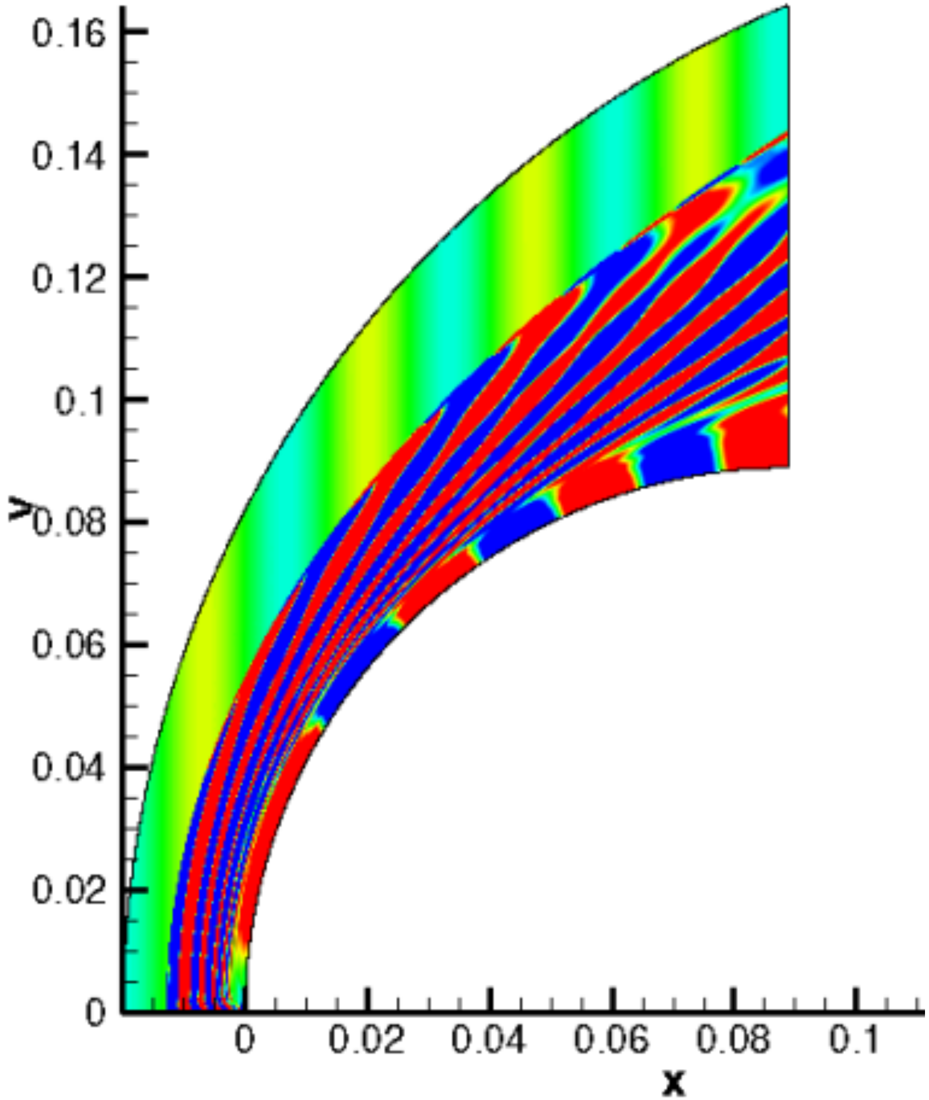




Grid converged solution
With large dissipation

Reduced numerical dissipation

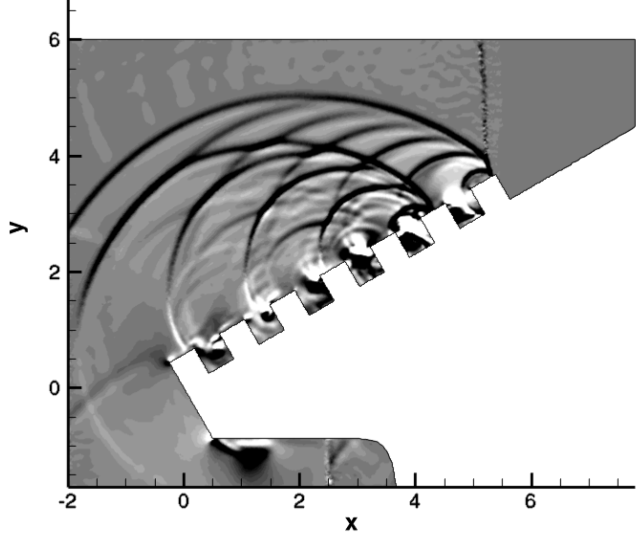
Acoustic Wave/Bow Shock Interaction over a hemisphere at Mach 6



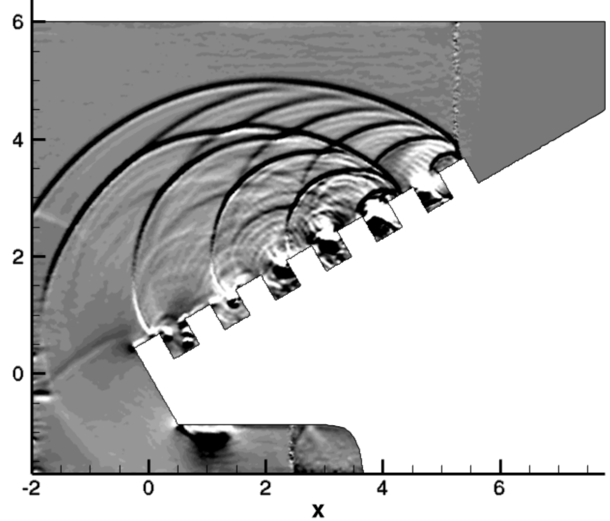
Supersonic flow over a multi-gutter wall

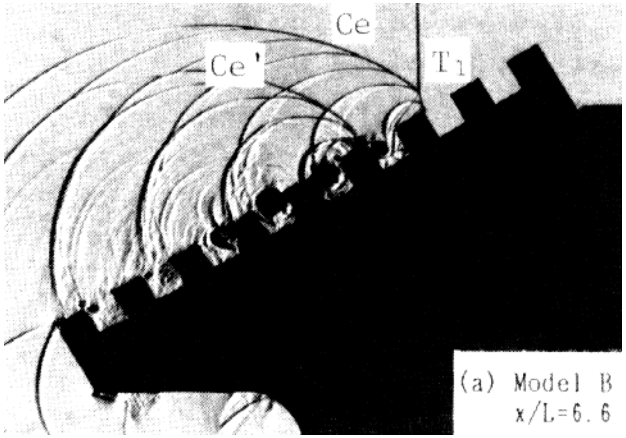
- Mach = 1.41, experiments by Suzuki et al.

2nd-order scheme



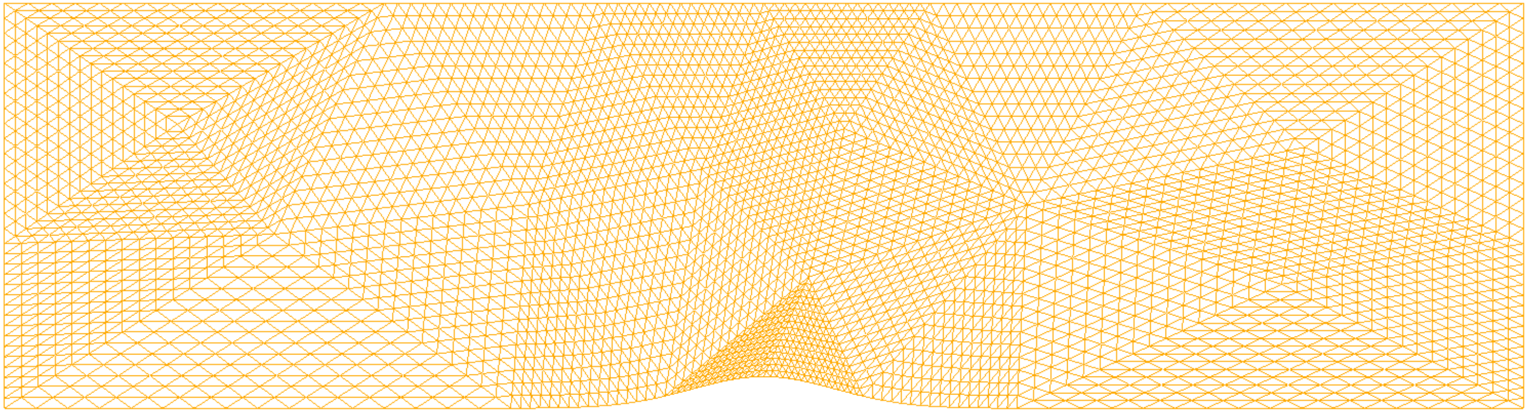
4th-order scheme





High-order Method Workshop Benchmark C1.1

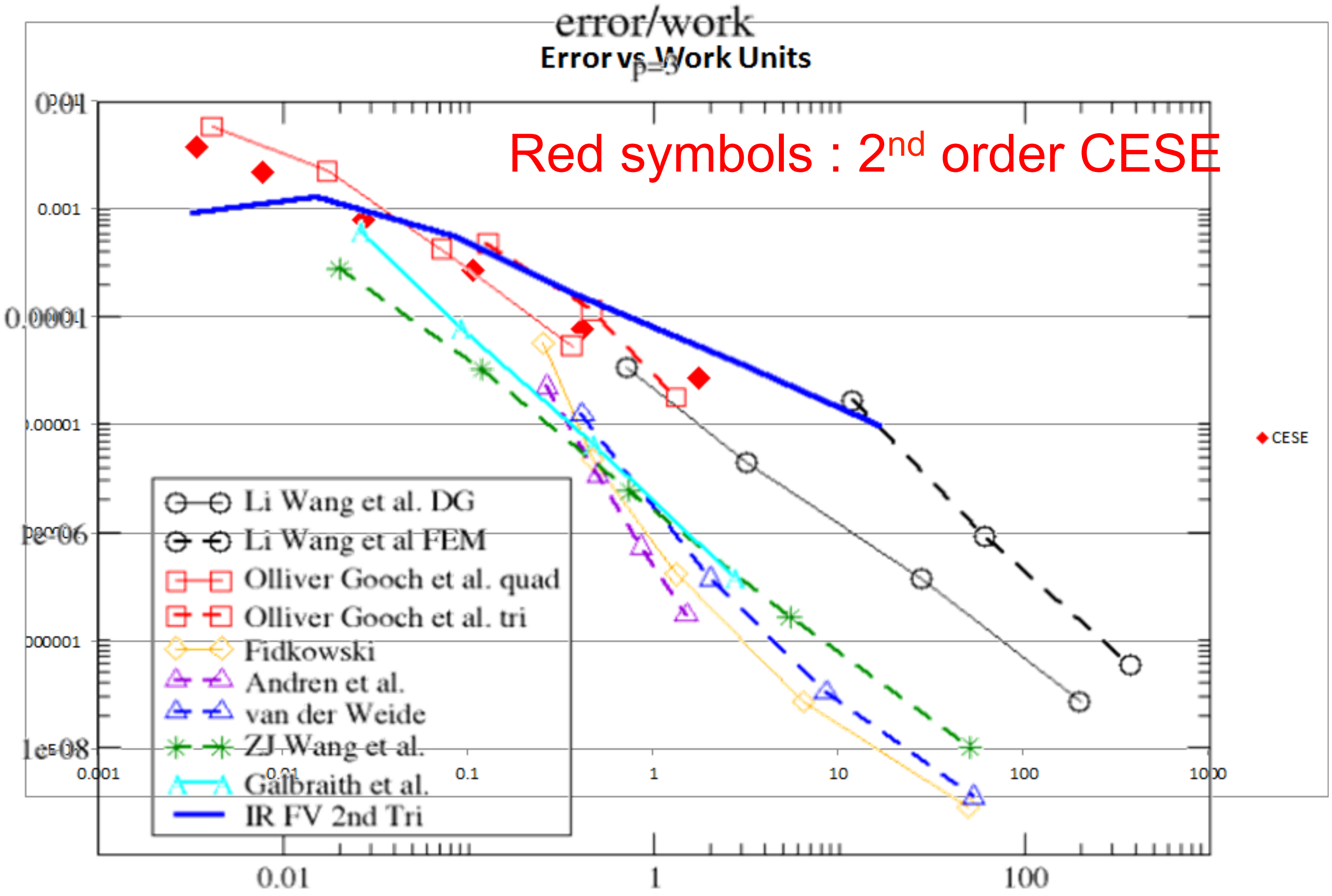
- Done by David Friedlander (GRC)
- Subsonic flow over a bump



Length Scale: 0.0063789
Number of Cells: 8,192

- Grids used were as provided by the workshop

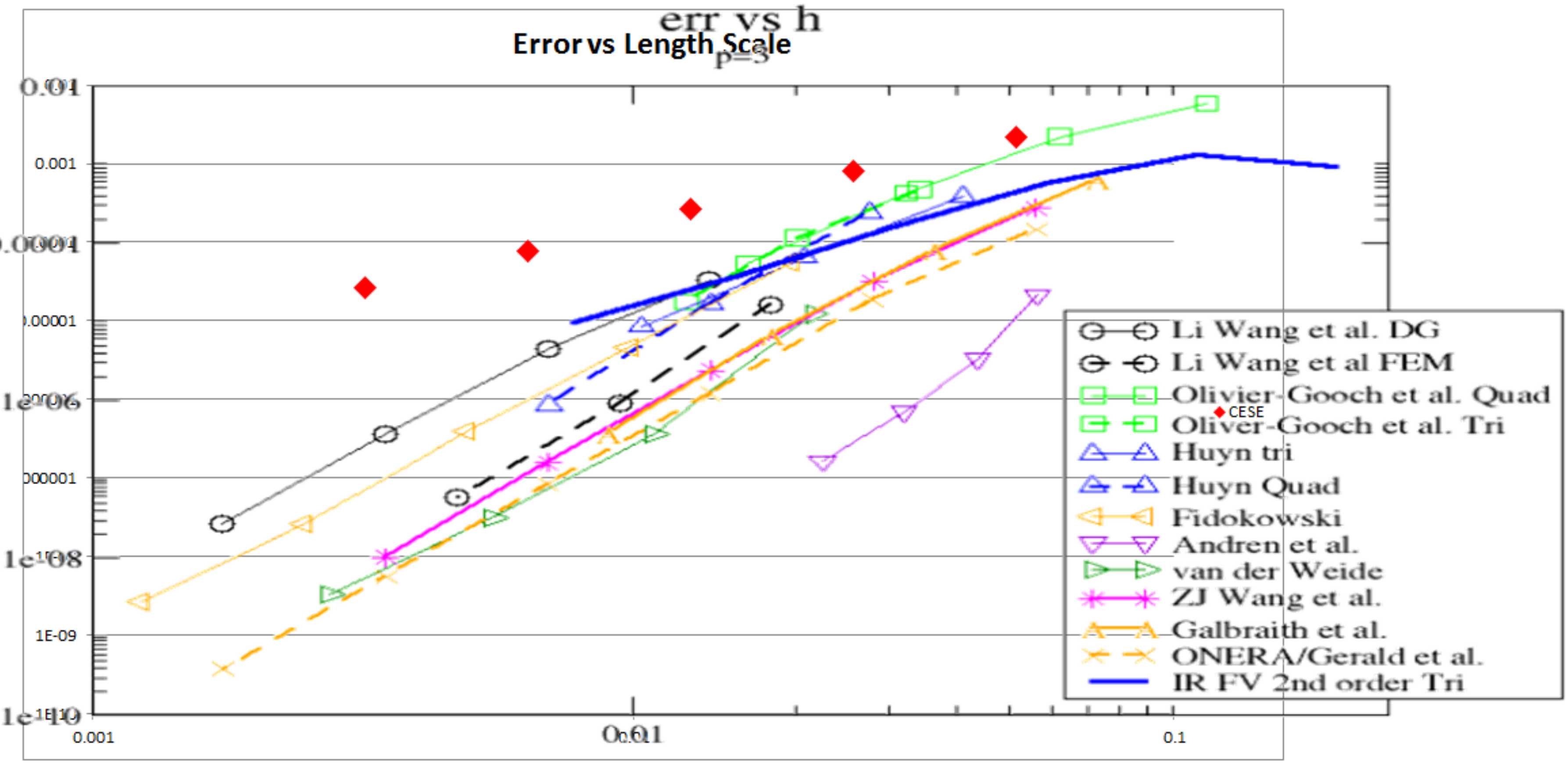
HOM Benchmark C1.1
Error Norm vs. Other Methods (p = 3)



By David Friedlander GRC

HOM Benchmark C1.1
Error Norm vs. other methods (p = 3)

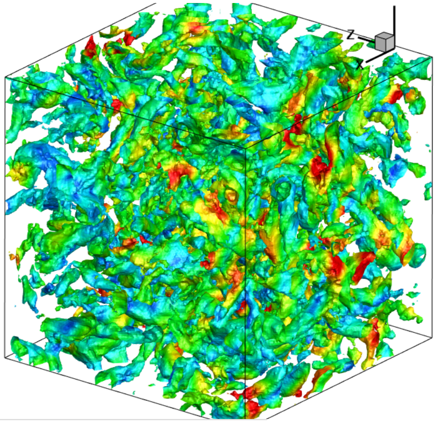
Red symbols : 2nd order CESE

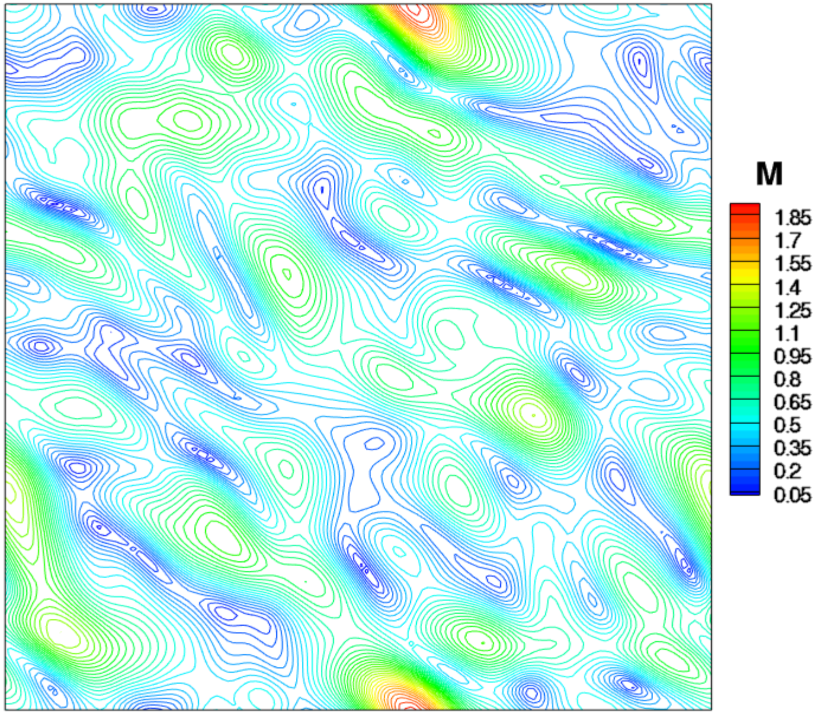


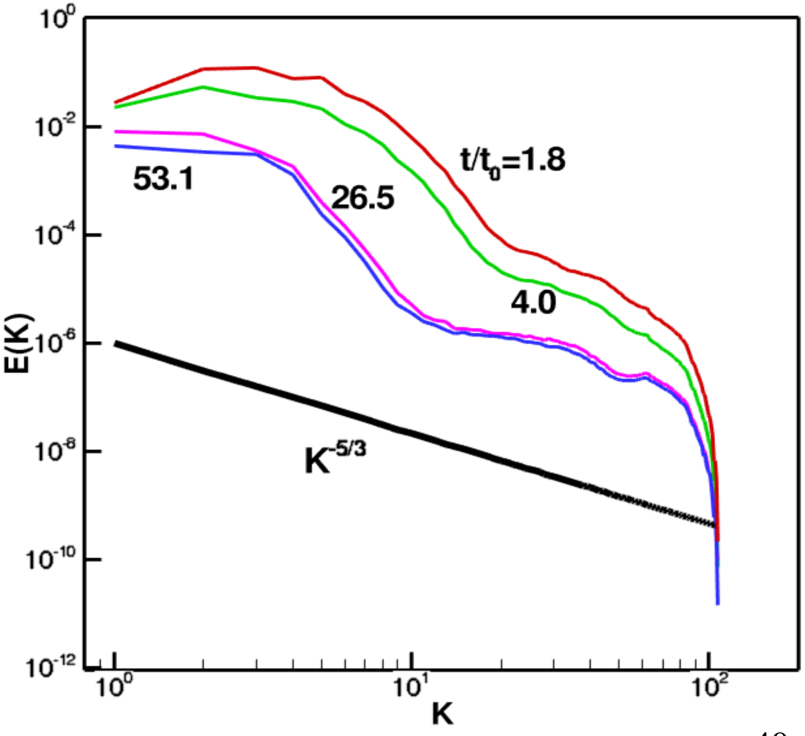
By David Friedlander GRC

Isotropic Turbulence Decay Simulation M_t=0.6, Re_t=100 (64^3 tetrahedrons)

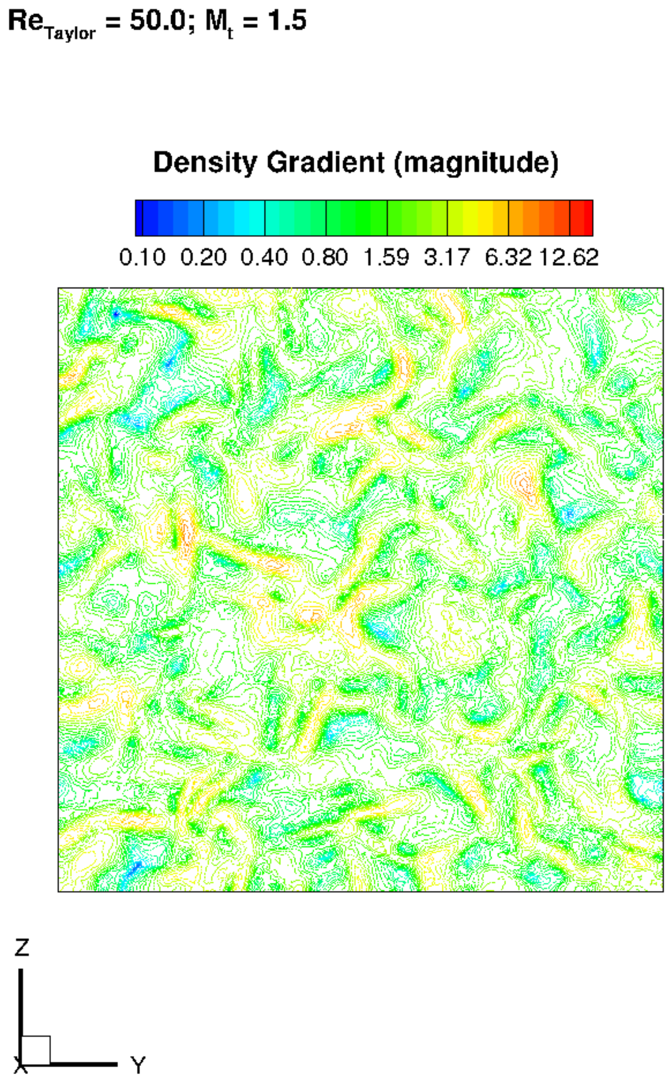
4th order CESE

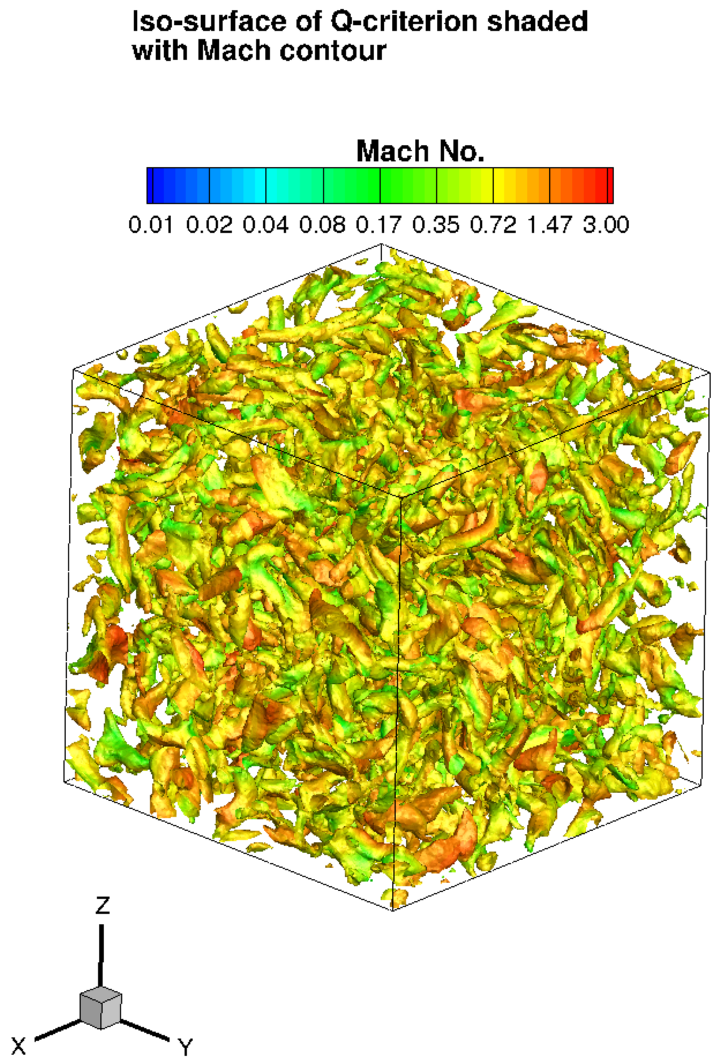




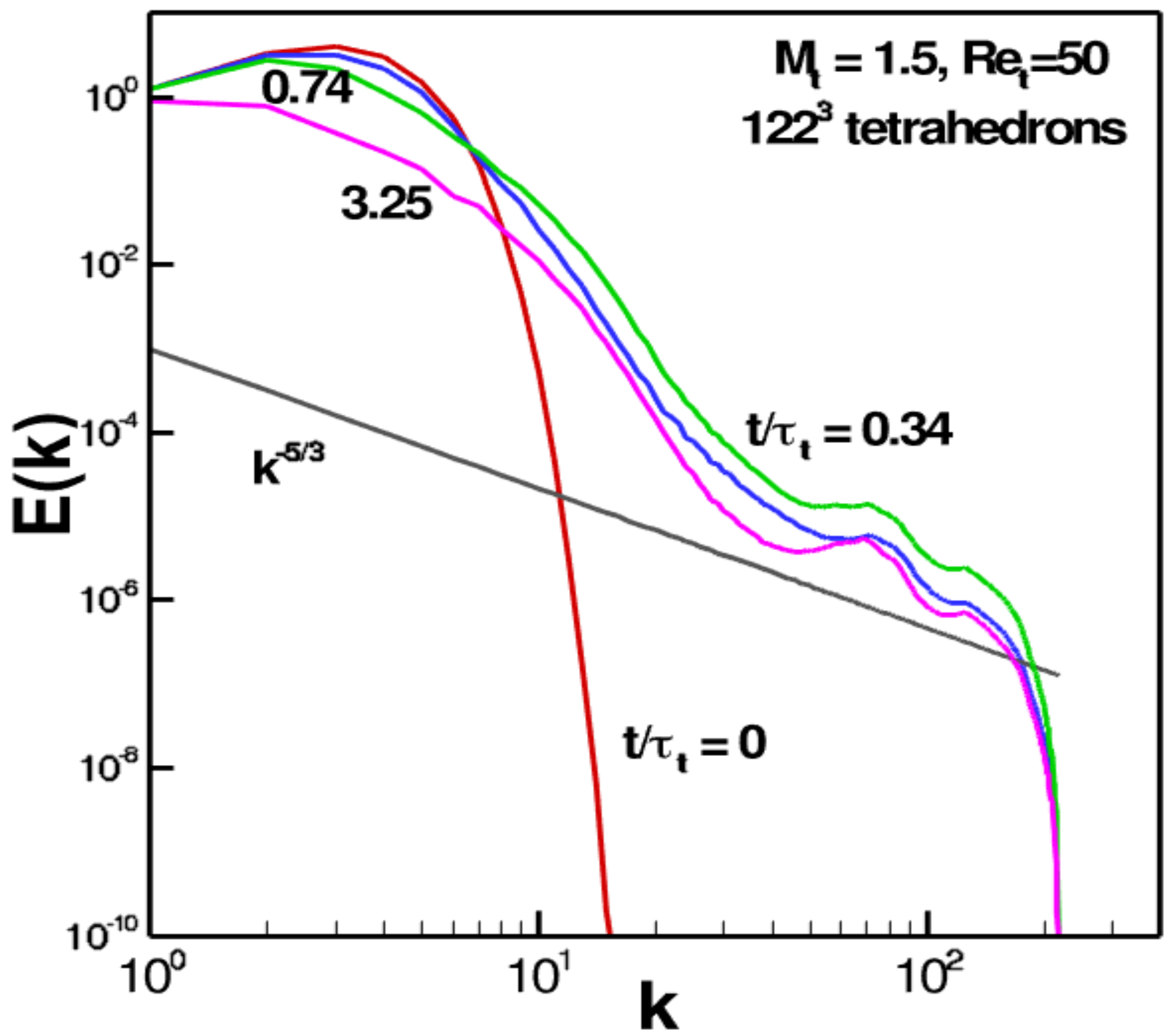


Isotropic Turbulence Decay Simulations M_t=1.5, Re_t=50 (122^3 tetrahedrons)



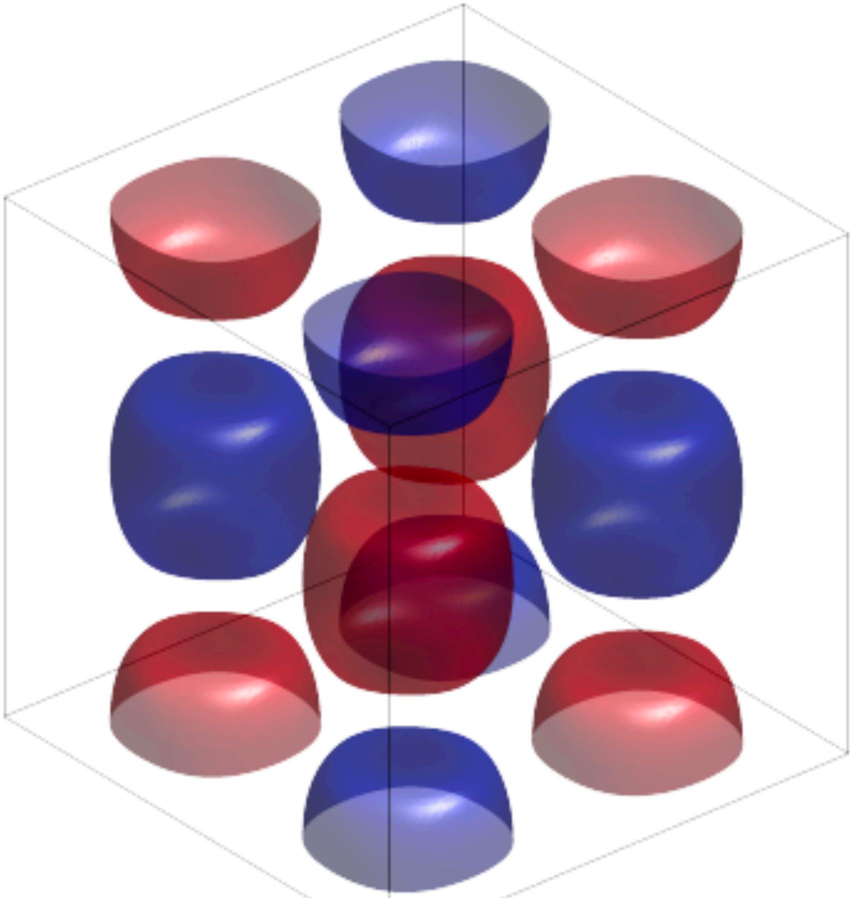


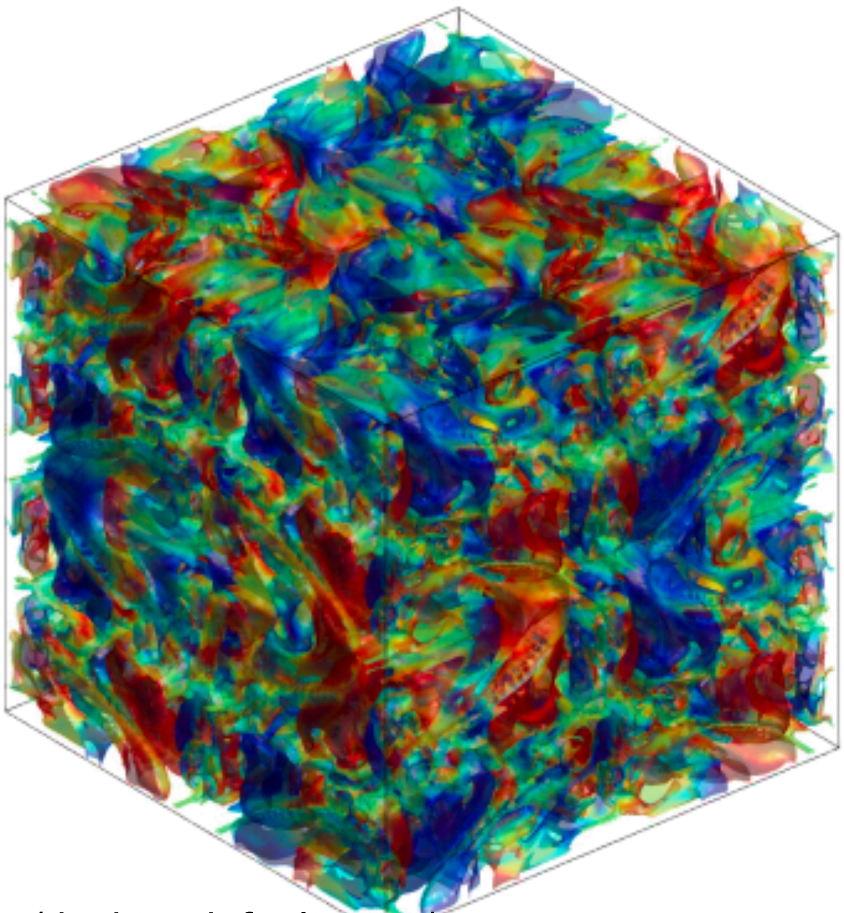
Isotropic Turbulence Decay Simulations M_t=1.5, Re_t=50 Spectra



Direct Numerical Simulation of Taylor Green Vortex – Inviscid & Re = 1600

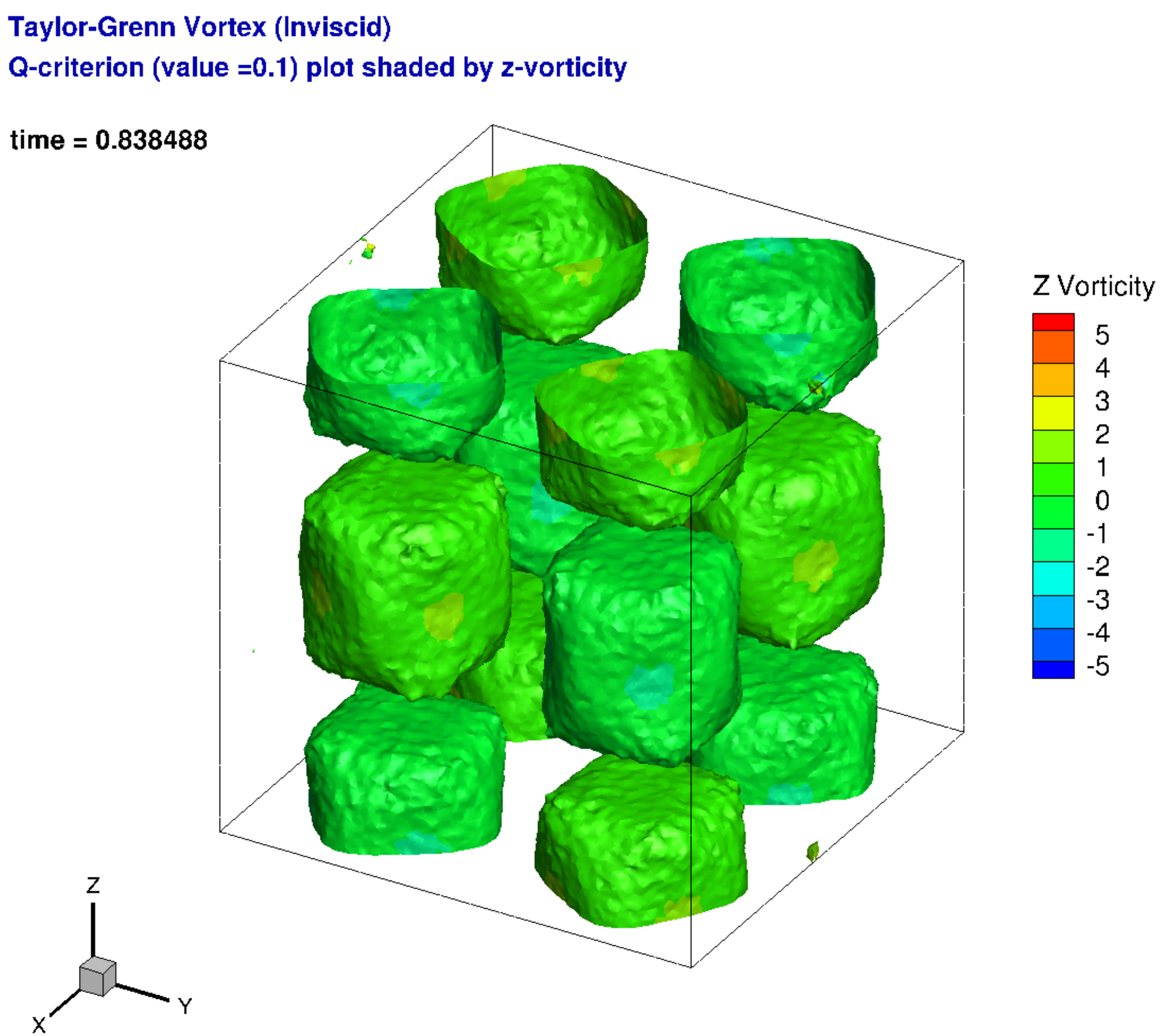
- HOM Benchmark C3.5



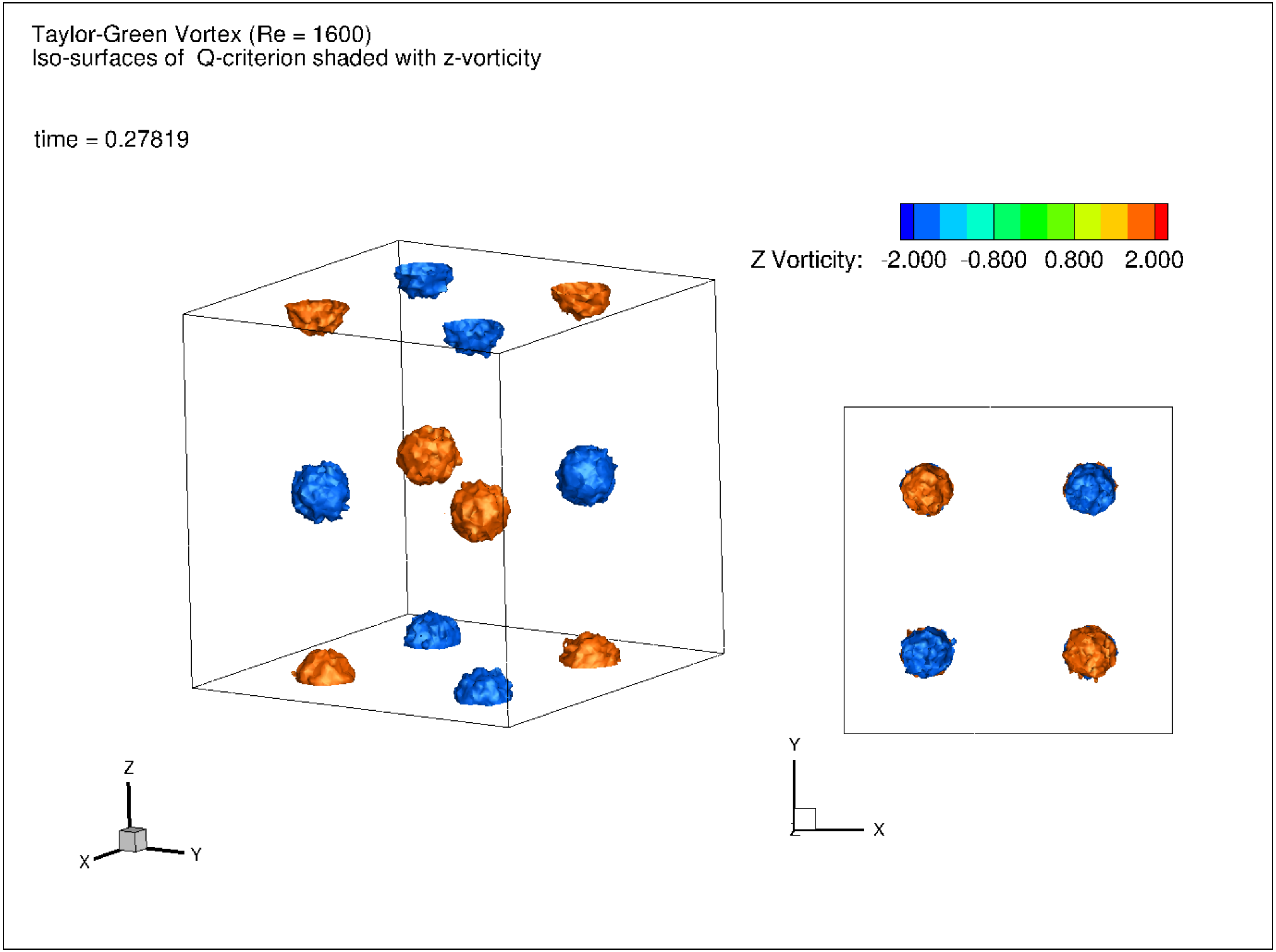


From HOM Workshop, http://www.dlr.de/as/desktopdefault.aspx/tabid-8170/13999_read-35550/

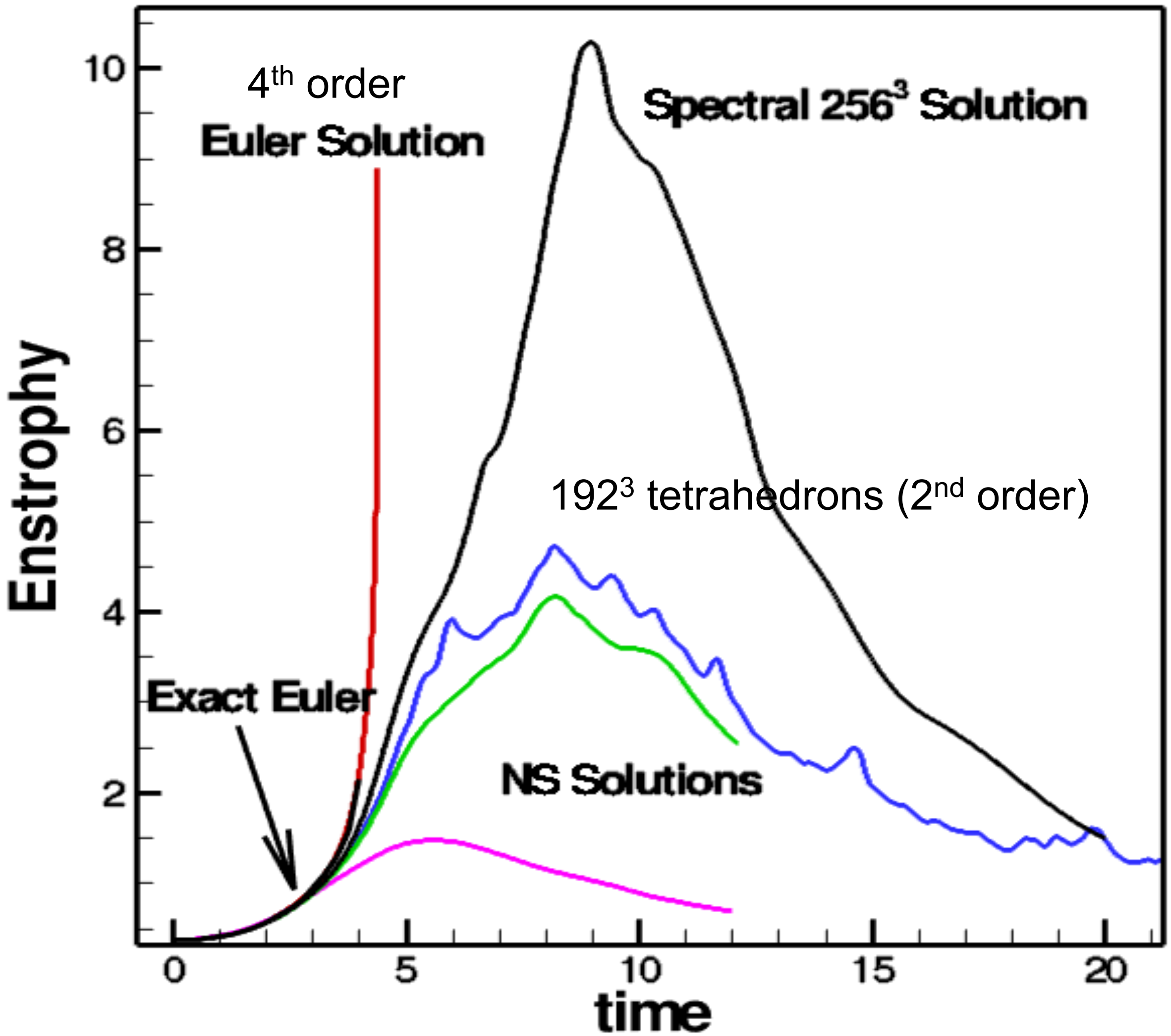
Direct Numerical Simulation of Taylor Green Vortex – Euler Solutions



Direct Numerical Simulation of Taylor Green Vortex – Re = 1600

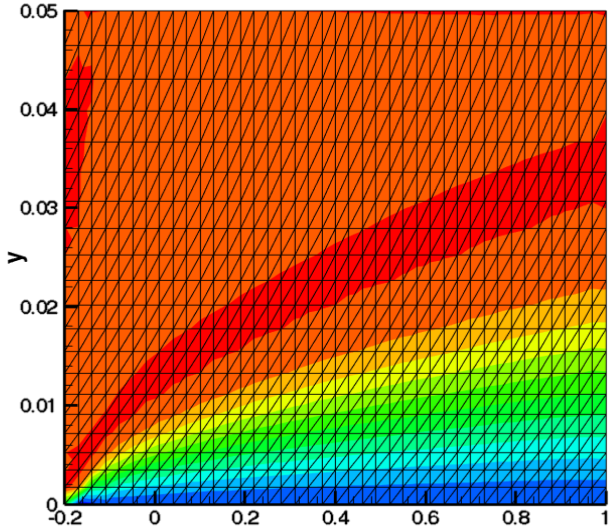


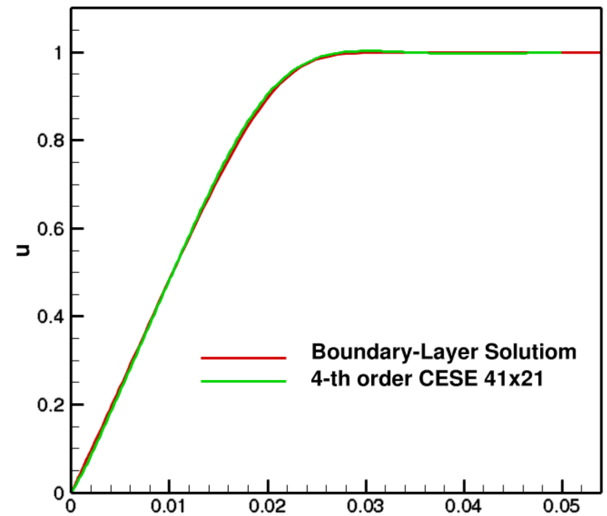
Direct Numerical Simulation of Taylor Green Vortex – Inviscid & Re = 1600



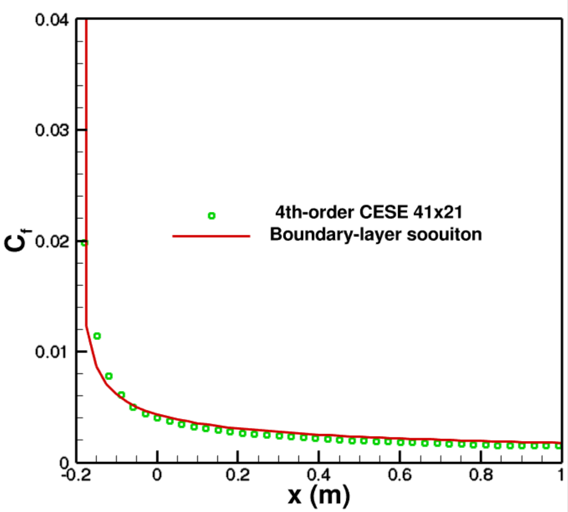
Mach 3 flat-plate boundary layer

Mesh with u velocity contours

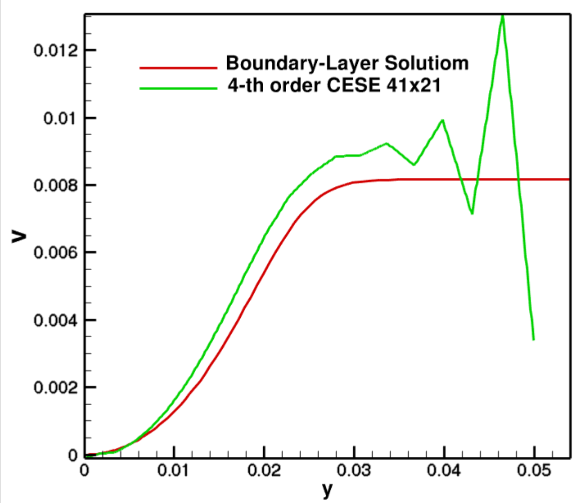




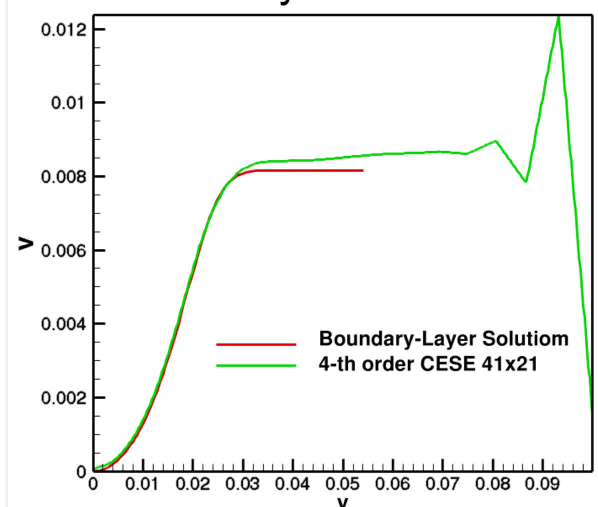
u velocity



Skin friction



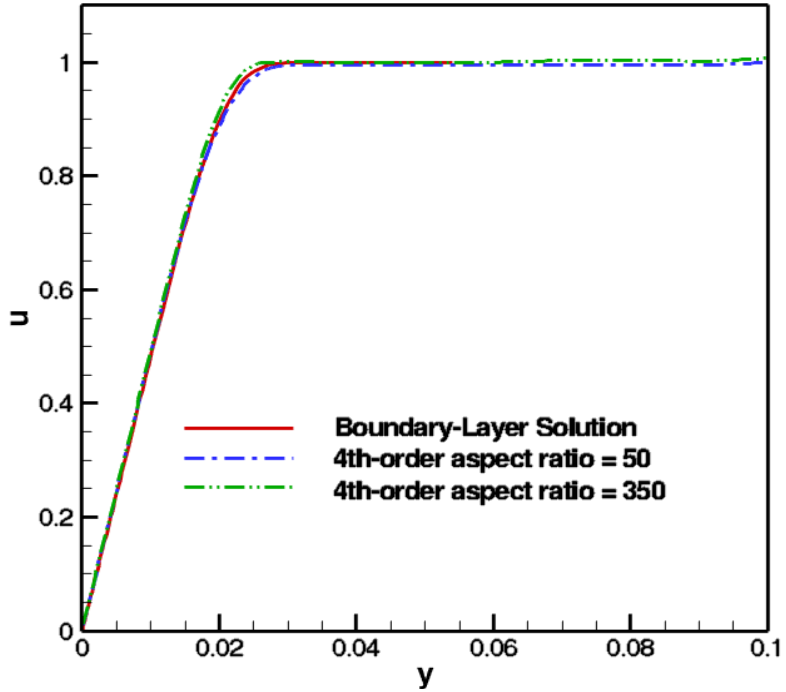
v velocity

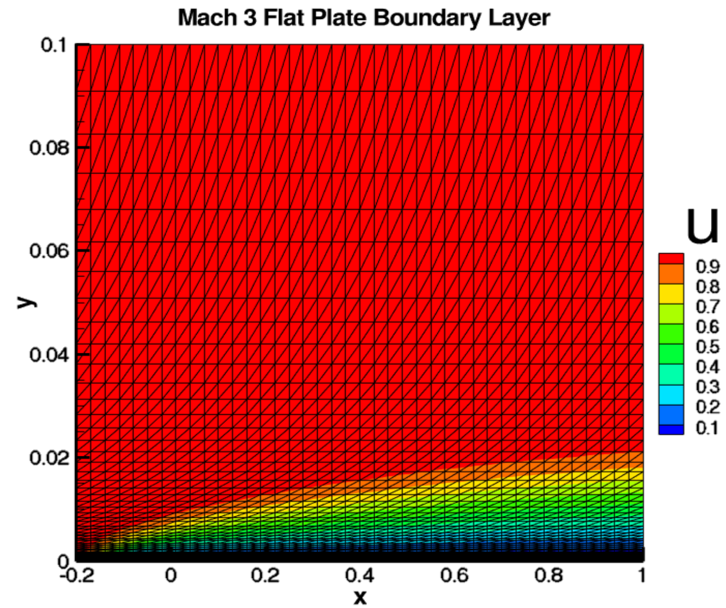


v velocity with larger domain

Integral High-Order Boundary Conditions

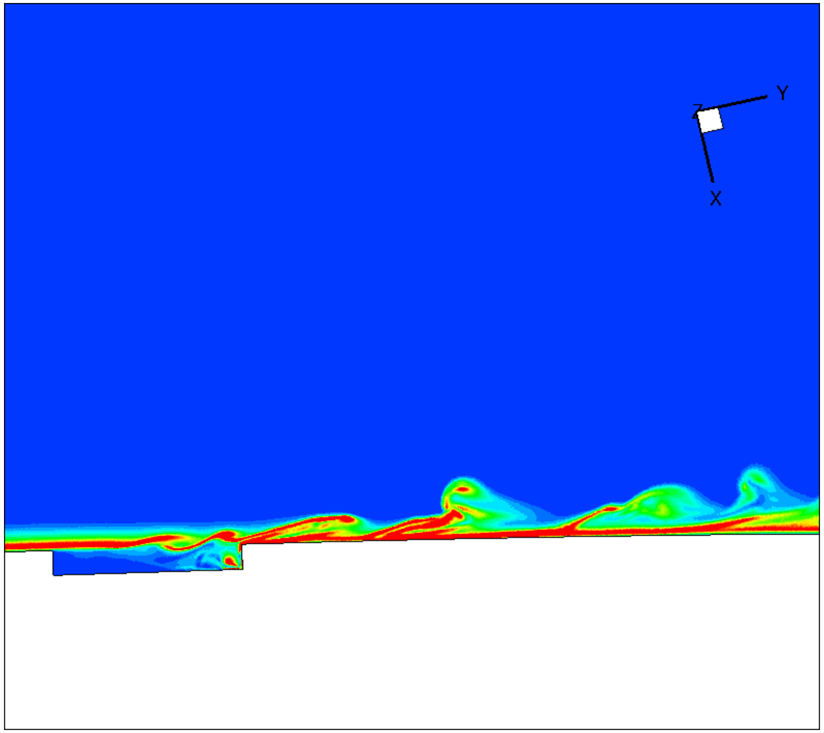
- Specified integrals at the boundary
  - Zero flux
  - Pressure or heat flux (high-order) integrals evaluated at boundary faces



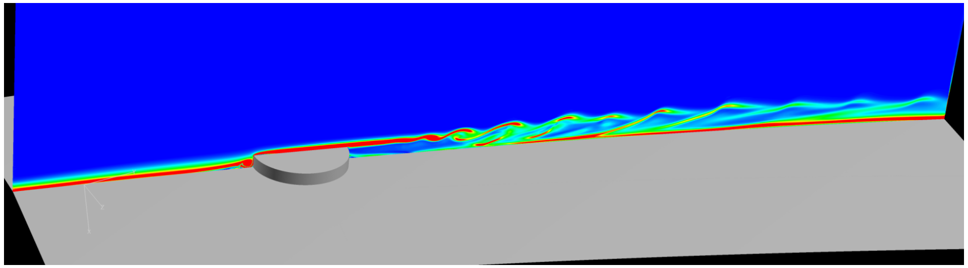


Mach 3 flat-plate boundary layer with adiabatic walls

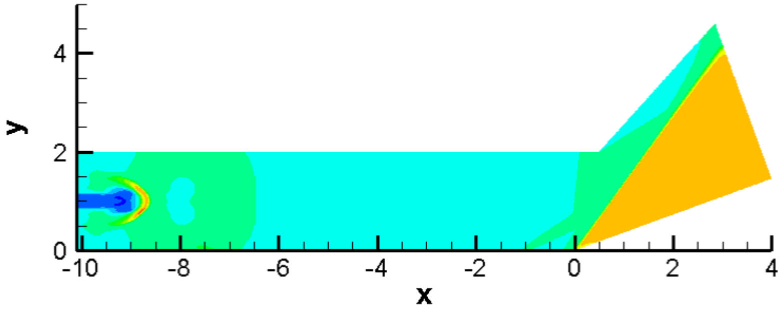
NASA Langley Research Center (*ez4d*)



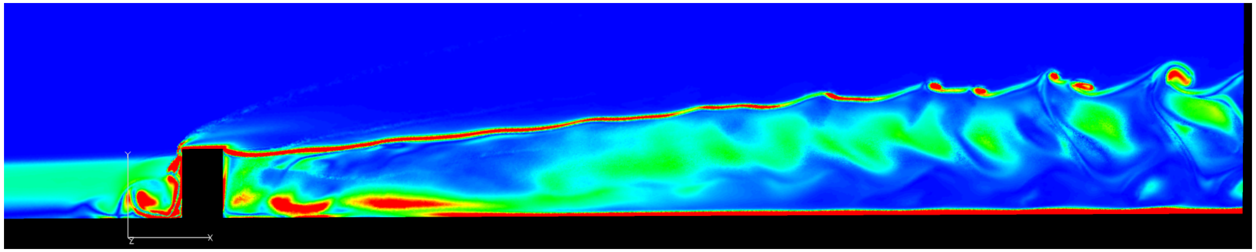
Subsonic (Mach 0.3) flow over a cavity



Subsonic (Mach 0.3) flow over an isolated cylinder



Hot spot/shock interaction (Mach 1.2) by Craig Streett, LaRC



Supersonic (Mach 6) flow over an isolated cylinder

CESE Applied to Multidiscipline Problems

- Stress waves propagation in solids (Ohio State)
- Fluid-structure interactions (LS-DYNA)
- Solid mechanics (China)
- Detonation waves (Ohio State, China)
- Multi-phase flows (Japan, China)
- LES of turbulent flows (Oxford University)

Solving Time-Dependent Schrödinger Equations (TDSE) using CESE

- Focused only on numerical aspects
- Model governing equations

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2}\nabla^2\Psi + V\Psi$$

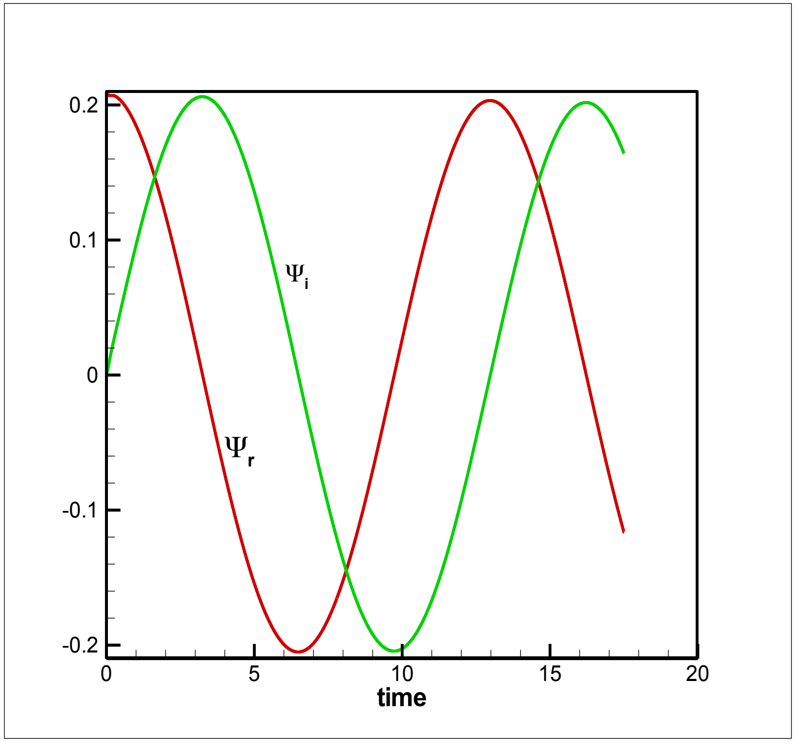
- Cast in conservation laws using only first derivatives and solve by the second-order CESE schemes
- Analytical solution is

$$\Psi = e^{i\omega t - |\vec{r}|}$$

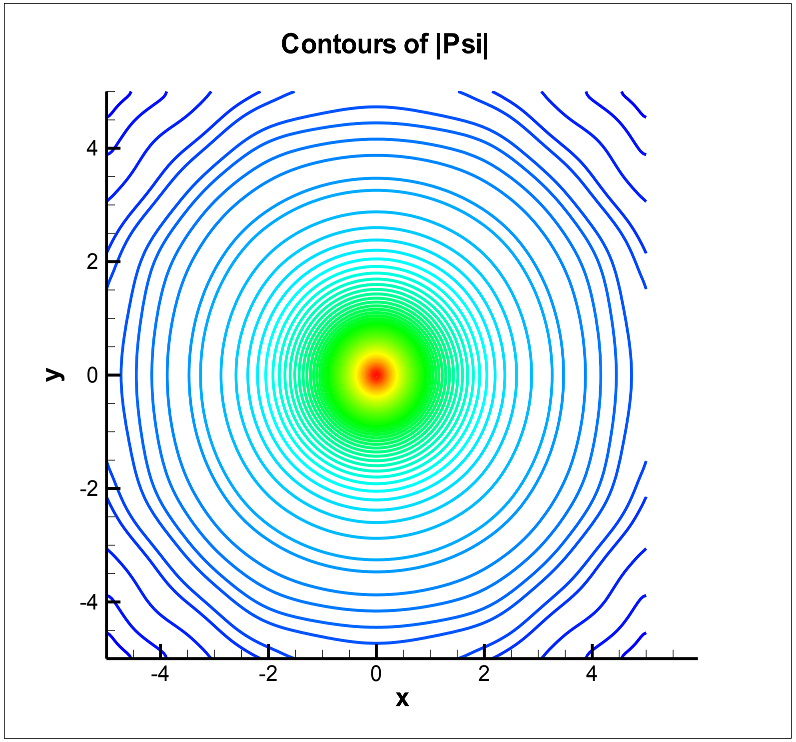
if $V = \frac{-1}{|\vec{r}|}$ $\vec{r} = \sqrt{x^2 + y^2 + z^2}$

Numerical Solutions of the Model TDSE

- Using 10x10, rectangular domain, non-reflecting boundary conditions
- Quadrilateral mesh, 200x200



Time trace at (0, 1)

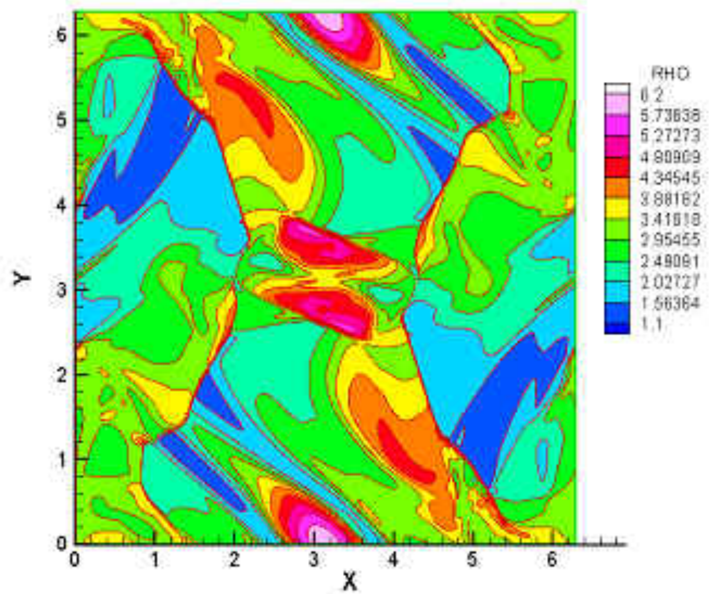


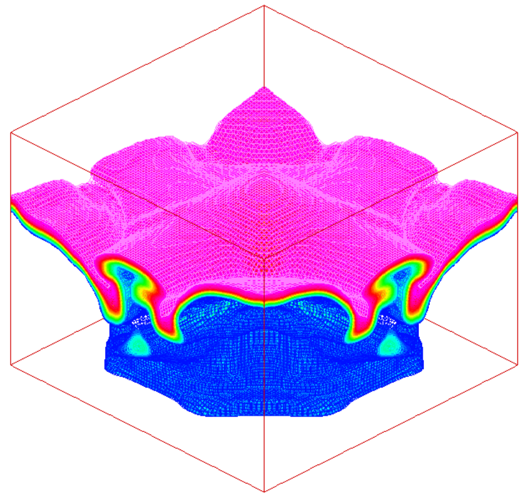
Ψ Contours

CESE Applications for Various Disciplines

Prof. S.-T. Yu, Ohio State University

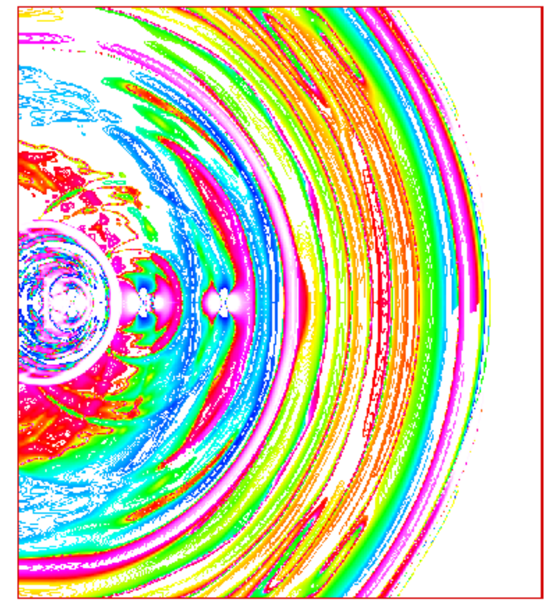
Ideal Magnetohydrodynamics (MHD) Simulations

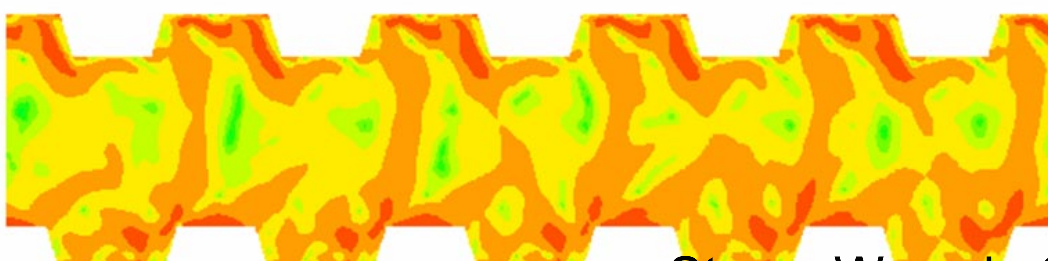




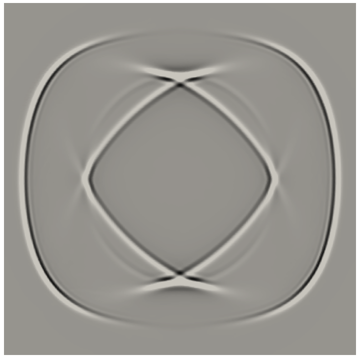
3D ZND (detonation)
Mass fraction

Pulse Detonation Engine
Mach 0.5 into M = 0





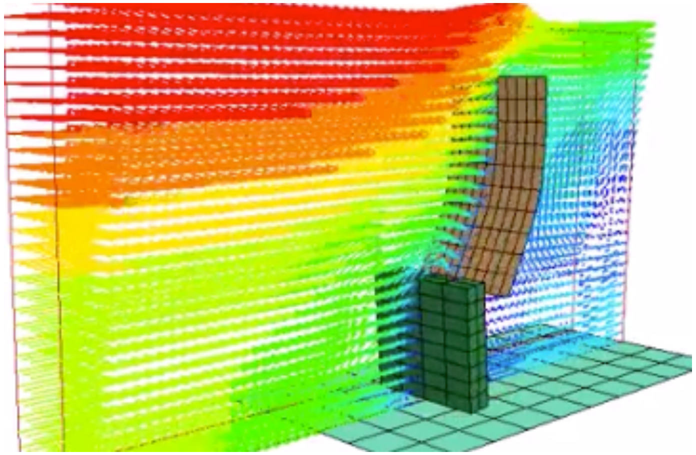
Stress Wave in Solids

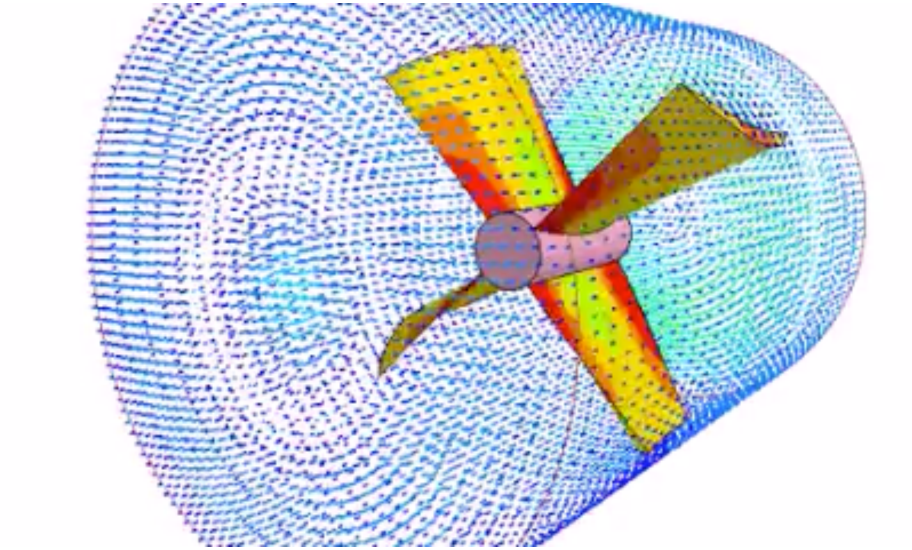


Yu, S.-T., Yang, L.X., and Lowe R. L., “Numerical Simulation of Linear and Nonlinear Waves in Hydroelastic Solids by the CESE Method,” *Wave Motion*, 47(3), pp. 168-182, 2010.

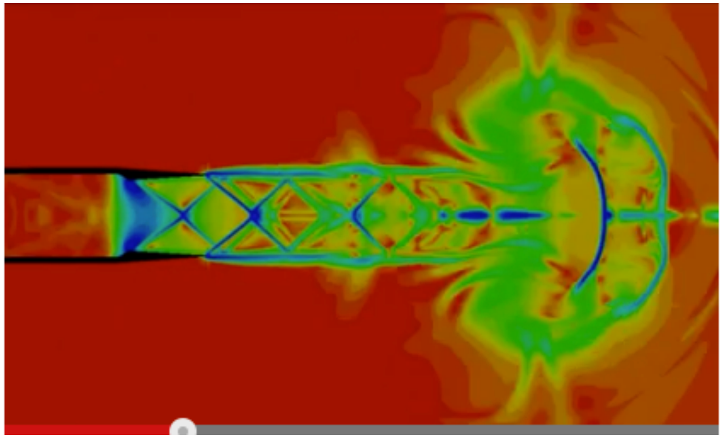
Livermore Software Technology Corporation
http://www.lstc.com

- LS-DYNA CESE software
  - 2D/Axisymetric/3D Navier-Stokes solver
  - Cavitation
  - Fluid/structure coupling →
  - Moving mesh





Rotating solid turbine blades



Supersonic jet

Concluding Remarks

- Improve unsteady numerical computations by addressing accuracy and efficiency
  - Time-accurate local time stepping method by preserving space-time flux conservation
    - Enhance accuracy for large grid size disparity
    - Improve efficiency by using large time steps for large cells
    - Used for both unsteady and steady-state computations
  - High-order CESE method
    - Retains the same CFL limit as 2^{nd} order schemes
    - Compact stencil
    - Provides 4^{th}, 3^{rd}, 2^{nd}, and 1^{st}-order accuracy for U, U_x, U_{xx}, and U_{xxx}
- Unstructured tetrahedral meshes offer improved small scale simulations
- Future work
  - Combined TALTS and high-order schemes
  - More DNS of complex physics/geometries using tetrahedral meshes
  - moving boundary problems