



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

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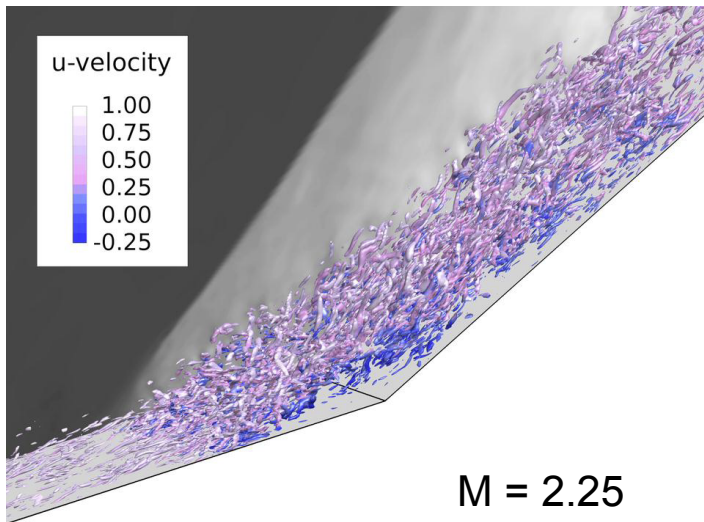


Outline

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

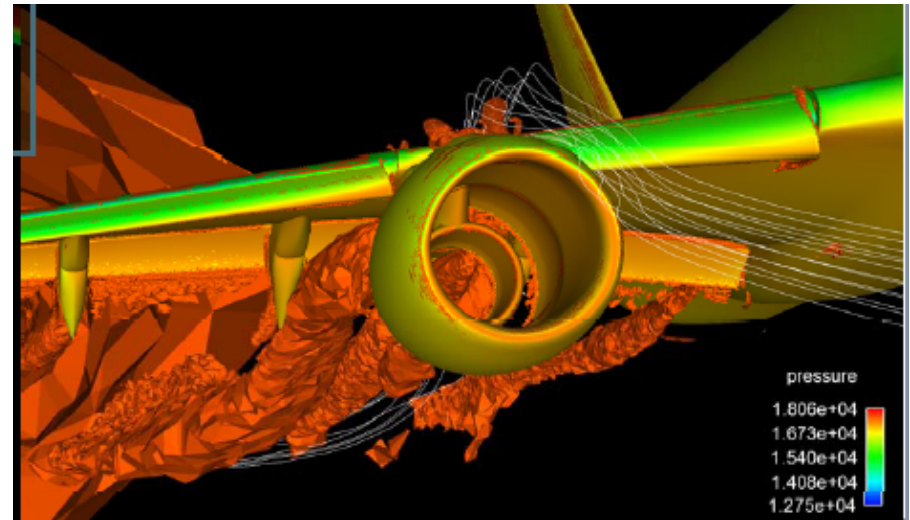


Examples of critical complex flow physics



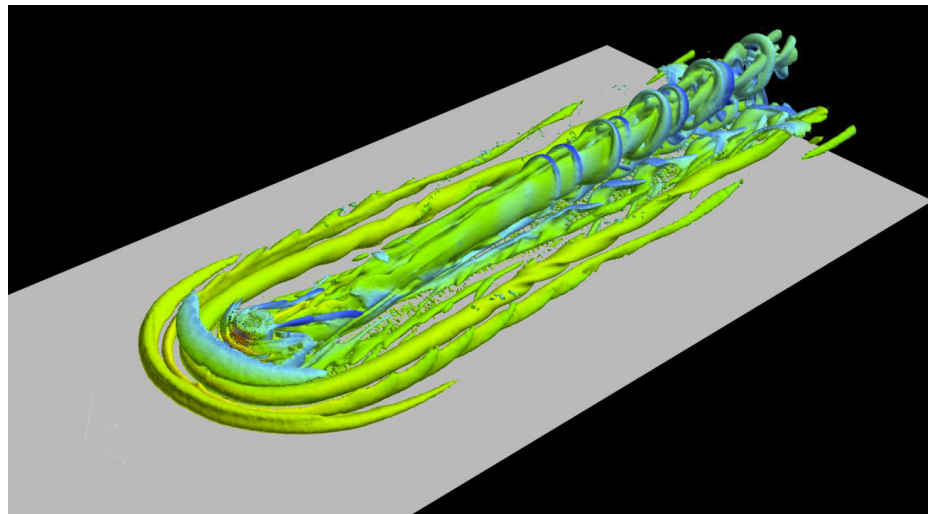
$M = 2.25$

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/dgIr/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 visualized of 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

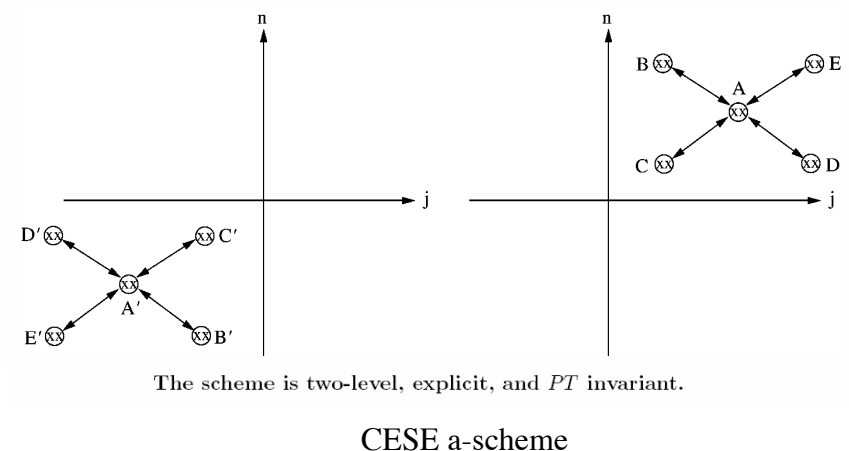
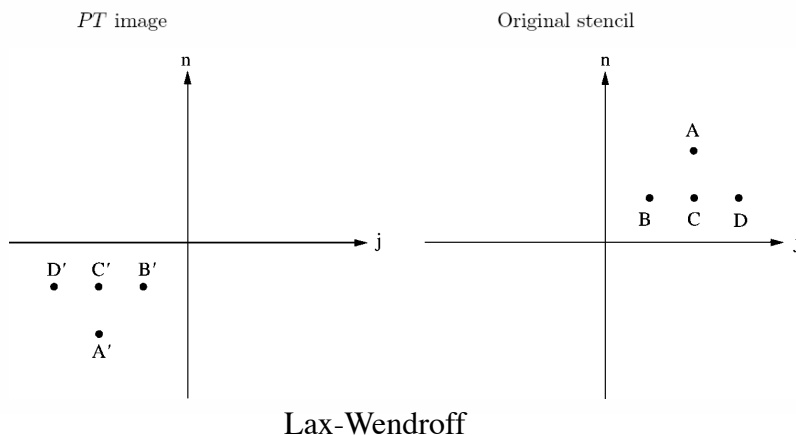
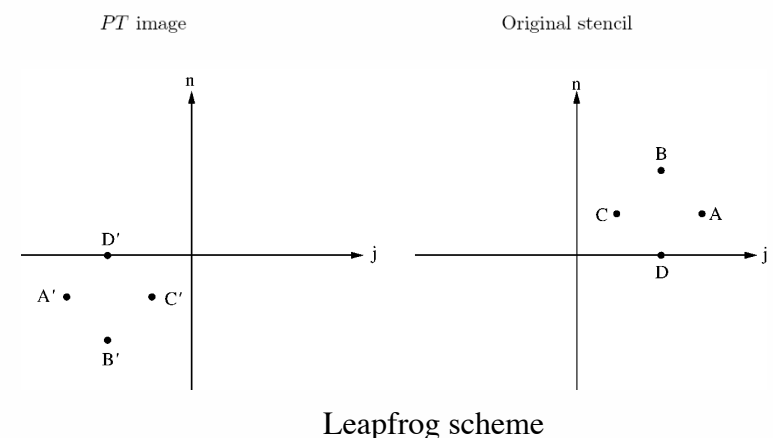
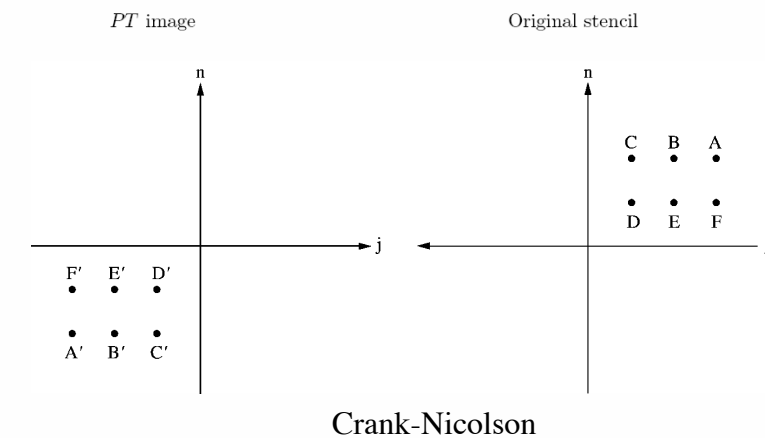
$$Q(x, y, t) = Q_0 + Q_t(t - t_0) + Q_x(x - x_0) + Q_y(y - y_0)$$

- 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

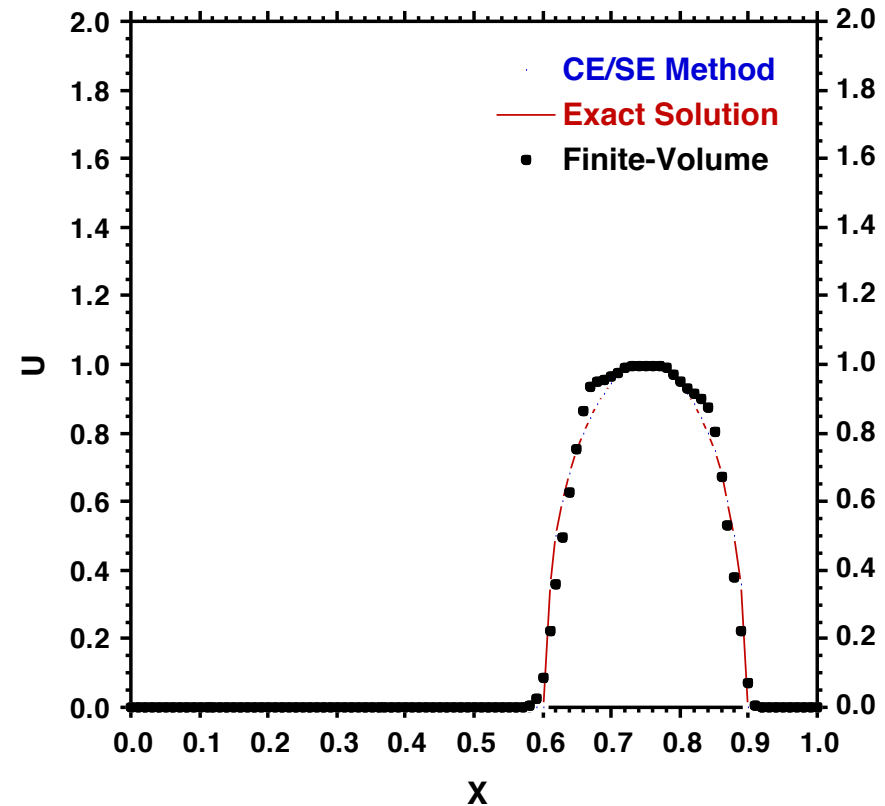
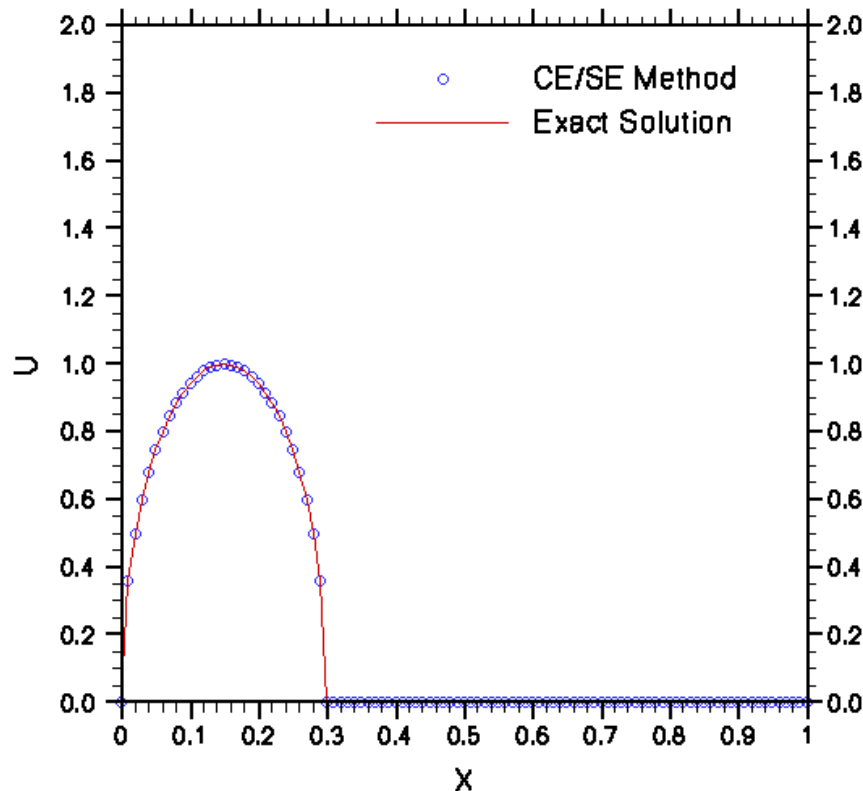




Elliptical Wave Propagation Using the CESE Method

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

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

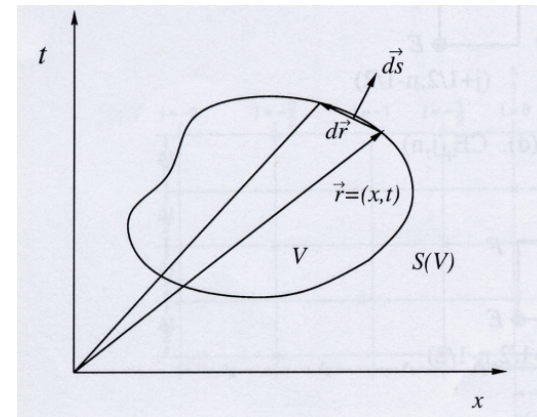
Explicit, implicit
time advancement

Spatial integration, FEM or FVM

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

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

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



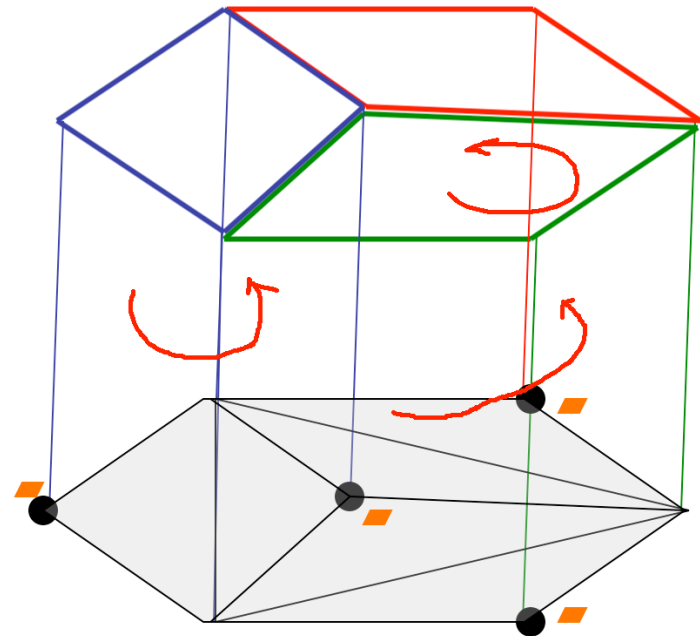
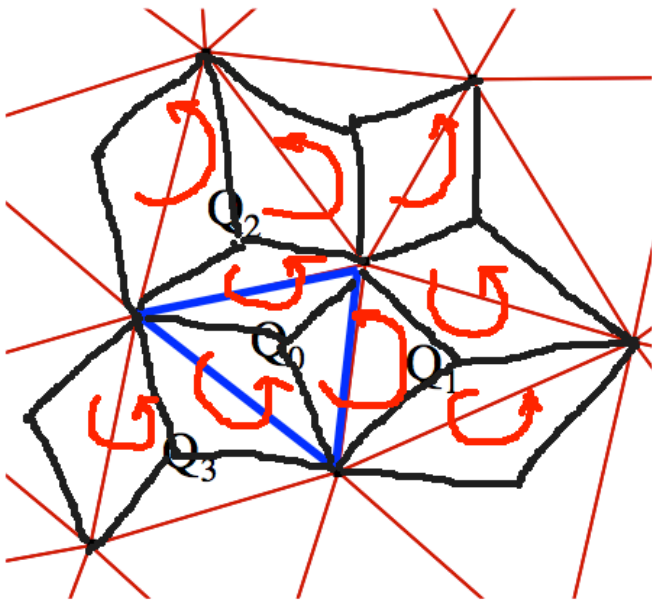
$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = 0$$

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





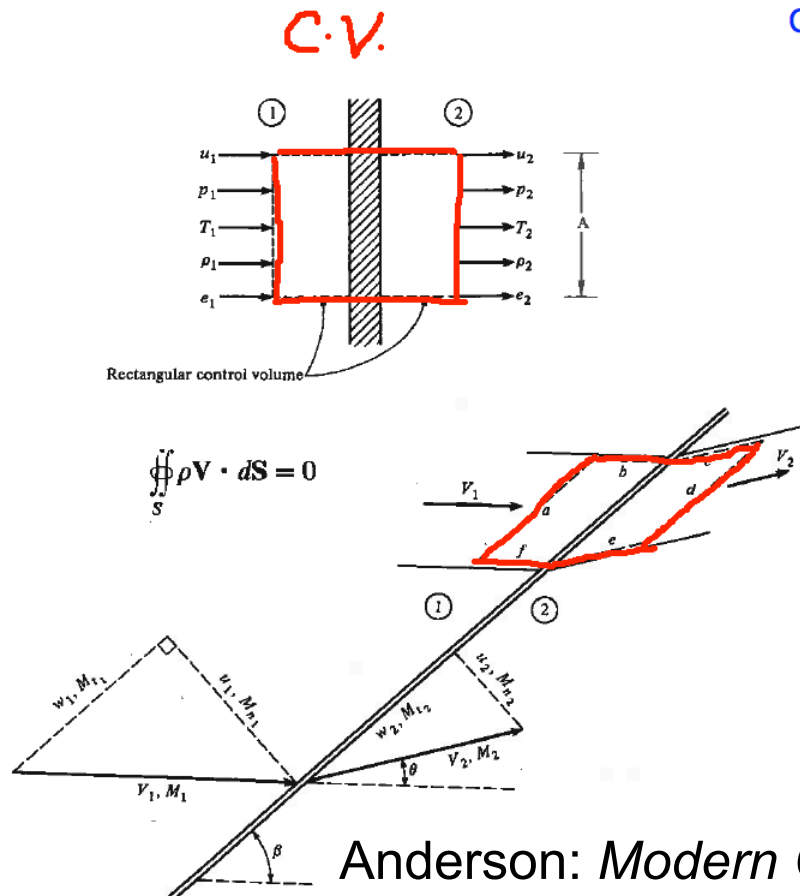
A Note on Entropy and Kinetic Energy Preserving Schemes

- 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

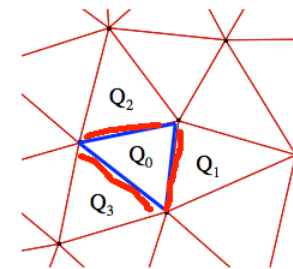


Core Ideas of the CESE Method (III)

- Distinguishing solution elements and conservation elements (control volume)

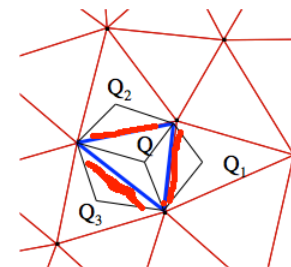


Conventional Unstructured Methods



— : Discontinuities?

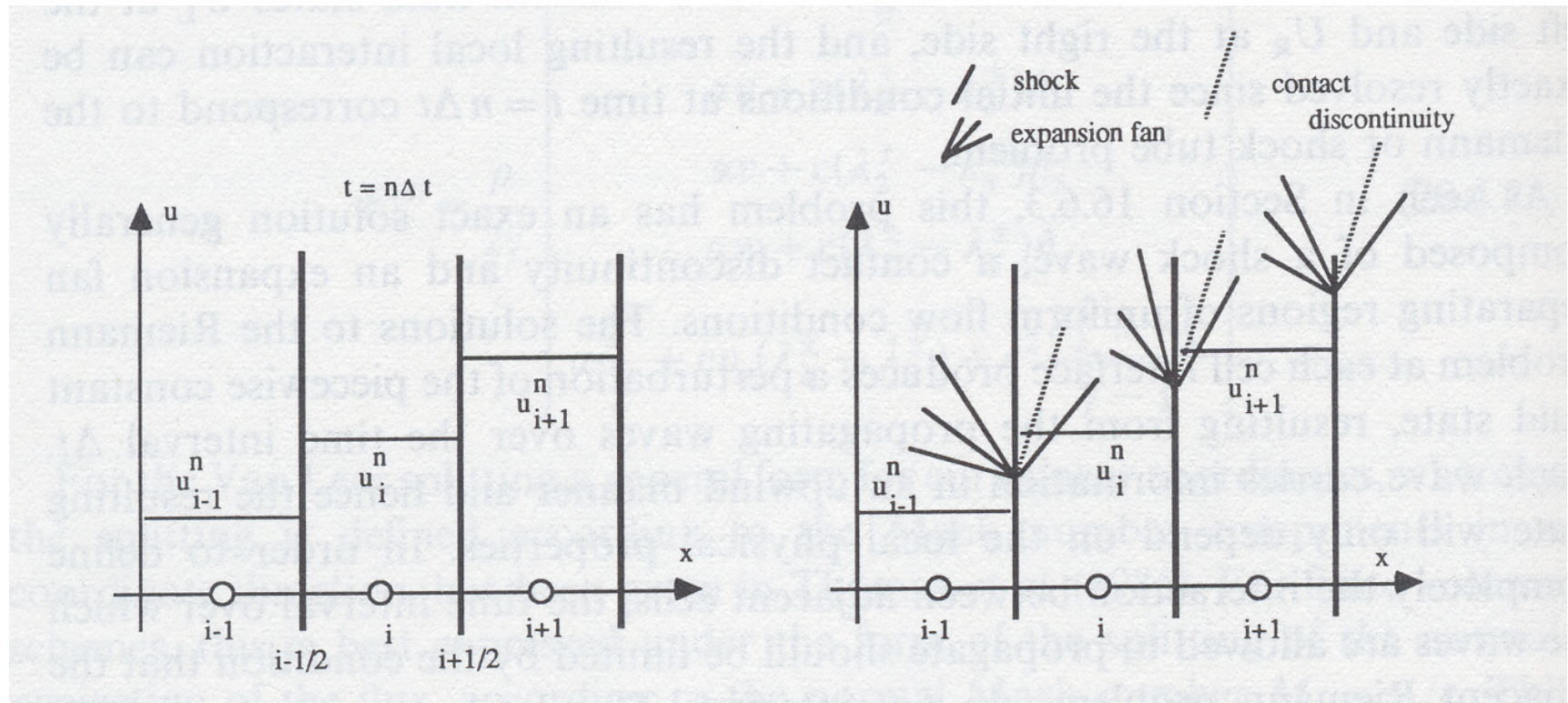
CESE



Anderson: *Modern Compressible Flows*



Cell Interfaces and Riemann Solvers



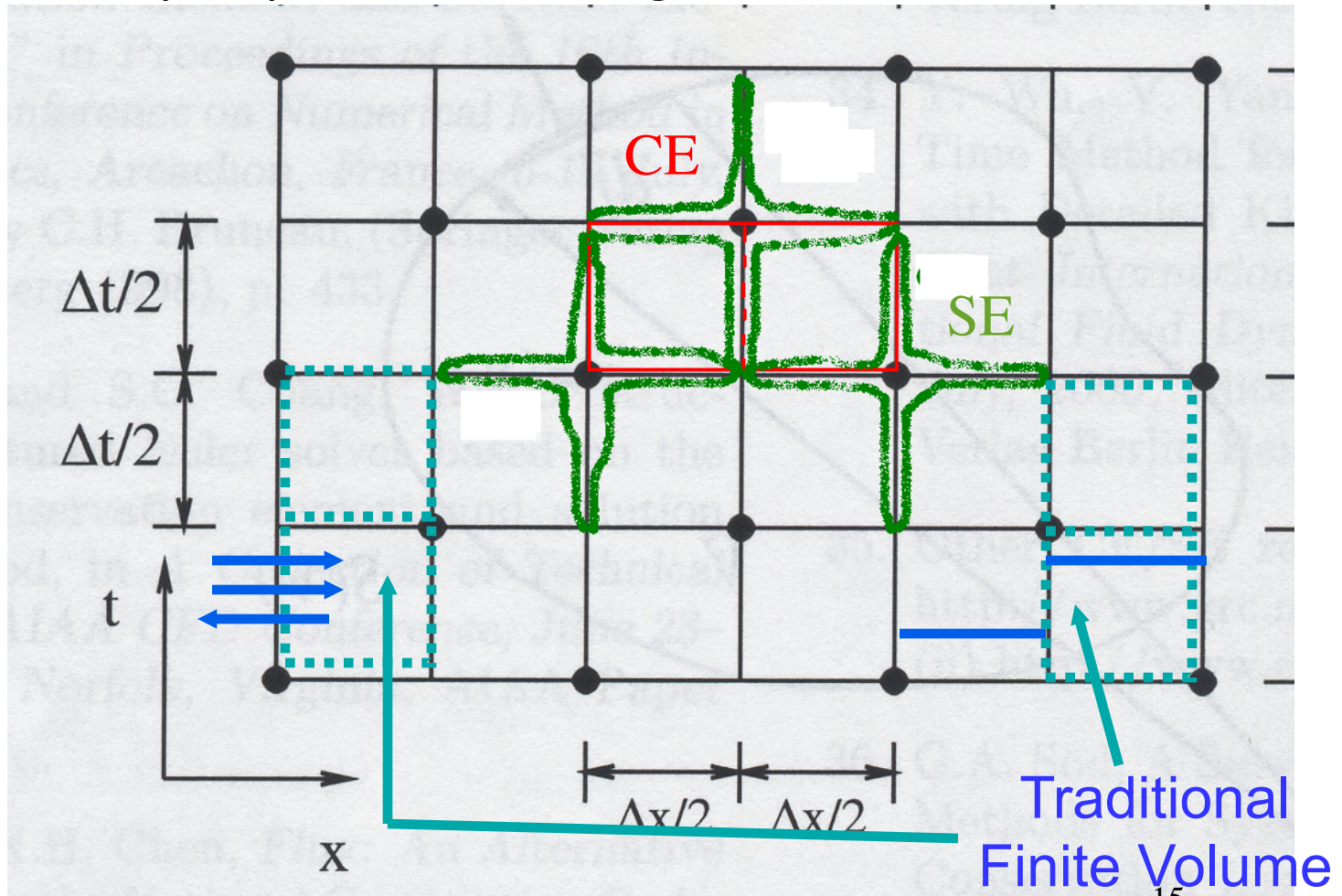
Seeking exact or approximate solution at the discontinuous interfaces

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



The CESE Method

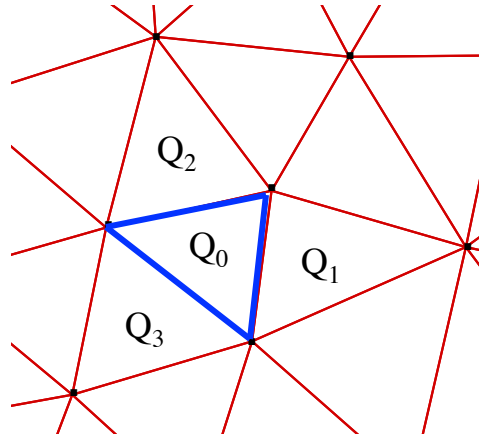
- Staggered solution element (SE) & conservation element (CE) for flux integration





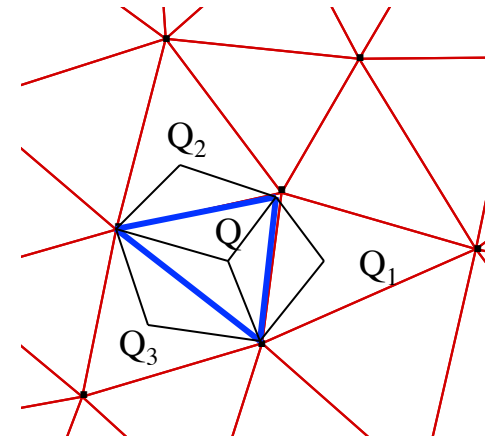
Numerical Flux Integration

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
 - No 1D 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

SlideShop.com

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

1995

1999

2002

2005

2007

2010

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 (4th 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

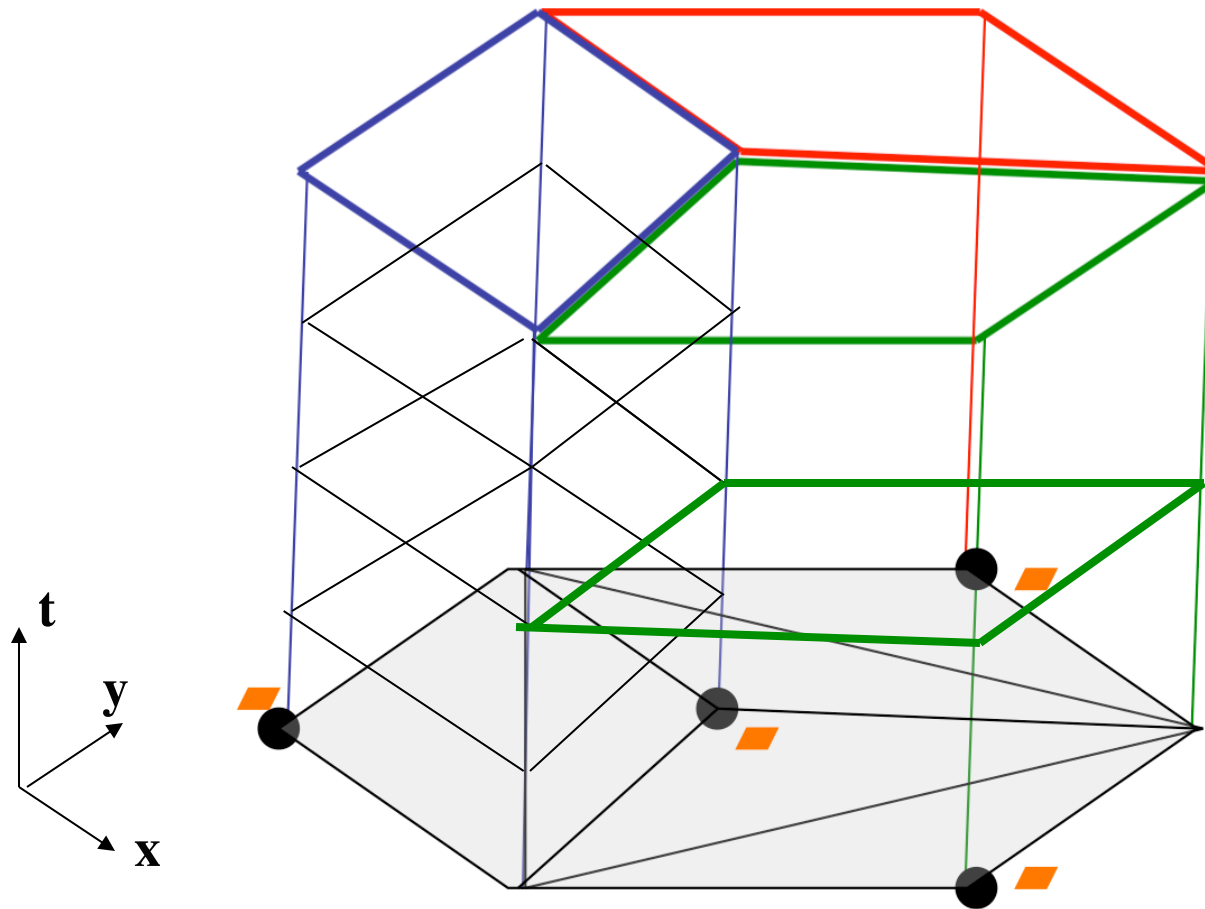


Time-accurate local time-stepping (TALTS) CESE method

- 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



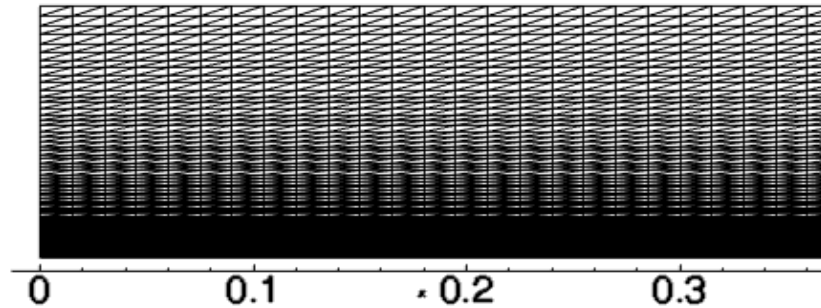
Topology for time-accurate local time-stepping flux integration





Acoustic Wave Propagation with Non-Uniform Mesh

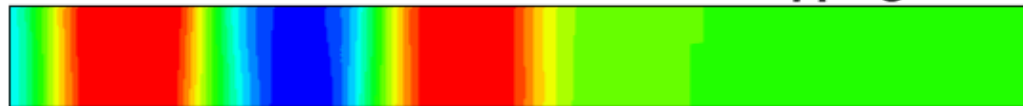
Near-Wall Stretched Mesh



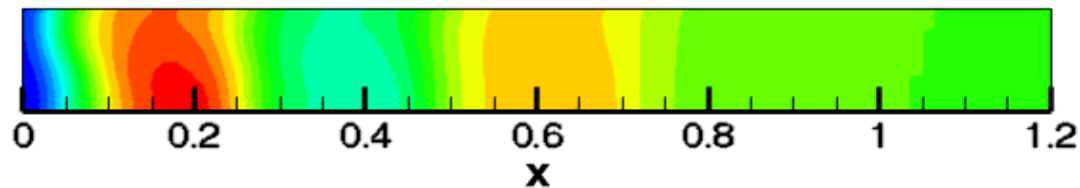
Density Contour



Time-accurate local time-stepping

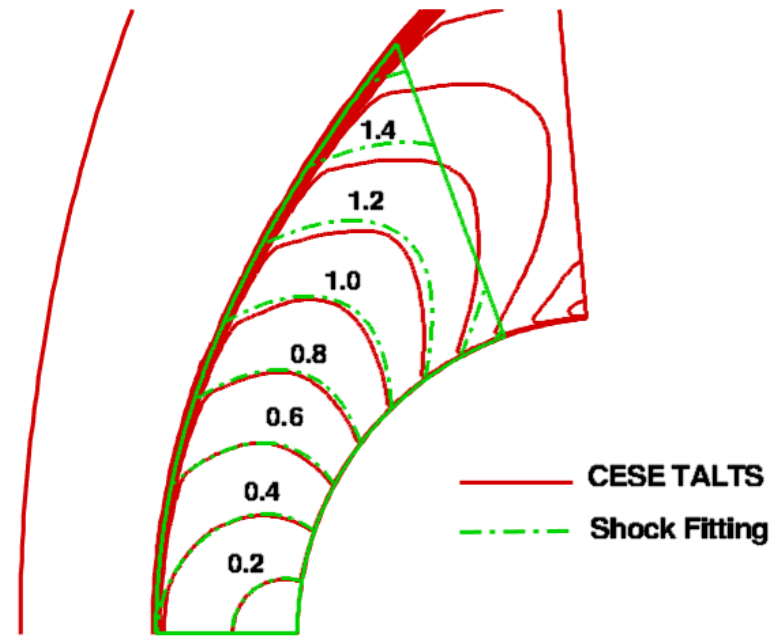
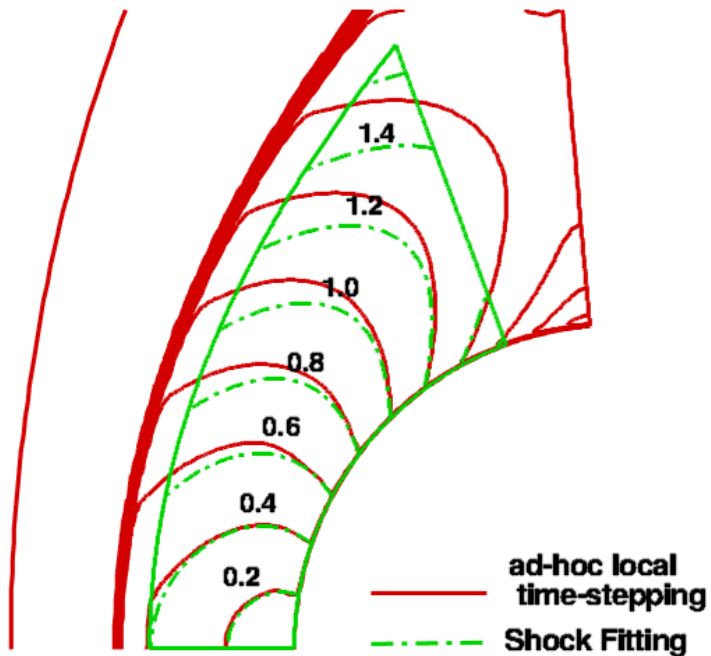


Constant time step



Mach 6 Flow over a Cylinder

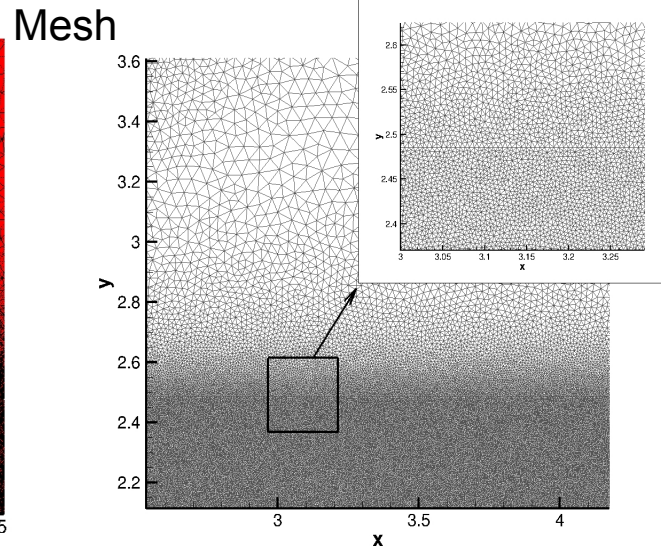
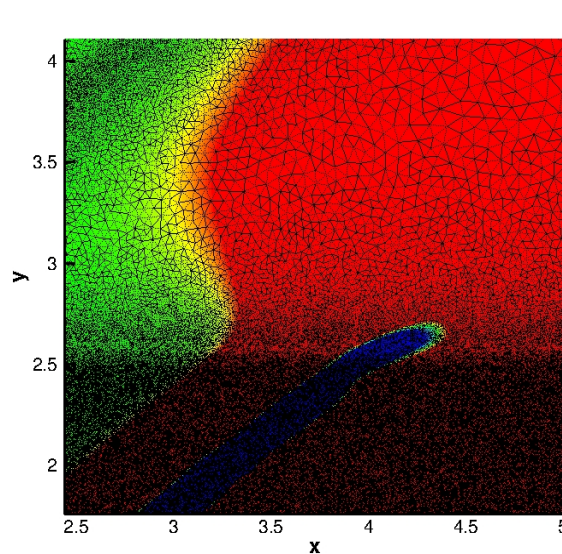
- Navier-Stokes computations with triangular mesh
 - Max. aspect ratio = 10^3 and $\Delta t_{\max}/\Delta t_{\min} = 2^{10}$



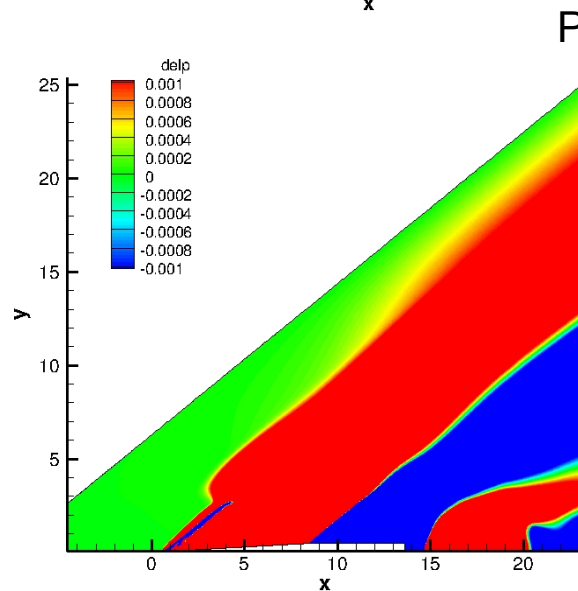
Shock-fitting solutions by: Salas, M. D. and Atkins, H. L., "On Problems Associated with Grid Convergence of Functionals," *Computers & Fluids*, Vol. 38, Issue 7, pp. 1145-1454, 2009.



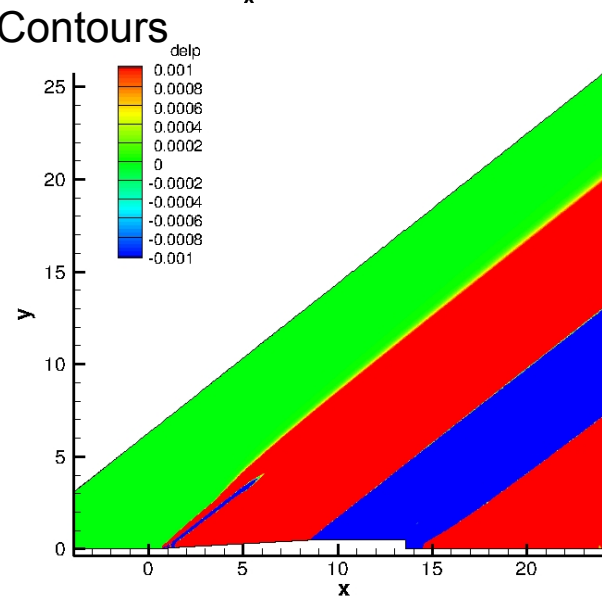
Mach 1.6 flow over a Cone with Counterflowing Jet



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



Constant time step

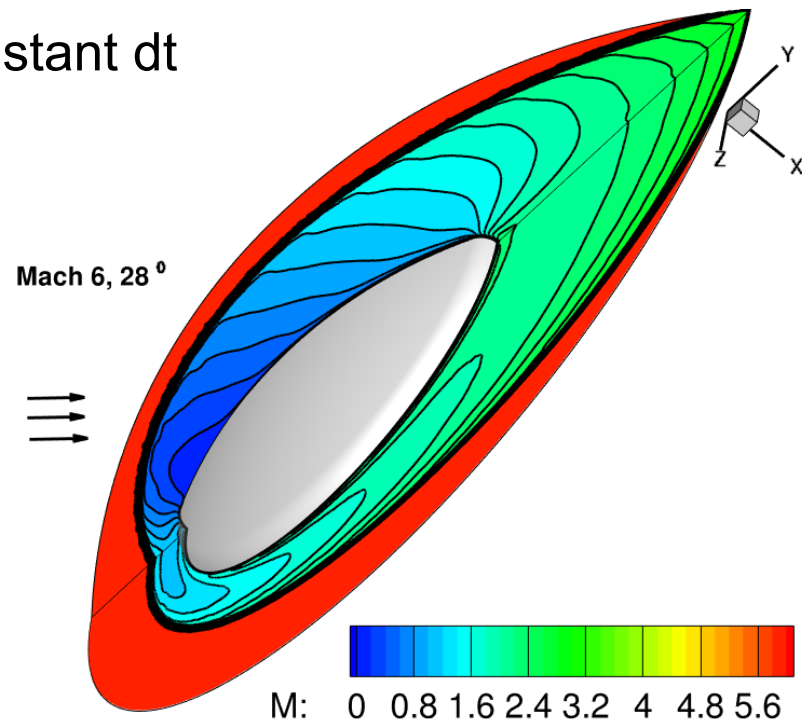


Time-accurate local time-stepping



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 4th, 6th, 8th, 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



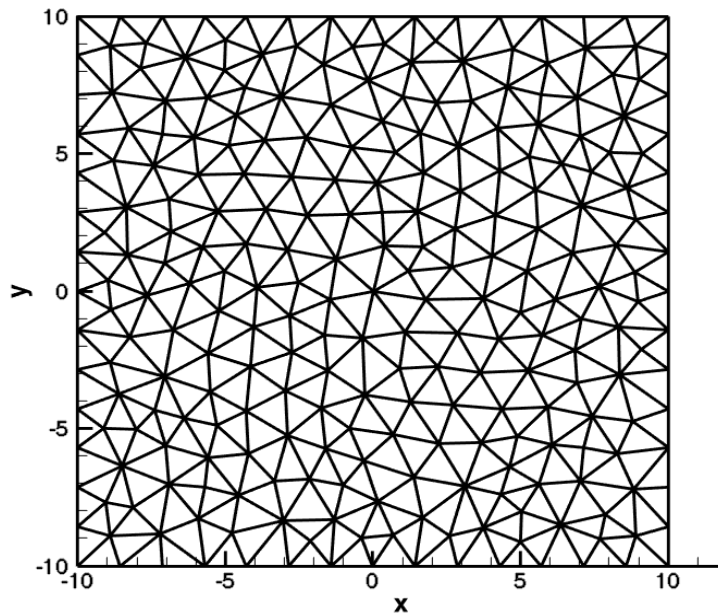
4th-order CESE Method

- Solve 2nd derivative equations using 2nd-order schemes
- Calculate 3rd 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 2nd order code

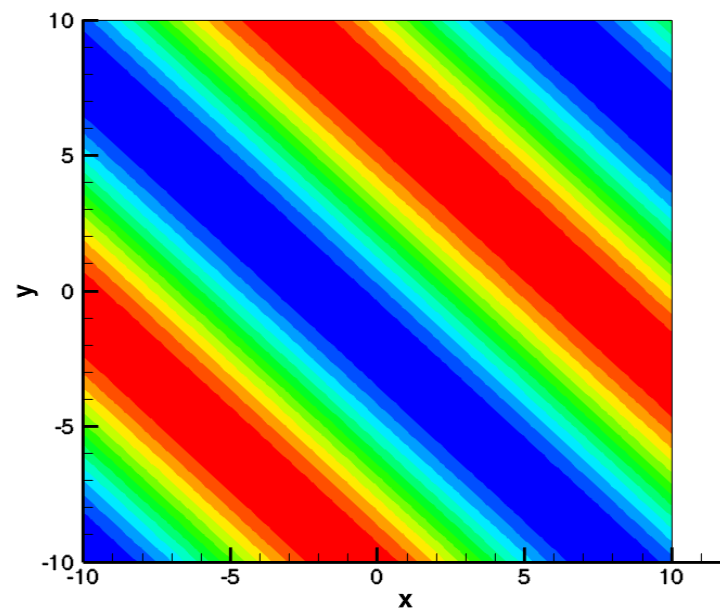


Verification with Full Euler Equations

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



Triangular mesh

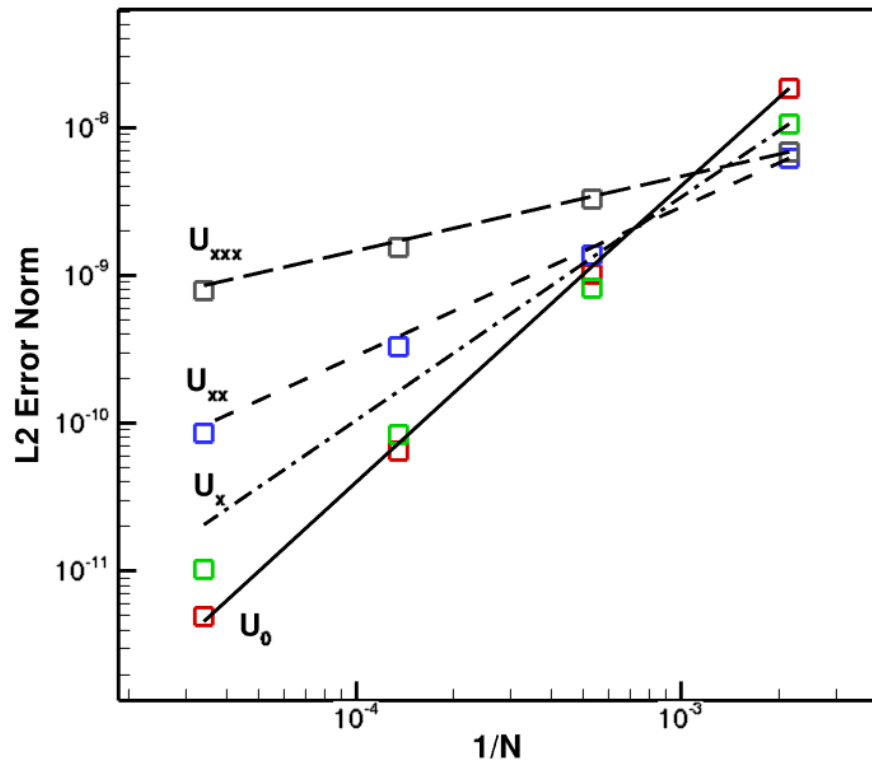


Velocity contours

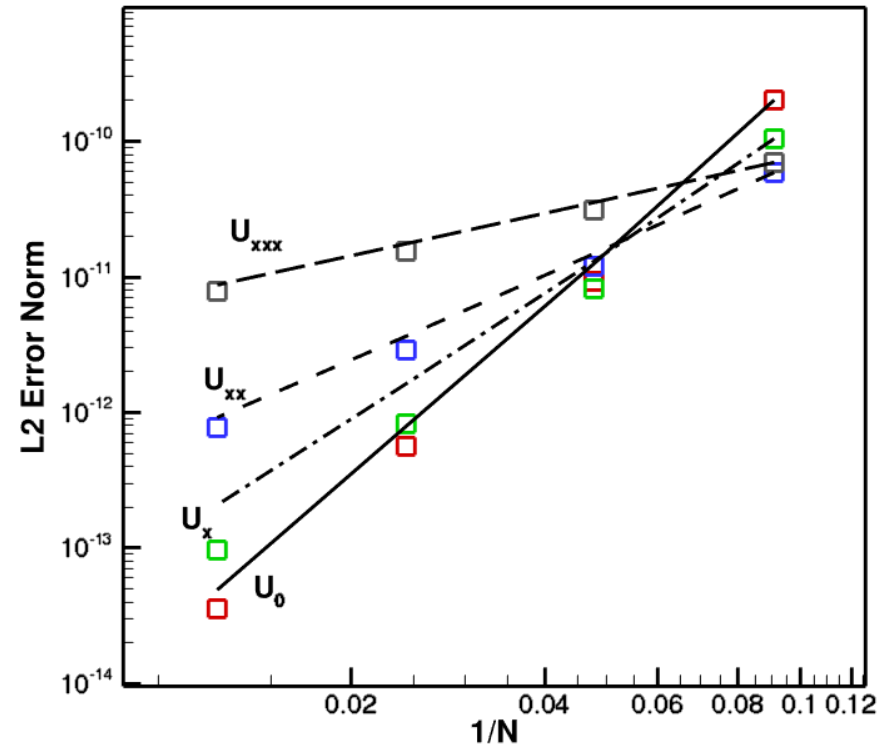


Verification with Full Euler Equations

Amplitude = 10^{-6}

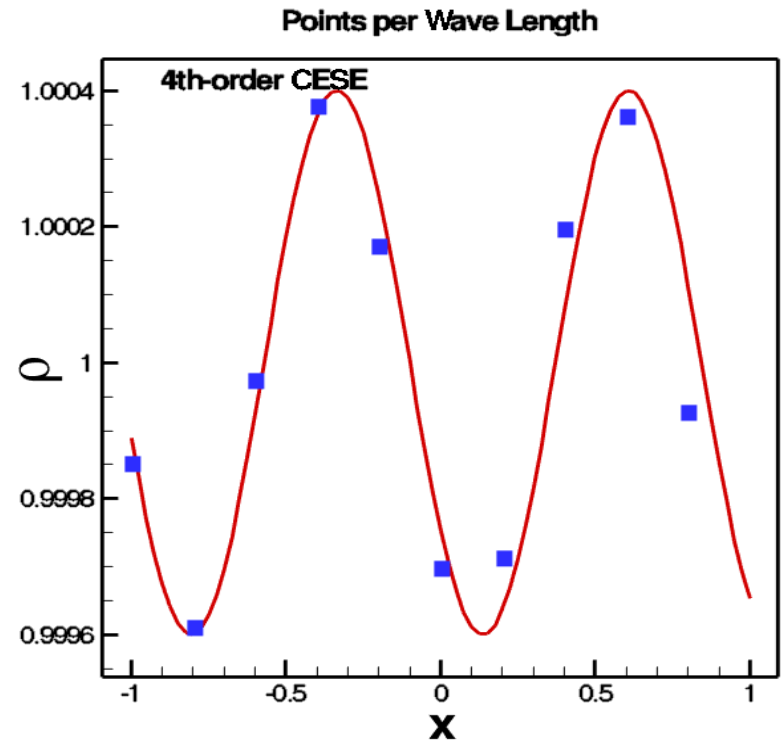
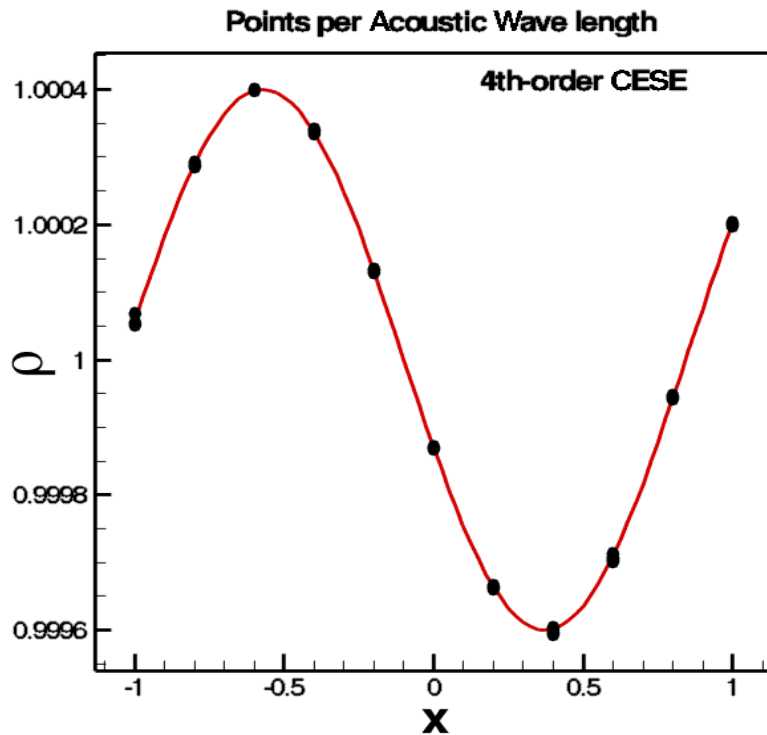


Amplitude = 10^{-8}





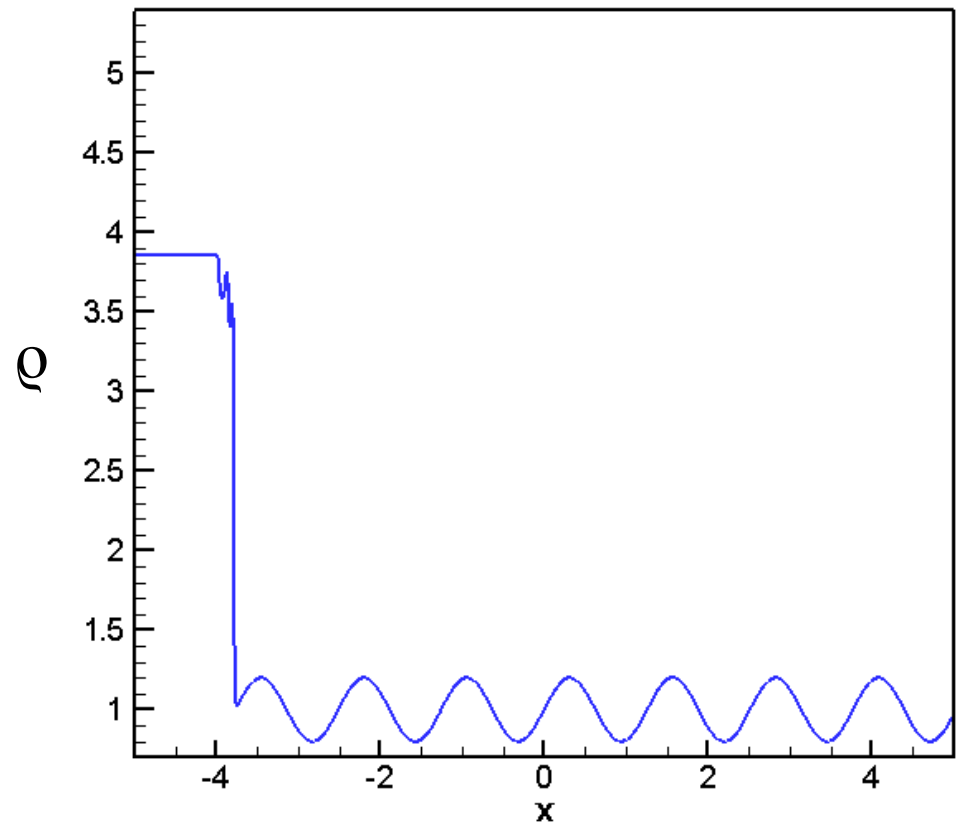
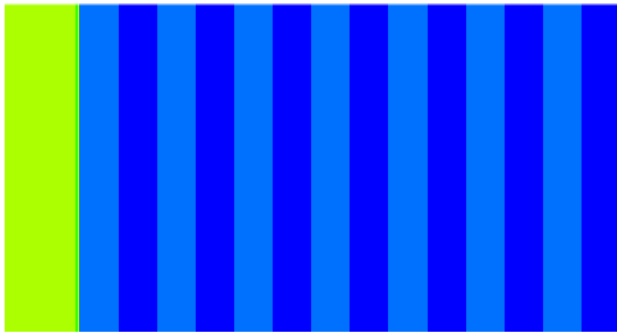
Grid Resolution Required for Waves





1D Shock-Acoustic Wave Interaction

Used by ENO, WENO, schemes to validate accuracy

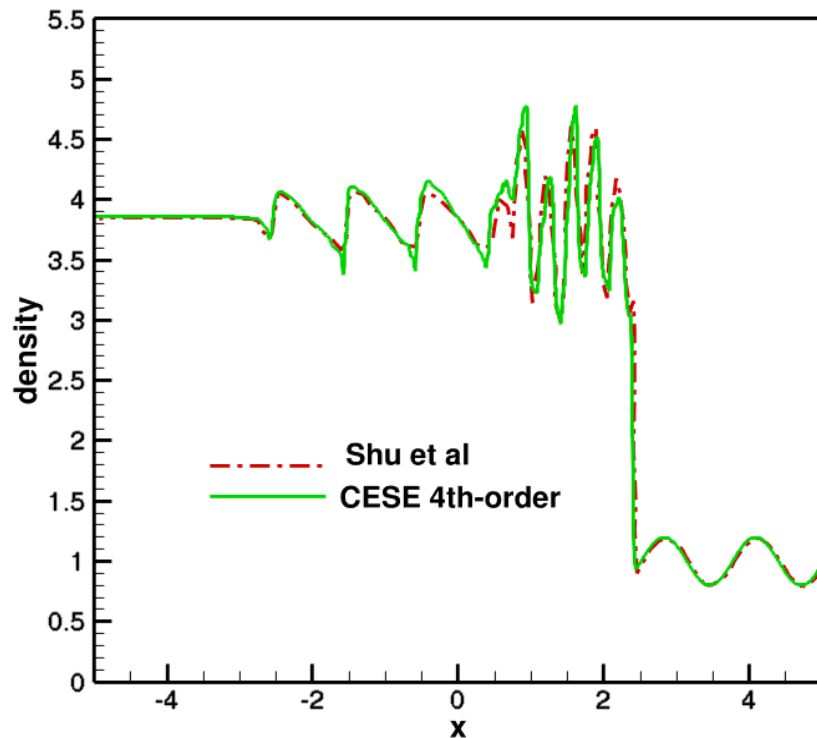


Density Contours and distribution

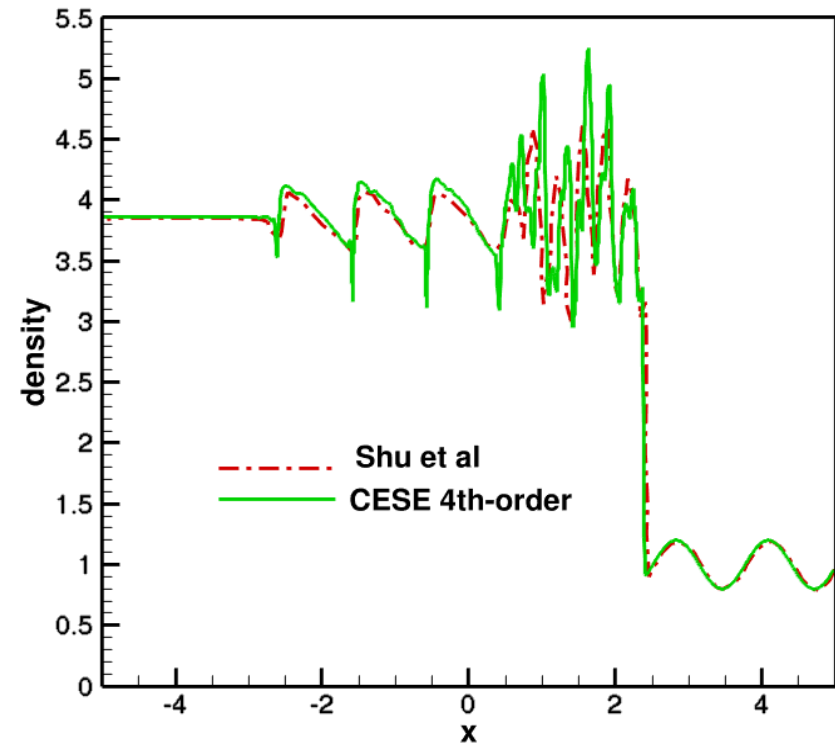


Shu & Osher Benchmark Problem (Shock/acoustic wave interaction)

1600 points



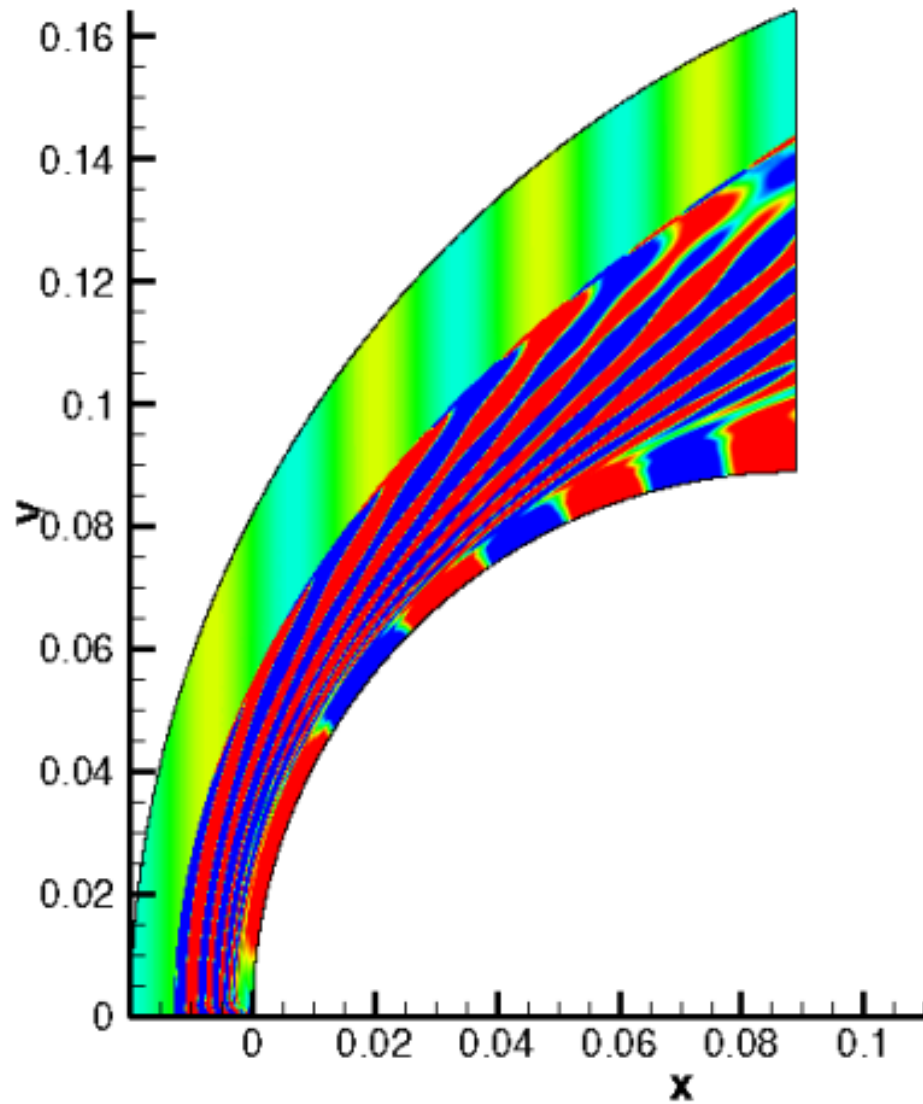
Grid converged solution
With large dissipation



Reduced numerical dissipation

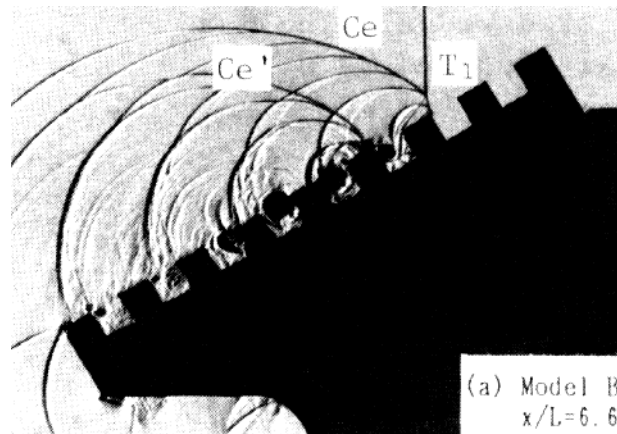
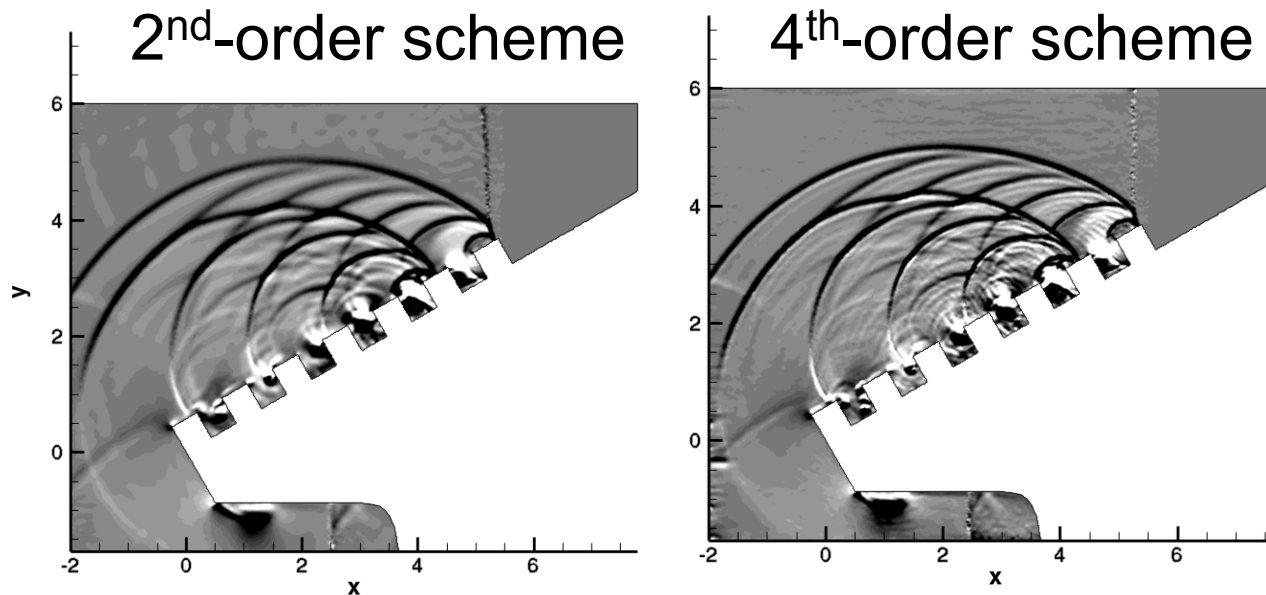


Acoustic Wave/Bow Shock Interaction over a hemisphere at Mach 6



Supersonic flow over a multi-gutter wall

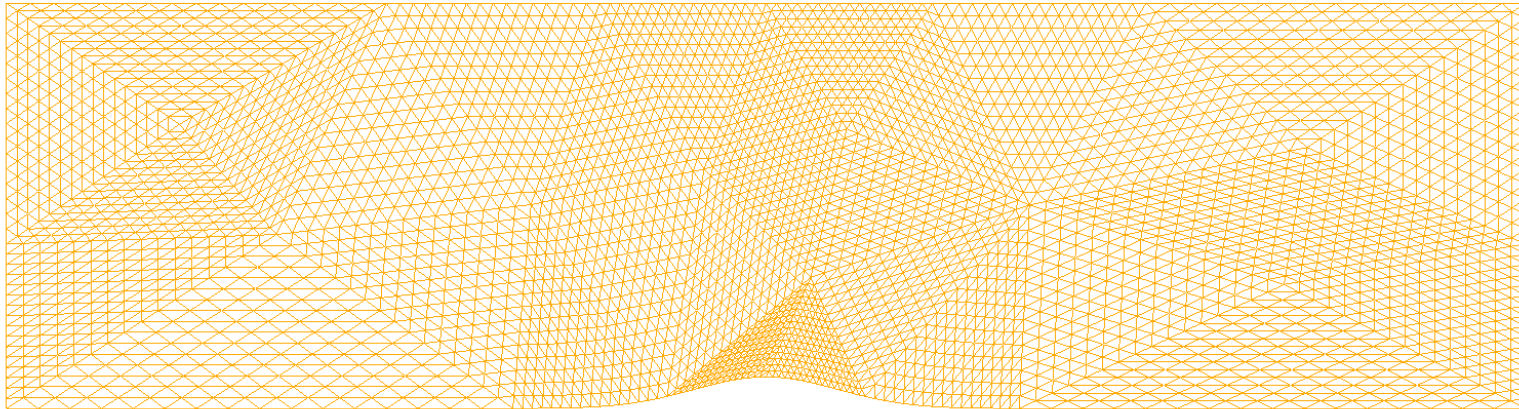
- Mach = 1.41, experiments by Suzuki et al.





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

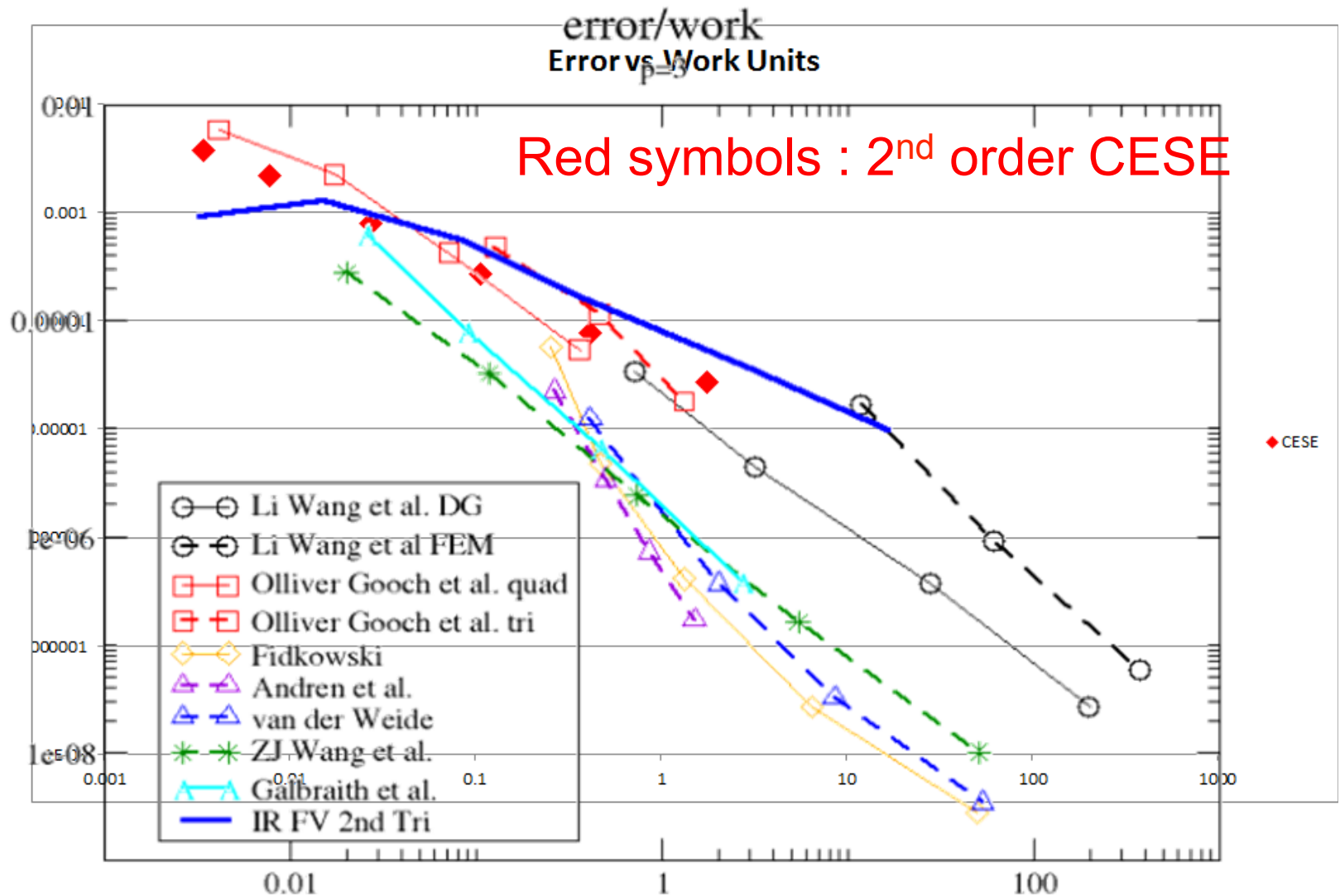
- Grids used were as provided by the workshop





HOM Benchmark C1.1

Error Norm vs. Other Methods ($p = 3$)



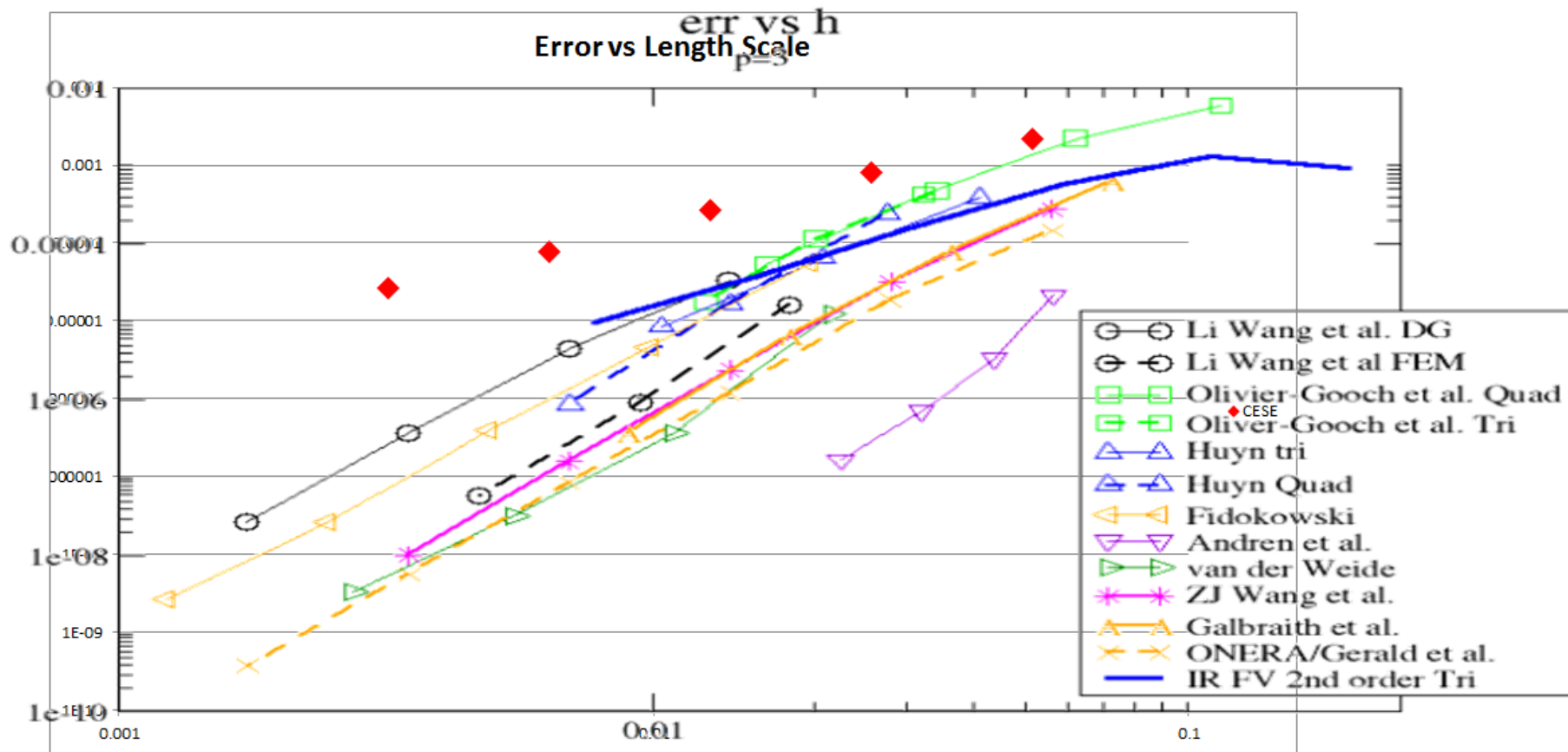
By David Friedlander GRC



HOM Benchmark C1.1

Error Norm vs. other methods ($p = 3$)

Red symbols : 2nd order CESE



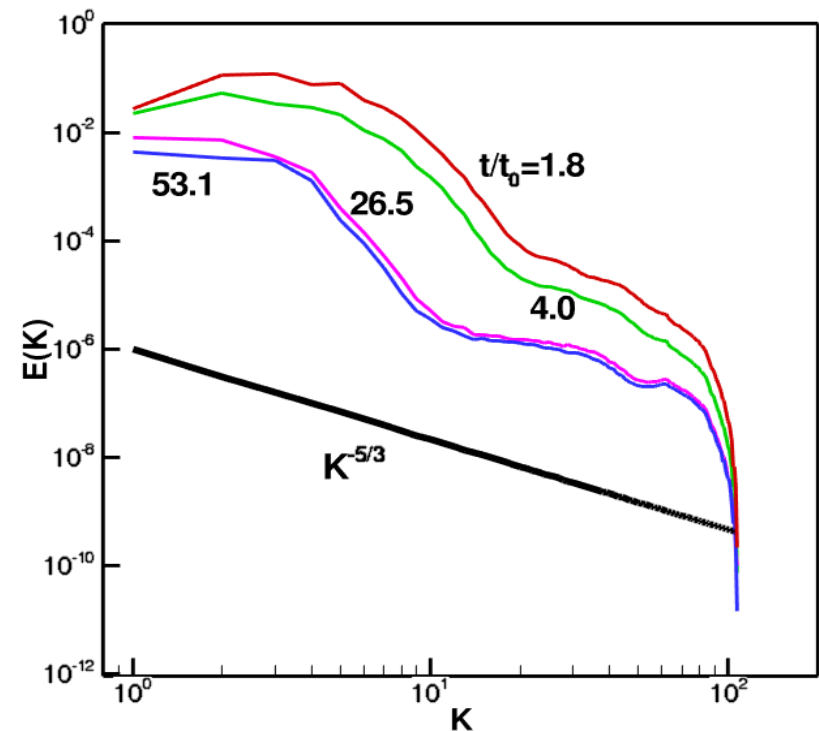
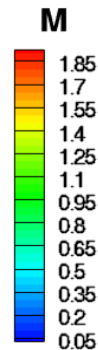
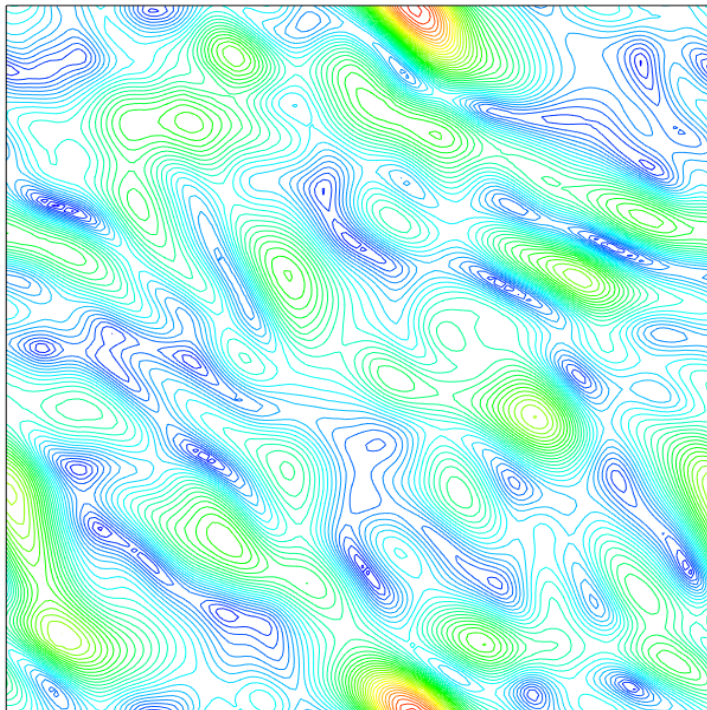
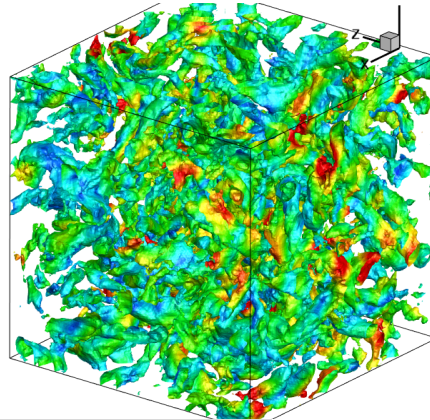
By David Friedlander GRC



Isotropic Turbulence Decay Simulation

$M_t=0.6$, $Re_t=100$ (64^3 tetrahedrons)

4th order CESE





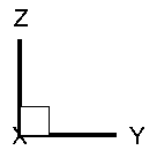
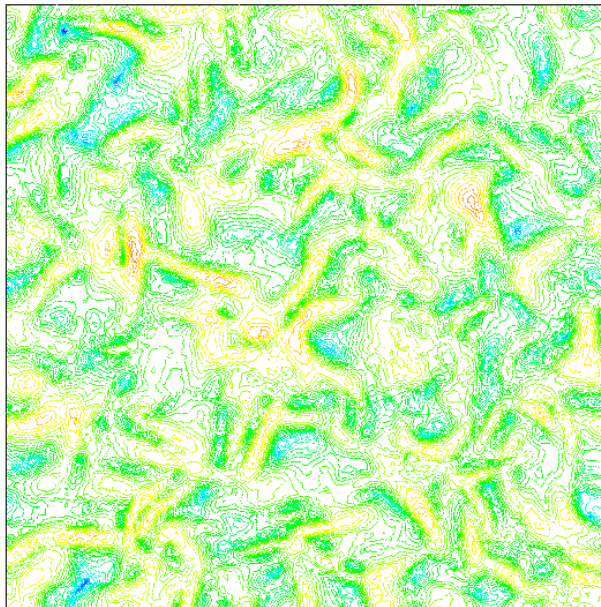
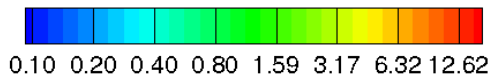
Isotropic Turbulence Decay Simulations

$M_t=1.5$, $Re_t=50$ (122^3 tetrahedrons)

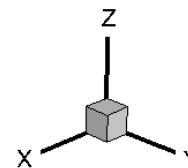
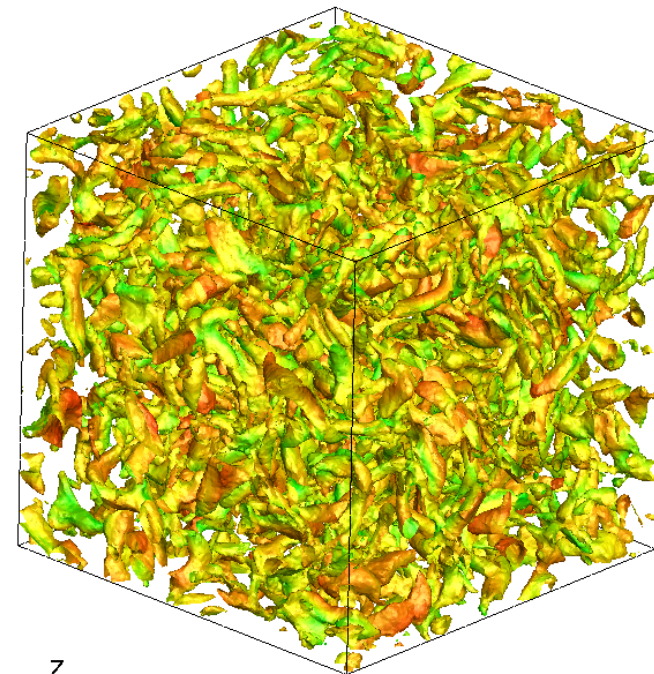
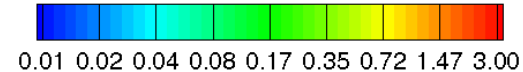
$Re_{Taylor} = 50.0$; $M_t = 1.5$

Iso-surface of Q-criterion shaded
with Mach contour

Density Gradient (magnitude)



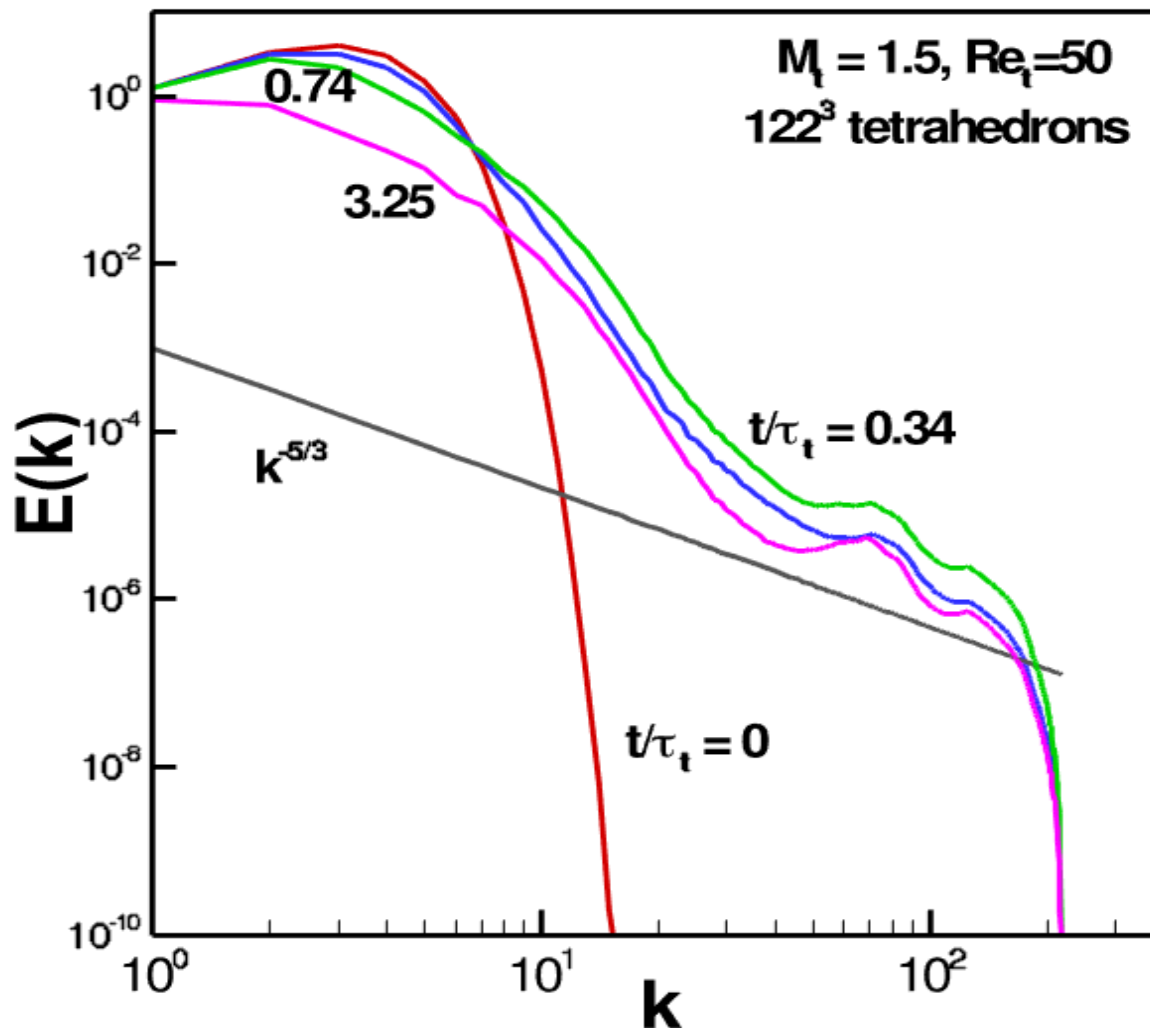
Mach No.





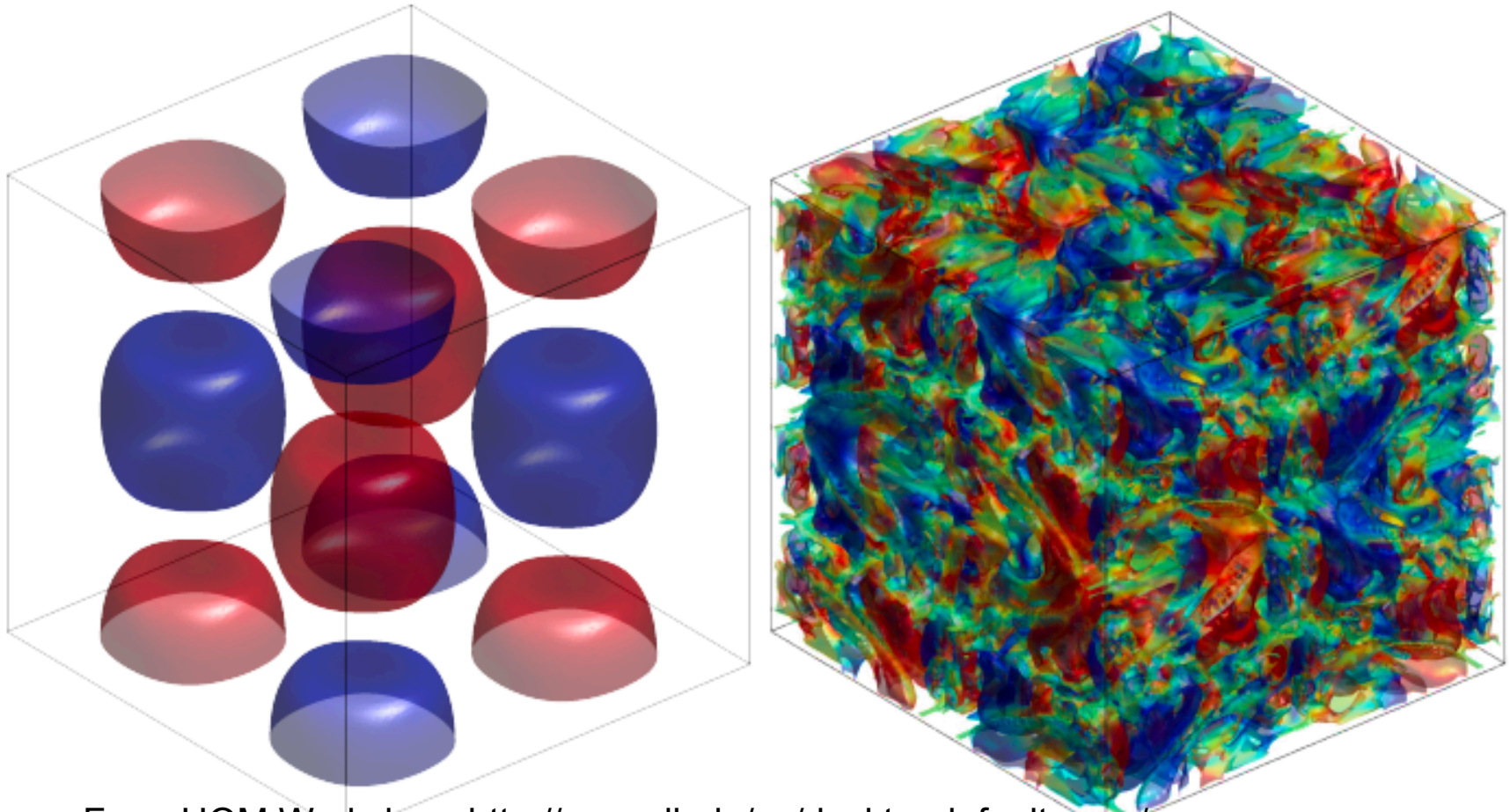
Isotropic Turbulence Decay Simulations

$M_t=1.5, Re_t=50$ Spectra



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

- HOM Benchmark C3.5



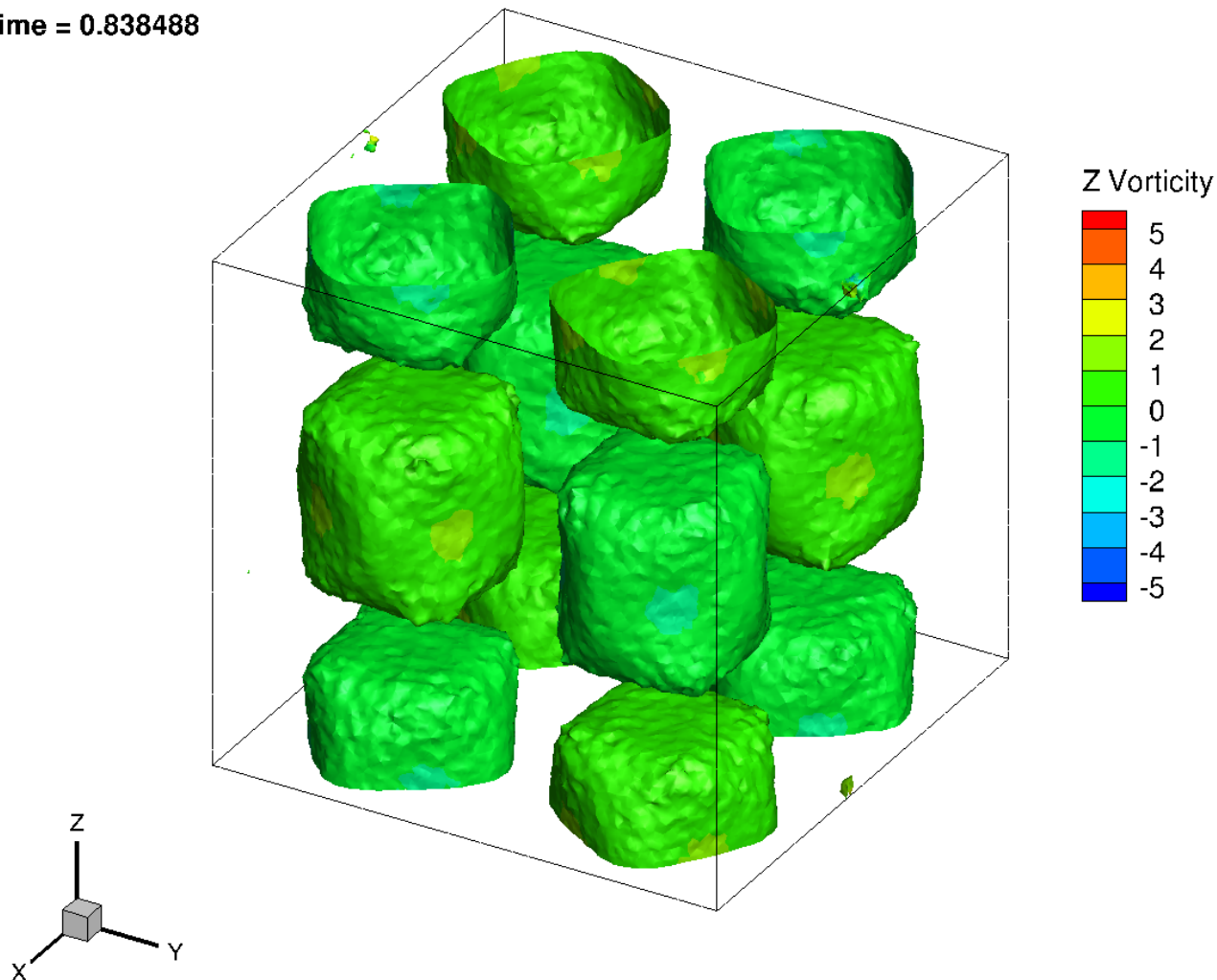
From HOM Workshop, http://www.dlr.de/as/desktopdefault.aspx/tabid-8170/13999_read-35550/

Direct Numerical Simulation of Taylor Green Vortex – Euler Solutions

Taylor-Green Vortex (Inviscid)

Q-criterion (value = 0.1) plot shaded by z-vorticity

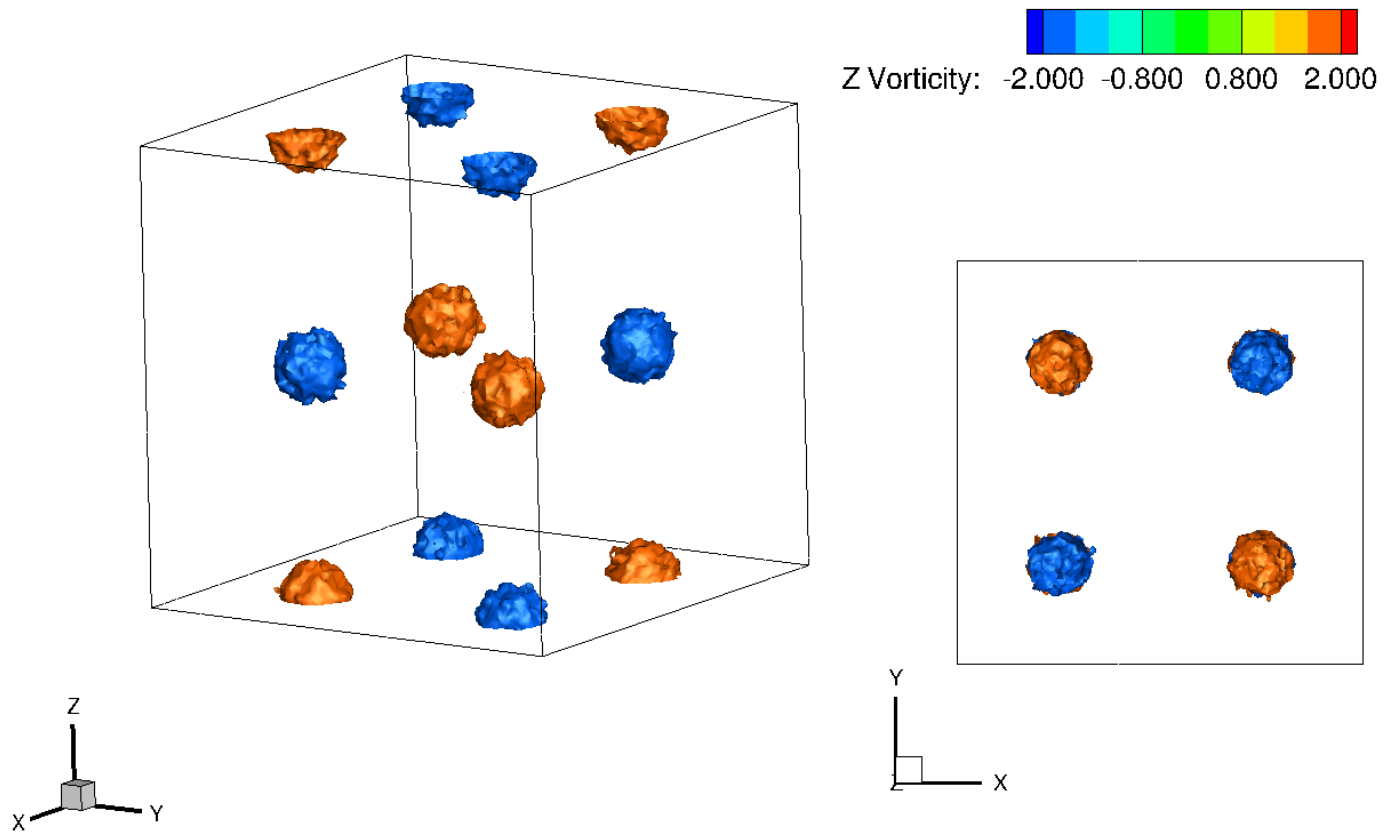
time = 0.838488



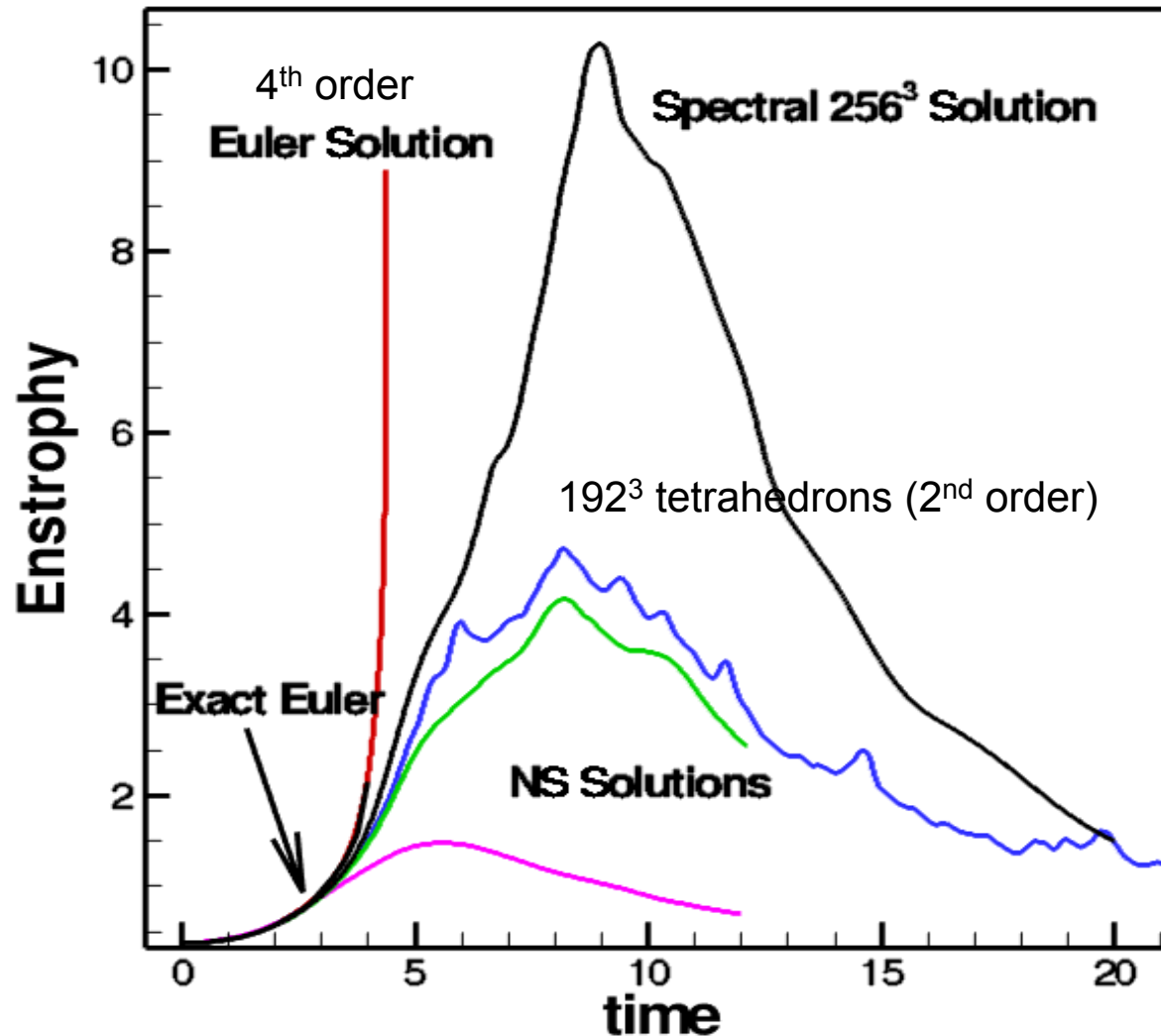
Direct Numerical Simulation of Taylor Green Vortex – $Re = 1600$

Taylor-Green Vortex ($Re = 1600$)
Iso-surfaces of Q -criterion shaded with z -vorticity

time = 0.27819



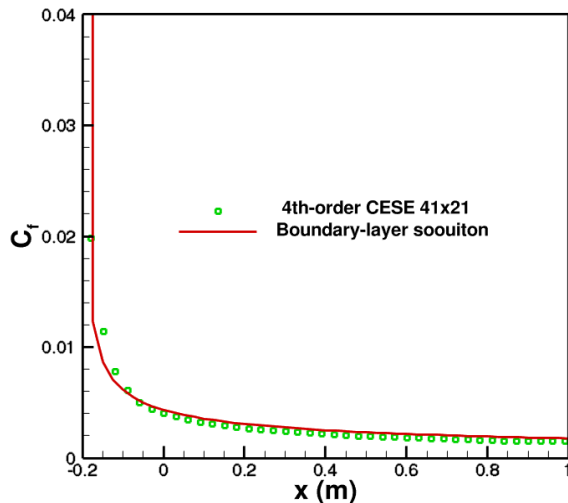
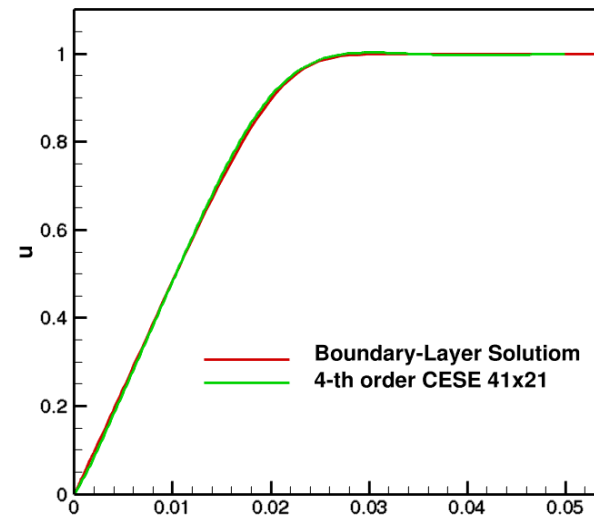
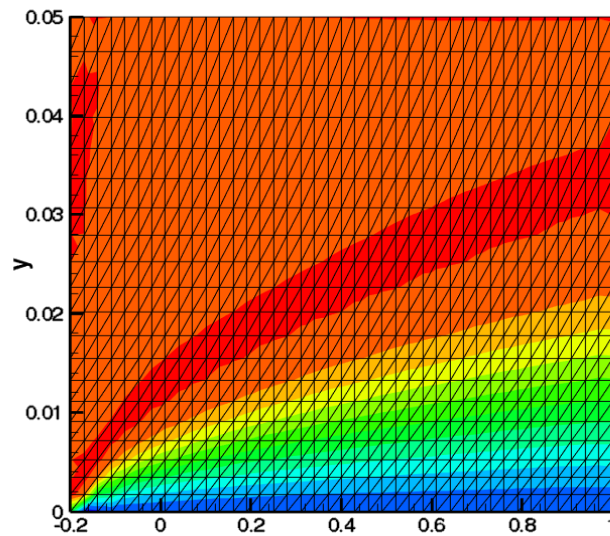
Direct Numerical Simulation of Taylor Green Vortex – Inviscid & $Re = 1600$



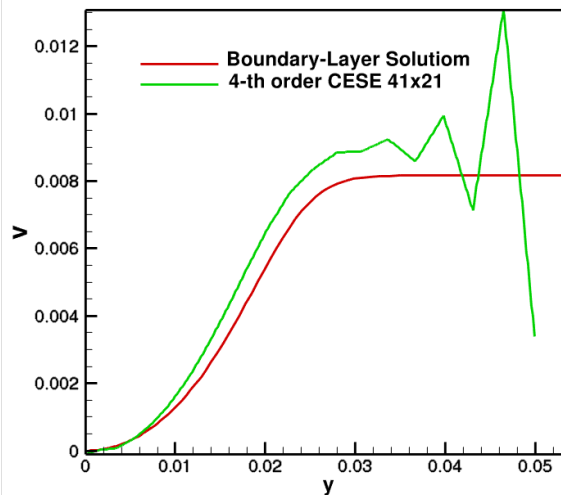


Mach 3 flat-plate boundary layer

Mesh with u velocity contours

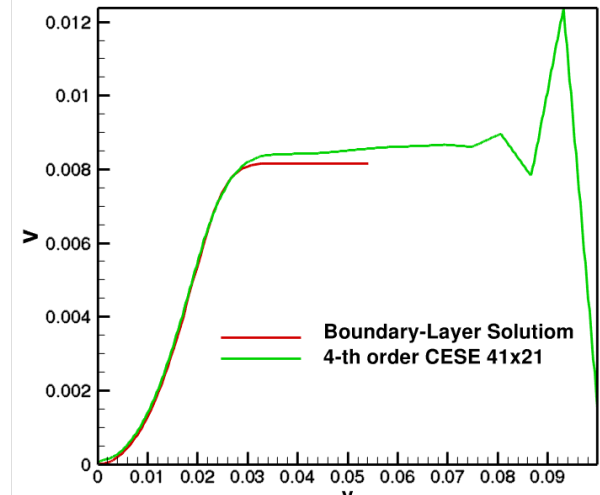


Skin friction



v velocity

u velocity

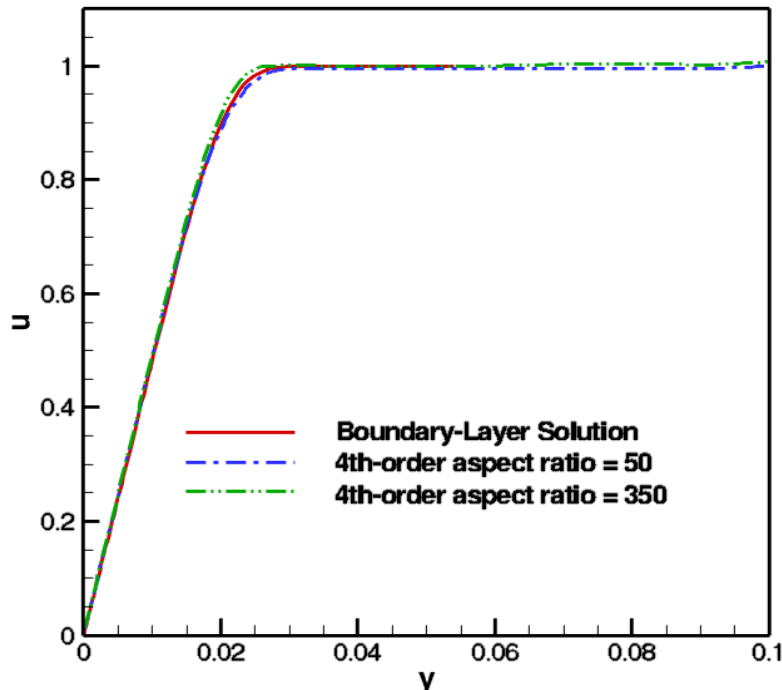


v velocity with
larger domain

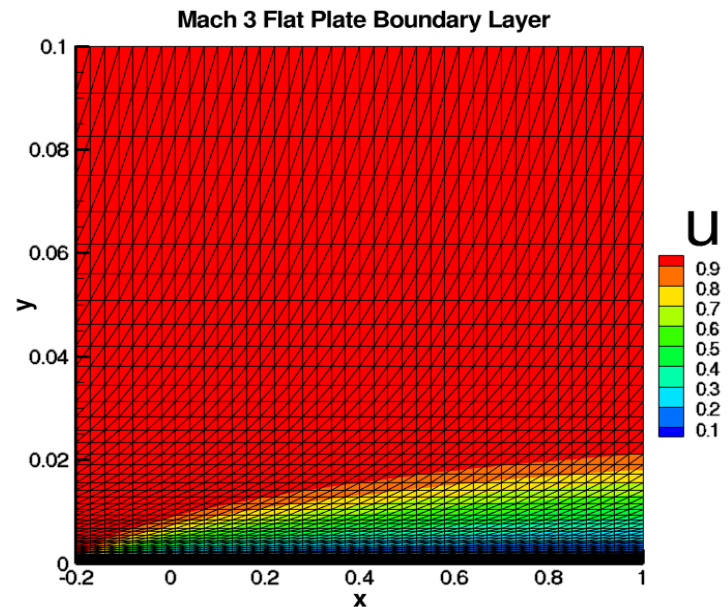


Integral High-Order Boundary Conditions

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

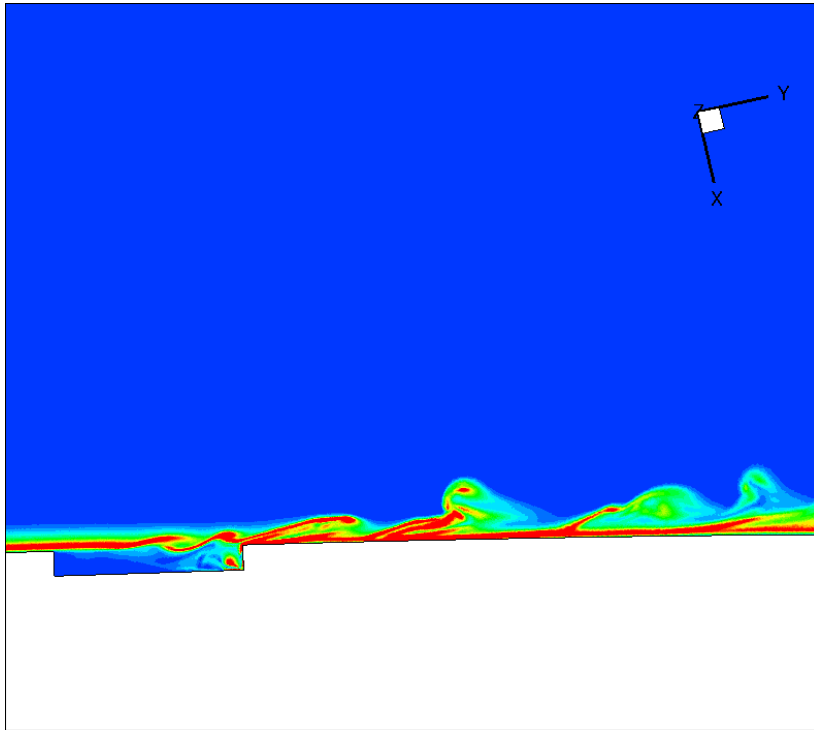


Mach 3 flat-plate boundary layer with adiabatic walls

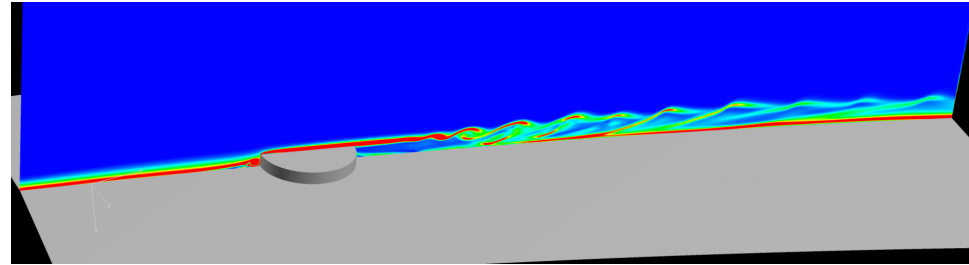




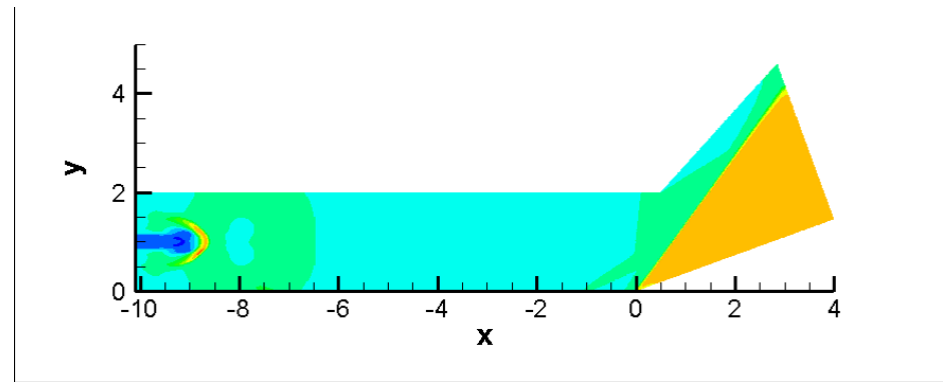
NASA Langley Research Center (ez4d)



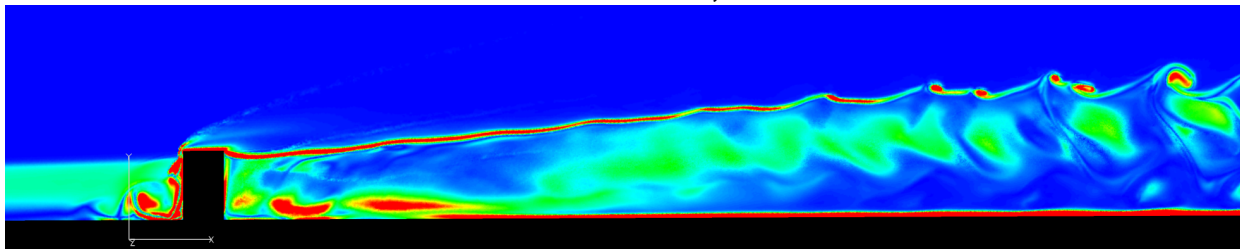
Subsonic (Mach 0.3) flow over a cavity



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

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

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

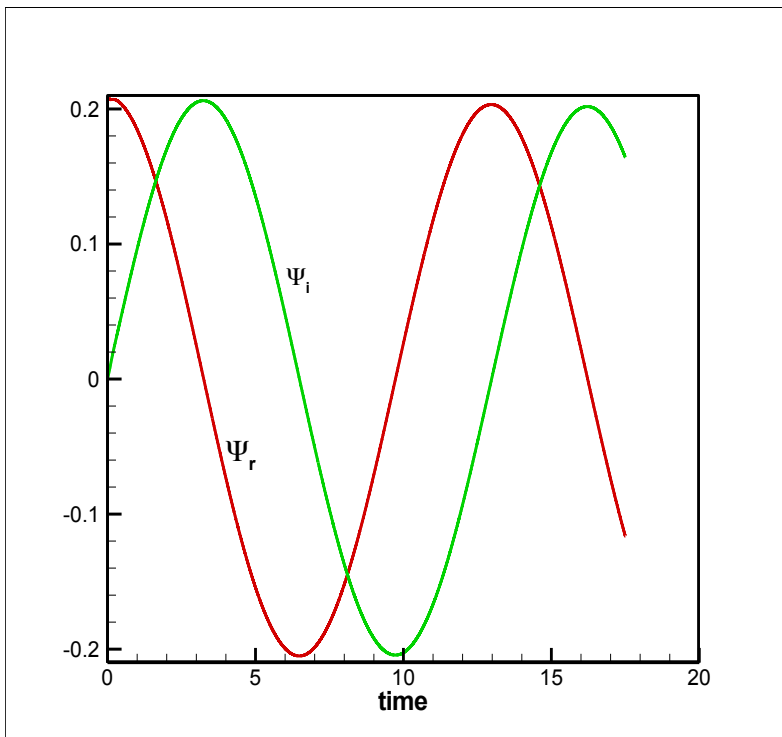
$$\Psi = e^{i\omega t - |\vec{r}|}$$

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

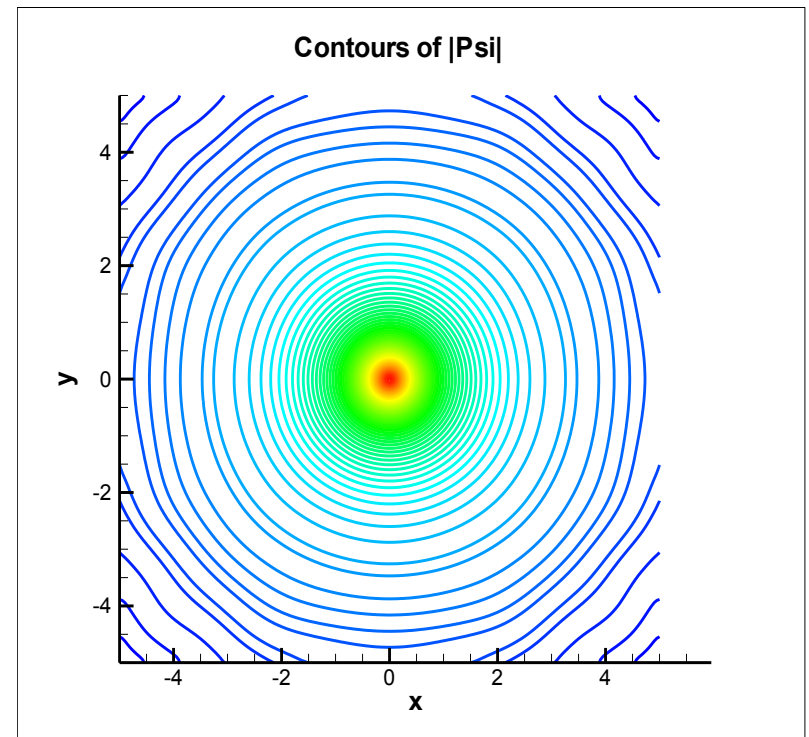


Numerical Solutions of the Model TDSE

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



Time trace at $(0, 1)$



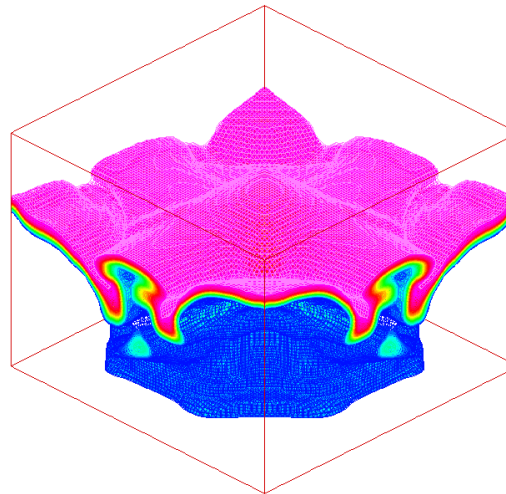
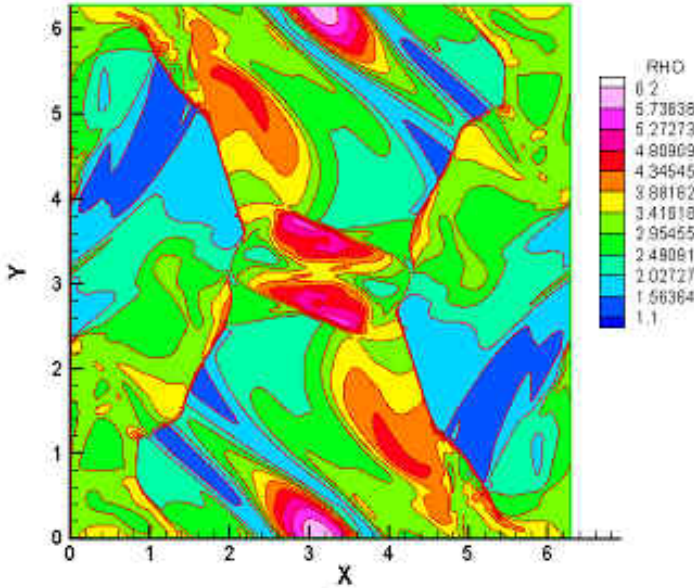
Ψ Contours₁



CESE Applications for Various Disciplines

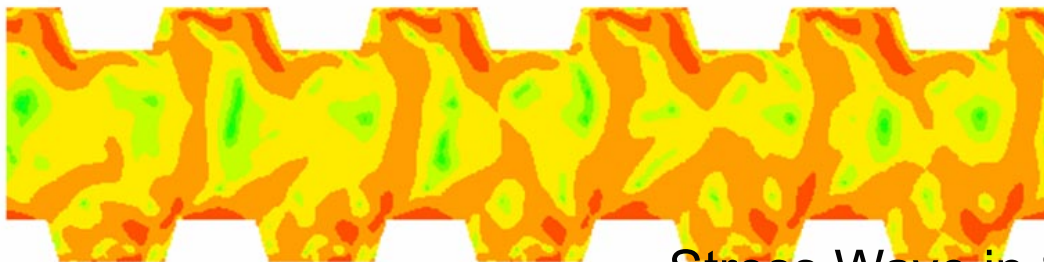
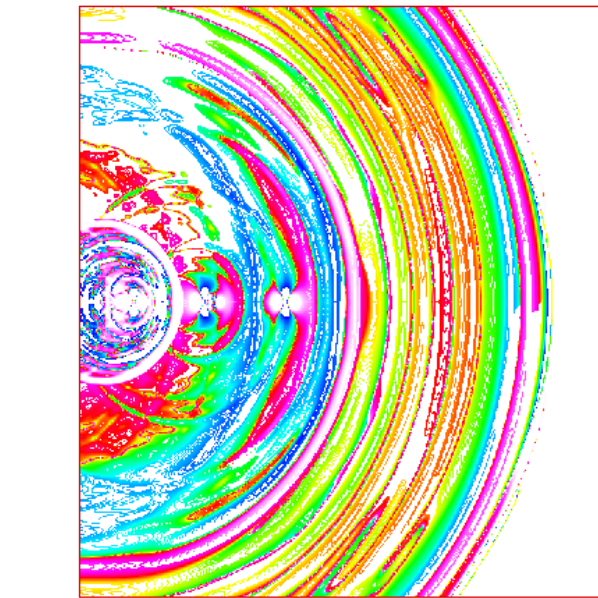
Prof. S.-T. Yu, Ohio State University

Ideal Magnetohydrodynamics (MHD)
Simulations



3D ZND (detonation)
Mass fraction

Pulse Detonation Engine
Mach 0.5 into $M = 0$

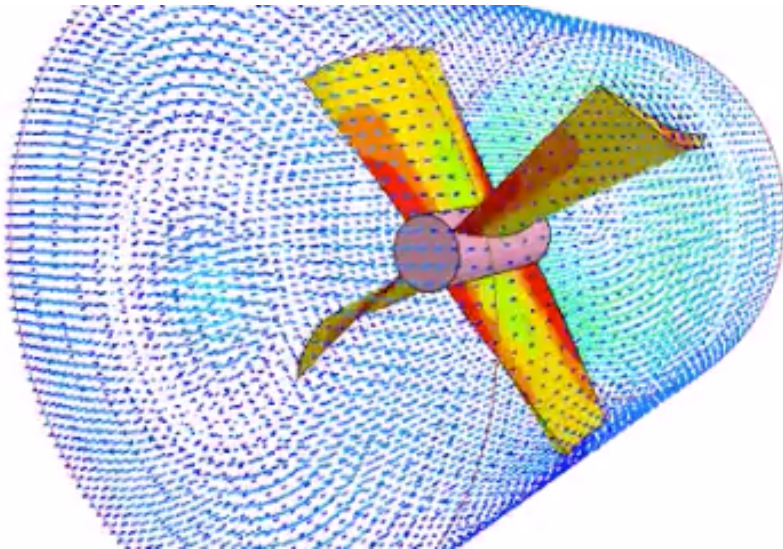
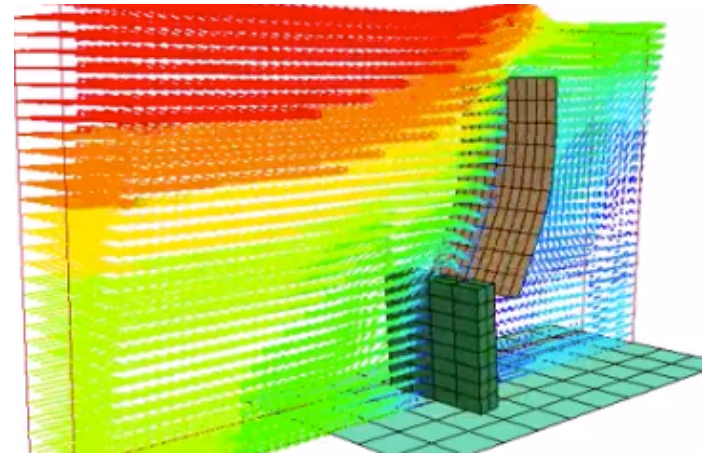


Stress Wave in Solids

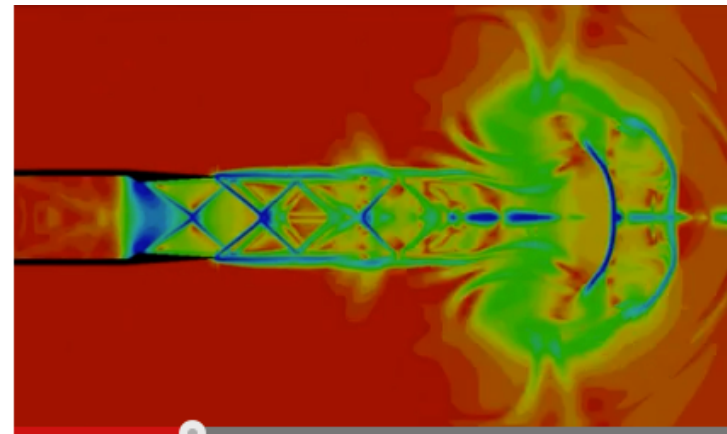


Yu, S.-T., Yang, L.X., and Lowe R. L., "Numerical Simulation of Linear and Nonlinear Waves in Hydroelastic Solids by the CESE Method," *Wave Motion*, 47(3), pp. 168-182, 2010.

- LS-DYNA CESE software
 - 2D/Axisymmetric/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 2nd order schemes
 - Compact stencil
 - Provides 4th, 3rd, 2nd, and 1st-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