High Fidelity Modeling for Numerical Simulations of Complex Combustion/Propulsion Systems

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MICHIGAN STATE UNIVERSITY

Objectives:

- Develop high-fidelity numerical models for high speed turbulent reacting flows
- Fundamental understanding of compressible turbulent reacting flows
- Study NASA's supersonic combustion problems for various flow and combustion parameters - Numerical experiments

- Long Term Goal: Integrated simulation of a "laboratory" high speed propulsion system – A virtual scramjet

Approach:

- A high-order, multi-block Eulerian-Lagrangian-Lagrangian LES/FMDF methodology is available for simulations of two-phase subsonic turbulent reacting flows in complex configurations
- LES/FMDF is being improved, extended and applied to high speed (supersonic and hypersonic) single-phase turbulent reacting flows
- DNS and experimental data is used for validation and improvement of LES/FMDF submodels

Large Eddy Simulations of Turbulent Reacting Flows

A Hybrid Eulerian-Lagrangian Methodology

Gasdynamics Field →

Filtered continuity and momentum equations via a generalized multi-block high-order finite difference **Eulerian** scheme for high speed turbulent flows in complex geometries

Compressible subgrid closures

Scalar Field (mass fractions and temperature) →

Filtered Mass Density Function (FMDF) equation via **Lagrangian** Monte Carlo method – Compressibility effects are added

Chemistry →

Kinetics: (I) reduced kinetics schemes with direct ODE solvers, and (II) reaction library with detailed mechanisms or complex reduced schemes
Fuels: methane, propane, decane, JP-10 kerosene, heptane, hydrogen, ethanol

LES/FMDF of Turbulent Reacting Flows

A Hybrid Eulerian-Lagrangian Methodology

$$\langle f \rangle_l = \int_{-\infty}^{+\infty} f(x',t) G(x'-x) dx', \quad \langle f \rangle_L = \frac{\langle \rho f \rangle_l}{\langle \rho \rangle_l}$$

Eulerian Component

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_i} = 0$$

$$\frac{\partial \langle \rho \rangle_l \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = -\frac{\partial \langle p \rangle_l}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle_l}{\partial x_i} - \frac{\partial \langle \Gamma_{ij} \rangle_l}{\partial x_i}$$

$$\frac{\partial \langle \rho \rangle_l \langle E \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle E \rangle_L}{\partial x_i} = -\frac{\partial \langle q_i \rangle_l}{\partial x_i} - \frac{\partial N_i}{\partial x_i} + \langle \rho S_e \rangle_l$$

$$\frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial \langle J_i^\alpha \rangle_l}{\partial x_i} - \frac{\partial M_i^\alpha}{\partial x_i} + \langle \rho S_\alpha \rangle_l, \quad \alpha = 1,2,\ldots,N_s$$

$$\langle p \rangle_l = \langle \rho \rangle_l R^0 \sum_{\alpha=1}^{N_\alpha} \langle Y_\alpha T \rangle_L / M_\alpha = \langle \rho \rangle_l \langle RT \rangle_L$$

LES/FMDF of Turbulent Reacting Flows

Scalar FMDF

Lagrangian Component

$$P_L(\psi, x, t) \equiv \int \rho(x', t)\xi[\psi, \phi(x', t)]G(x' - x)dx'$$

$[\psi, \phi(x,t)] \equiv$ Mass Fractions and Energy

$$\xi[\psi, \phi(x,t)] = \delta[\psi - \phi(x,t)] \equiv \prod_{\alpha=1}^{N_s} \delta[\psi_\alpha - \phi_\alpha(x,t)]$$

Fine-Grained Density

Scalar FMDF Equation

$$\frac{\partial P_L}{\partial t} + \frac{\partial\left[\langle u_i \rangle_L P_L\right]}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\langle \rho \rangle_L \left(\langle D \rangle_L + D_l\right)\frac{\partial\left(P_L / \langle \rho \rangle_l\right)}{\partial x_i}\right]$$

$$+ \sum_{\alpha=1}^{N_s+1} \frac{\partial}{\partial \psi_\alpha}\left[\Omega_m\left(\psi_\alpha - \langle \phi_\alpha \rangle_L\right)P_L\right] - \sum_{\alpha=1}^{N_s+1} \frac{\partial}{\partial \psi_\alpha}\left[\hat{S}_\alpha P_L\right]$$

$S_\alpha \equiv$ **Reaction terms**

LES/FMDF of Turbulent Reacting Flows

Subgrid-Scale Closures

Subgrid Stresses in Momentum Eq. : $T_{ij} = \langle \rho \rangle_l \left(\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L \right)$

Subgrid Convection in FMDF Eq. : $\left[\langle u_i | \psi \rangle_L - \langle u_i \rangle_L \right] P_L = -\gamma_t \dfrac{\partial \left(P_L / \langle \rho \rangle_l \right)}{\partial x_i}$

Subgrid Mixing in FMDF Eq. (LMSE/IEM model) :

$$\frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left[\left\langle \gamma \frac{\partial \phi_a}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \middle| \psi \right\rangle_L P_L / \rho \right] = -\frac{\partial}{\partial \psi_a} \left[\Omega_m \left(\psi_\alpha - \langle \phi_a \rangle_L \right) P_L \right]$$

Subgrid Reaction: *No model is needed in FMDF methodology!*

LES of Turbulent Reacting Flows

Velocity-Scalar FMDF

$$F_L(V,\psi,x;t) \equiv \int_{-\infty}^{+\infty} \rho(x',t)\xi[V,U(x',t),\psi,\phi(x',t)]G(x'-x)dx'$$

Fine-Grained Density $\xi[V,U(x,t),\psi,\phi(x,t)] = \delta[V-U(x,t)]\delta[\psi-\phi(x,t)]$

Velocity-Scalar FMDF Transport Equation

$$\frac{\partial F_L}{\partial t} + v_i \frac{\partial F_L}{\partial x_i} = \left(\frac{1}{\hat{\rho}}\frac{\partial \langle p \rangle_l}{\partial x_i}\right)\frac{\partial F_L}{\partial v_i} - \frac{\partial\left[\hat{S}_\alpha(\psi)F_L\right]}{\partial \psi_\alpha} + \frac{\partial}{\partial v_i}\left[\left\langle -\frac{\partial \tau_{ij}}{\partial x_j} \middle| V,\psi \right\rangle F_L/\hat{\rho}\right]$$

$$+ \frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial J_i^\alpha}{\partial x_i} \middle| V,\psi \right\rangle F_L/\hat{\rho}\right] + \frac{\partial}{\partial v_i}\left[\left(\left\langle \frac{\partial p}{\partial x_i} \middle| V,\psi \right\rangle_l - \frac{\partial \langle p \rangle_l}{\partial x_i}\right)F_L/\hat{\rho}\right]$$

Turbulent convection and chemical reaction terms are closed

Main Features of LES/FMDF

- Large scale, unsteady, non-universal, geometry-depended quantities are explicitly computed in LES/FMDF

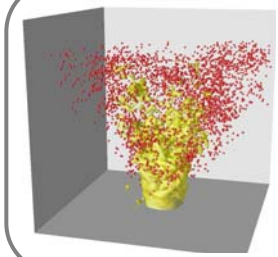
- LES/FMDF is applicable to 3D simulations of high speed reacting flows in complex geometries

- FMDF accounts for the effects of chemical reactions in an exact manner and may be used for various types of chemical reactions (slow, fast, endothermic, exothermic, etc.)

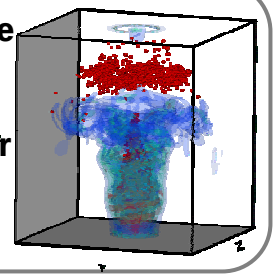
- FMDF contains high order information on subgrid or small scale fluctuations

- The Lagrangian Monte Carlo solution of the FMDF is free of artificial (diffusion) numerical errors

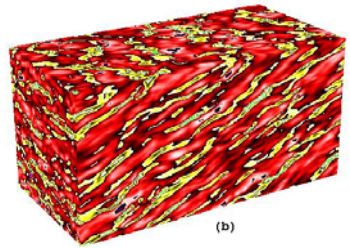
Application of LES/FMDF to Subsonic Flows

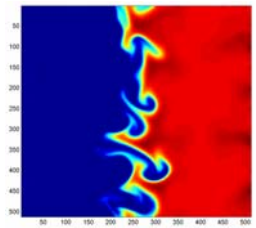


Double Swirl Spray Burner

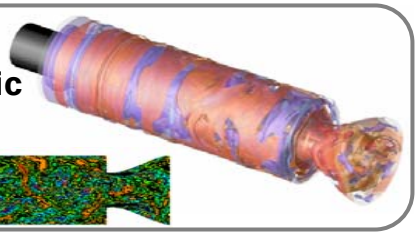


Homogeneous Compressible Turbulent Combustion

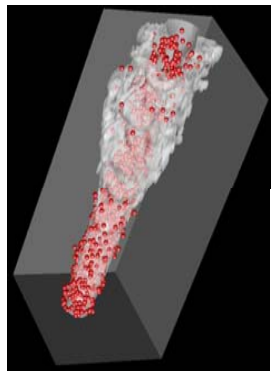


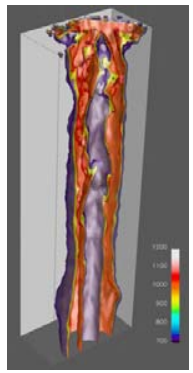


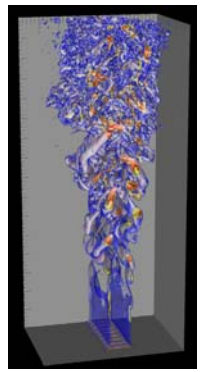
Axisymmetric Combustor

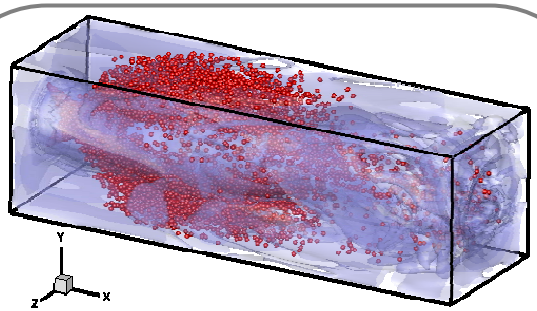


Round and Planar Single- and Two-Phase Reacting Jets

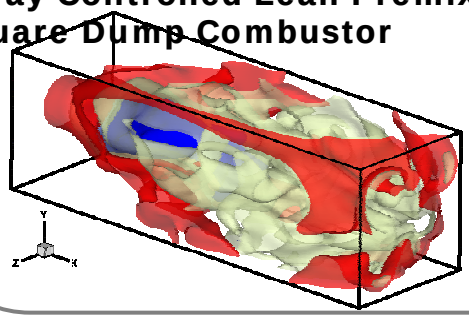




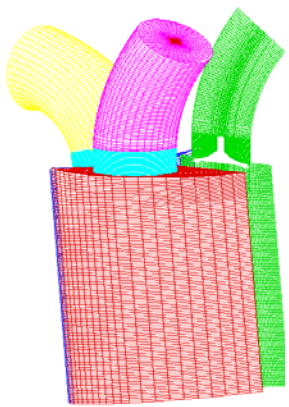


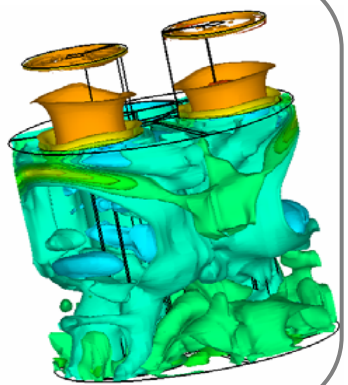


Spray Controlled Lean Premixed Square Dump Combustor



Direct Injection Gasoline Engine With Moving Valves and complex Piston & Cylinder Head





Validation of LES Models and Numerical Schemes

Comparison with experiment

- Jet and bluff body flames
- Two-phase turbulent jet
- Dump combustor
- Swirl-stabilized burner

Comparison with DNS

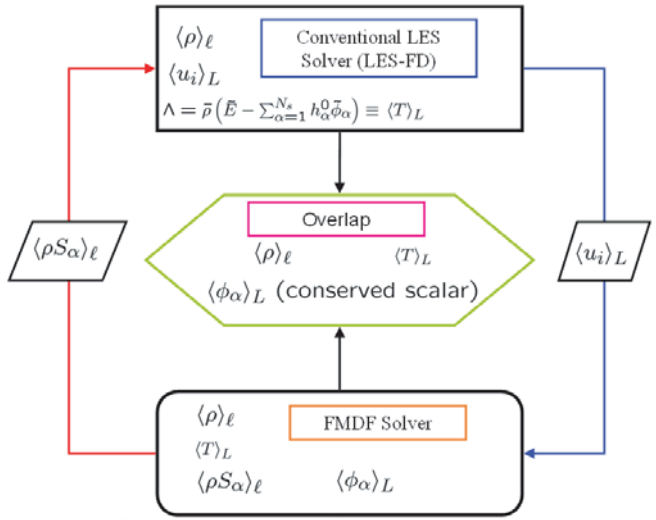
- Turbulent mixing layer
- Planar turbulent Jet
- Homogeneous turbulent flow

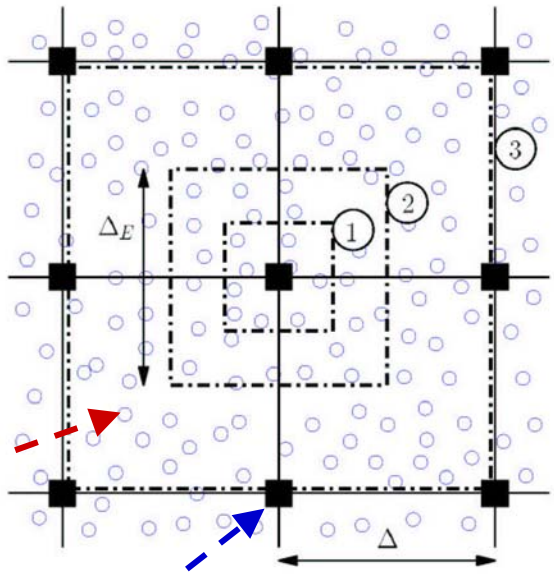
Comparison between different LES methods

- A generalized high-order finite difference vs. finite volume and spectral schemes
- Consistency of Eulerian and Lagrangian fields

A Hybrid Eulerian-Lagrangian Numerical Method

- Eulerian: Transport equations for the SGS moments
  - Deterministic simulations
- Lagrangian: Transport equation for the FMDF
  - Monte Carlo simulations
- Coupling of Eulerian & Lagrangian fields and a certain degree of "redundancy"



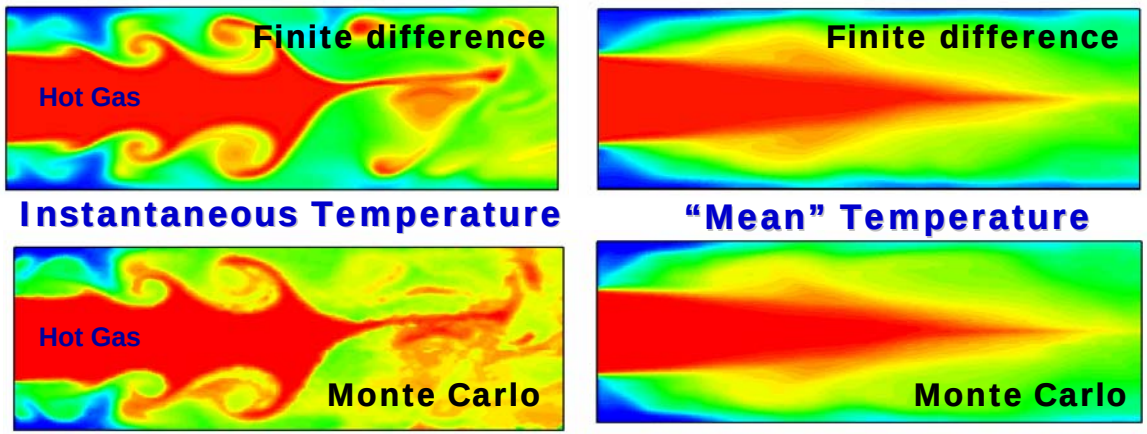


Lagrangian Monte Carlo Particle

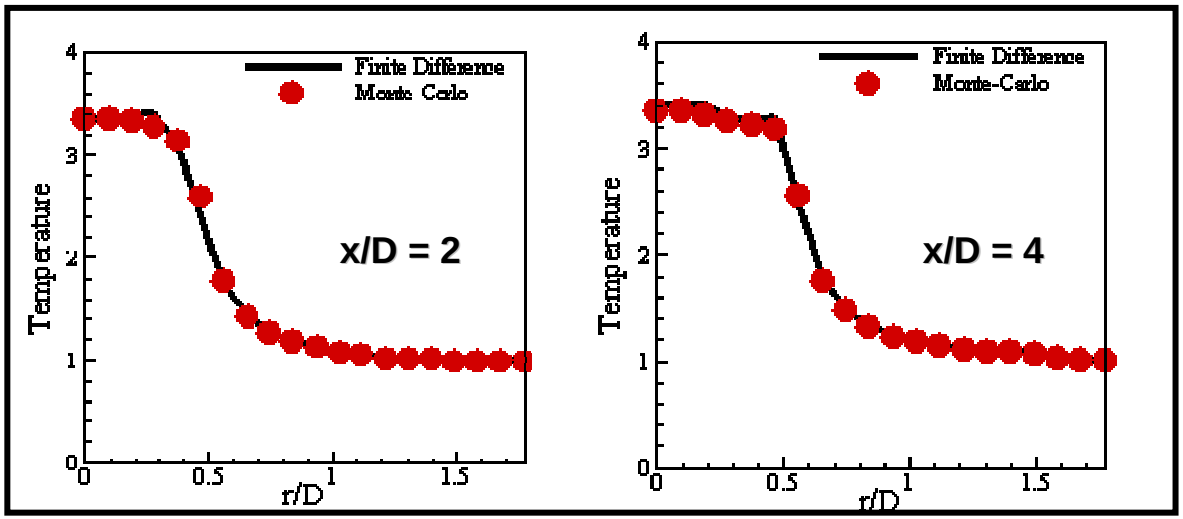
Eulerian Grid Point

LES/FMDF of Dump Combustors

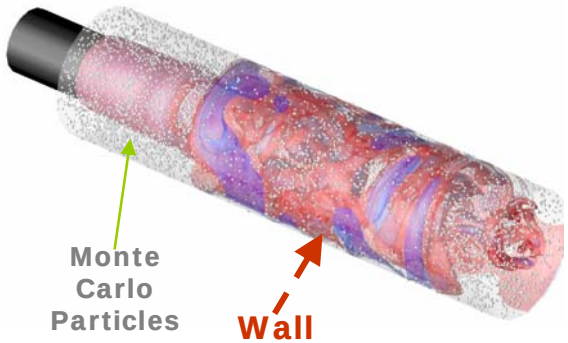
consistency between Eulerian and Lagrangian components



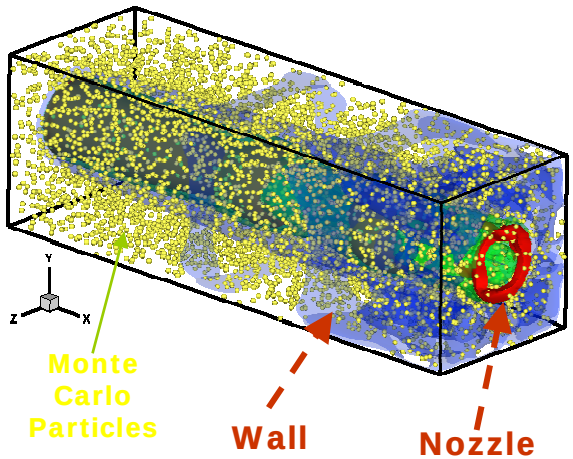
Consistency for Non-Reacting, Non-Isothermal Flows



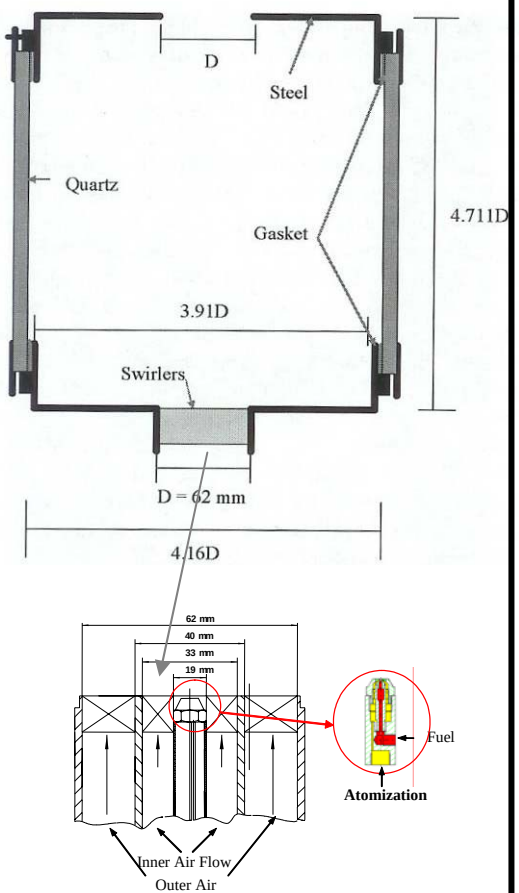
Axisymmetric Sudden Expansion



Rectangular Sudden Expansion

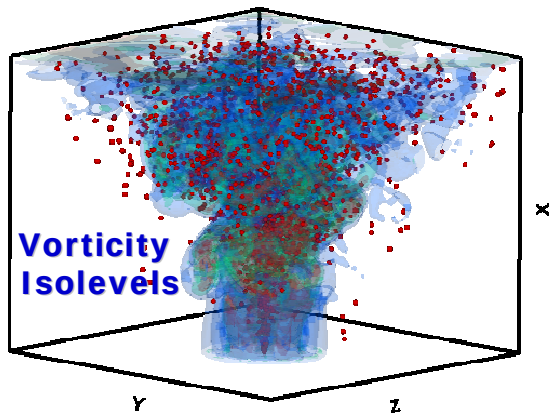


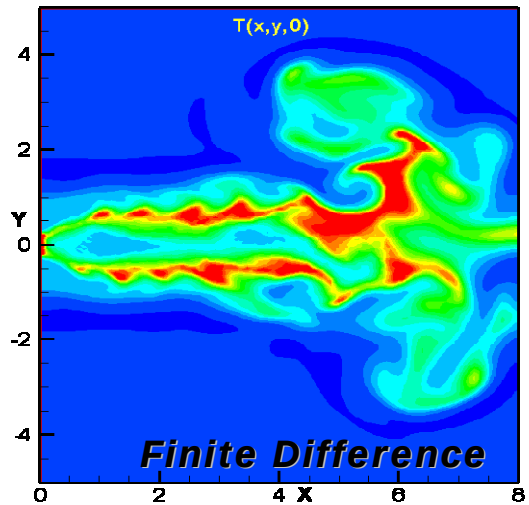
LES/FMDF of Double Swirl Spray Burner

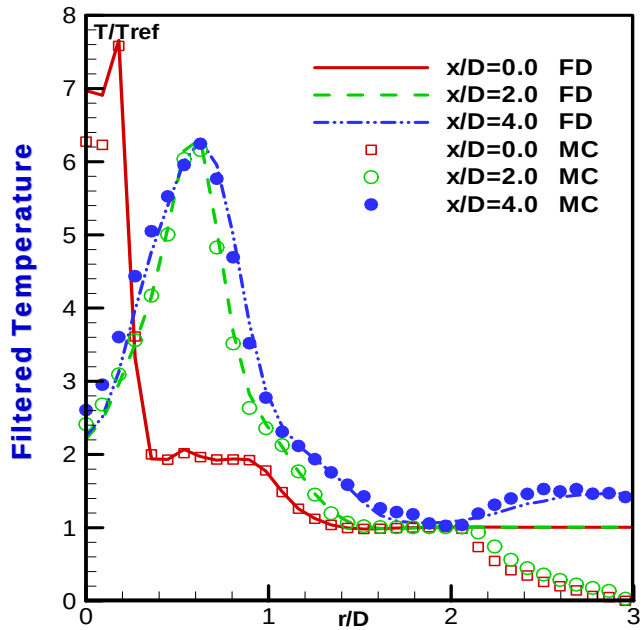


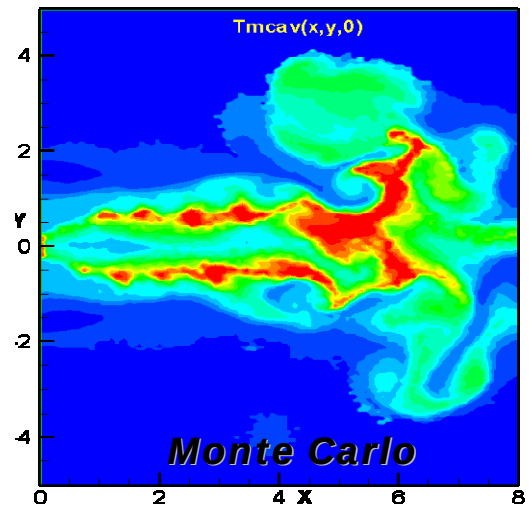
A Schematic of Double Swirl-Stabilized Spray Burner

Consistency for Reacting Flow with Spray





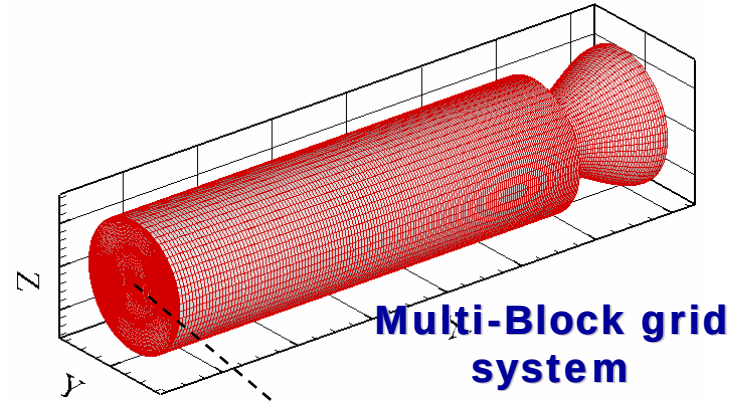




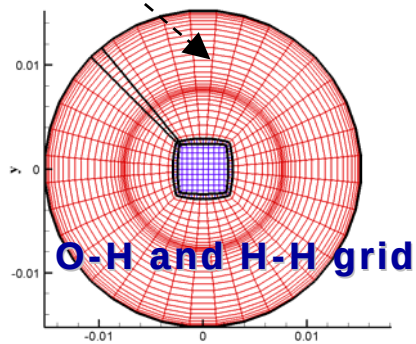
Temperature Contours

LES/FMDF of Axisymmetric Dump Combustor (Gould et al. 1994)

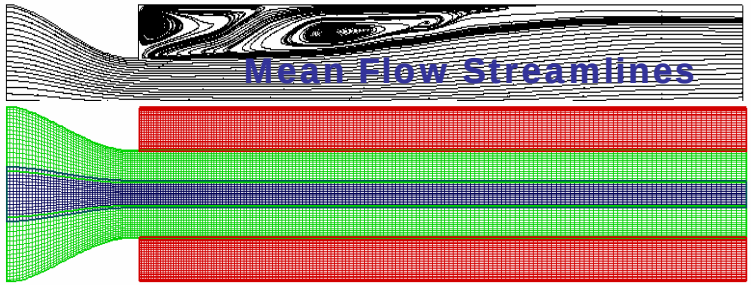
Comparison with experiment

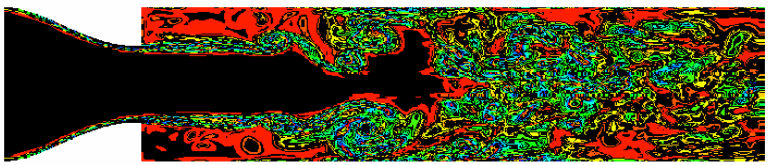


Multi-Block grid system

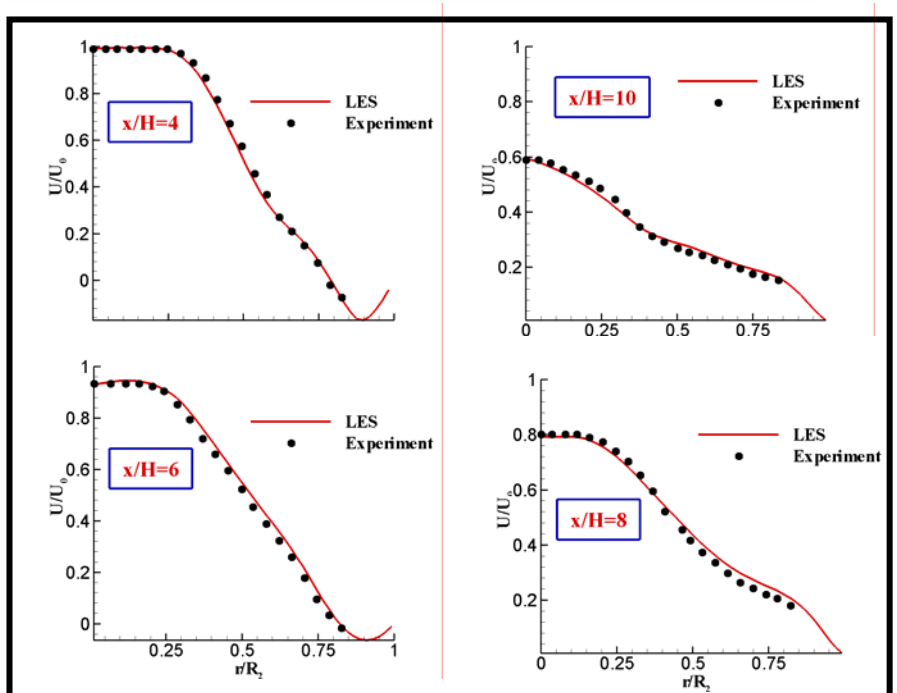


O-H and H-H grid

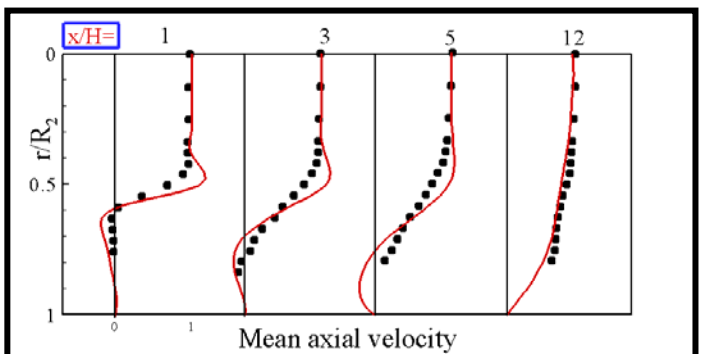




Vorticity Contours



Cold Flow – mean axial velocity



Reacting Flows

Extension and Application of LES/FMDF to High Speed Flows

- In its present form, LES/FMDF is a robust and efficient methodology for single- and two-phase subsonic turbulent reacting flows in complex geometries
- Large-scale compressibility effects are explicitly calculated
- Robust high-order Eulerian finite difference methods (e.g. WENO, MP, Compact+MP) for LES of high speed turbulent flows have been developed
- Work is in progress to develop improved subgrid and wall (e.g. DES) models for supersonic and hypersonic flows
- Subgrid compressibility effects are being added to existent scalar FMDF model
- PDF-based subgrid compressible velocity-scalar FMDF models are being developed for supersonic flows
- Close collaborations with NASA scientists and other university investigators- continuously including their inputs into our work (flow configurations, experimental data, chemistry models,…….)

Application of LES to High Speed Flows

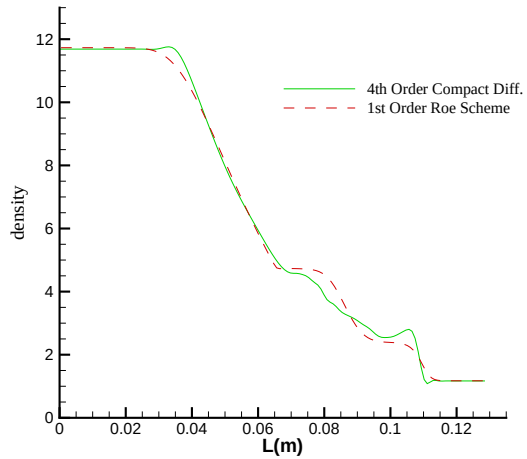
Numerical Methods

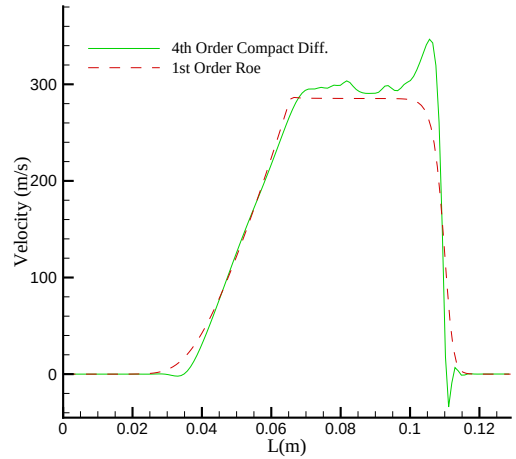
1) High-order Compact-RK scheme + Filtering and/or local upwind limiters (Rizzetta et al. 2001) – 3D code is developed and tested
2) High-order WENO-RK scheme (Shi et al. 2003)- 3D code is developed and tested
3) High-order Monotonicity Preserving (MP)-RK scheme (Huynh 2007) - 2D code is developed and tested, 3D code is developed)

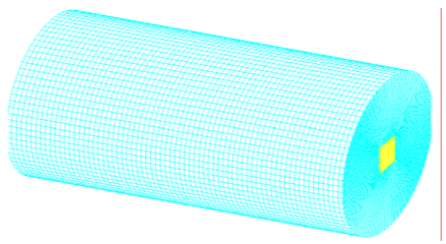
Test Problems

1) 1D Problems: Advection (Wave), Burgers, Lax, Shock Tube, (1D calculations with 3D codes)
2) 2D Problems: Rayleigh-Taylor Instability, Double Mach Reflection, Isotropic Turbulence (2D calculations with 3D codes)
3) Converging-Diverging Nozzle – 3D LES calculations
4) Supersonic Channel Flow – 3D DNS and LES calculations
5) Supersonic Boundary Layer and Compression Ramp – 3D LES calculations
6) Co-Annular Reacting Supersonic Jet – 3D LES calculations

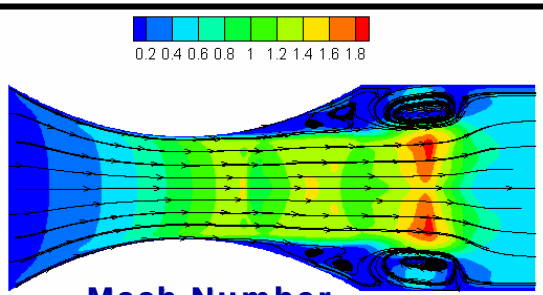
Application of LES to High Speed Flows



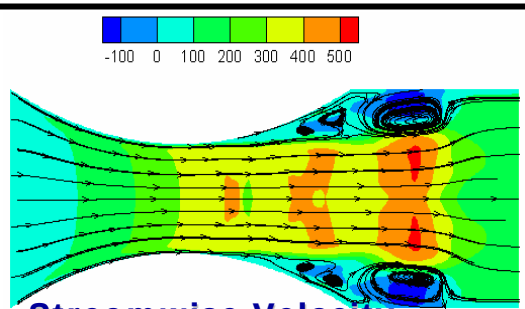




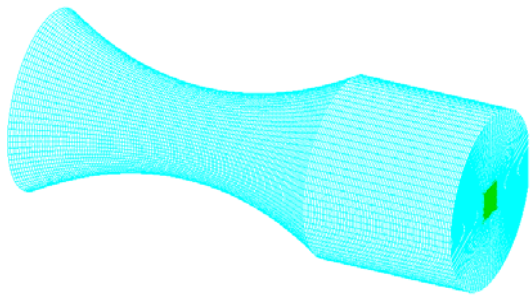
Shock Tube
3D calculations with Compact Scheme

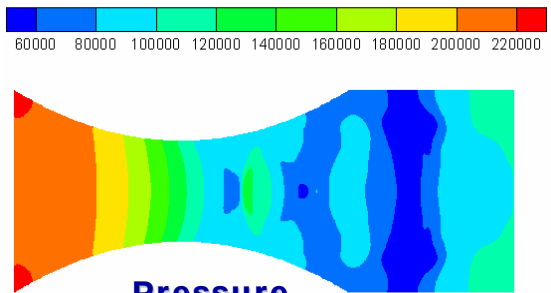


Mach Number

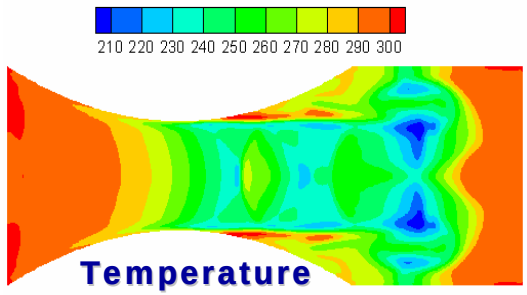


Streamwise Velocity





Pressure



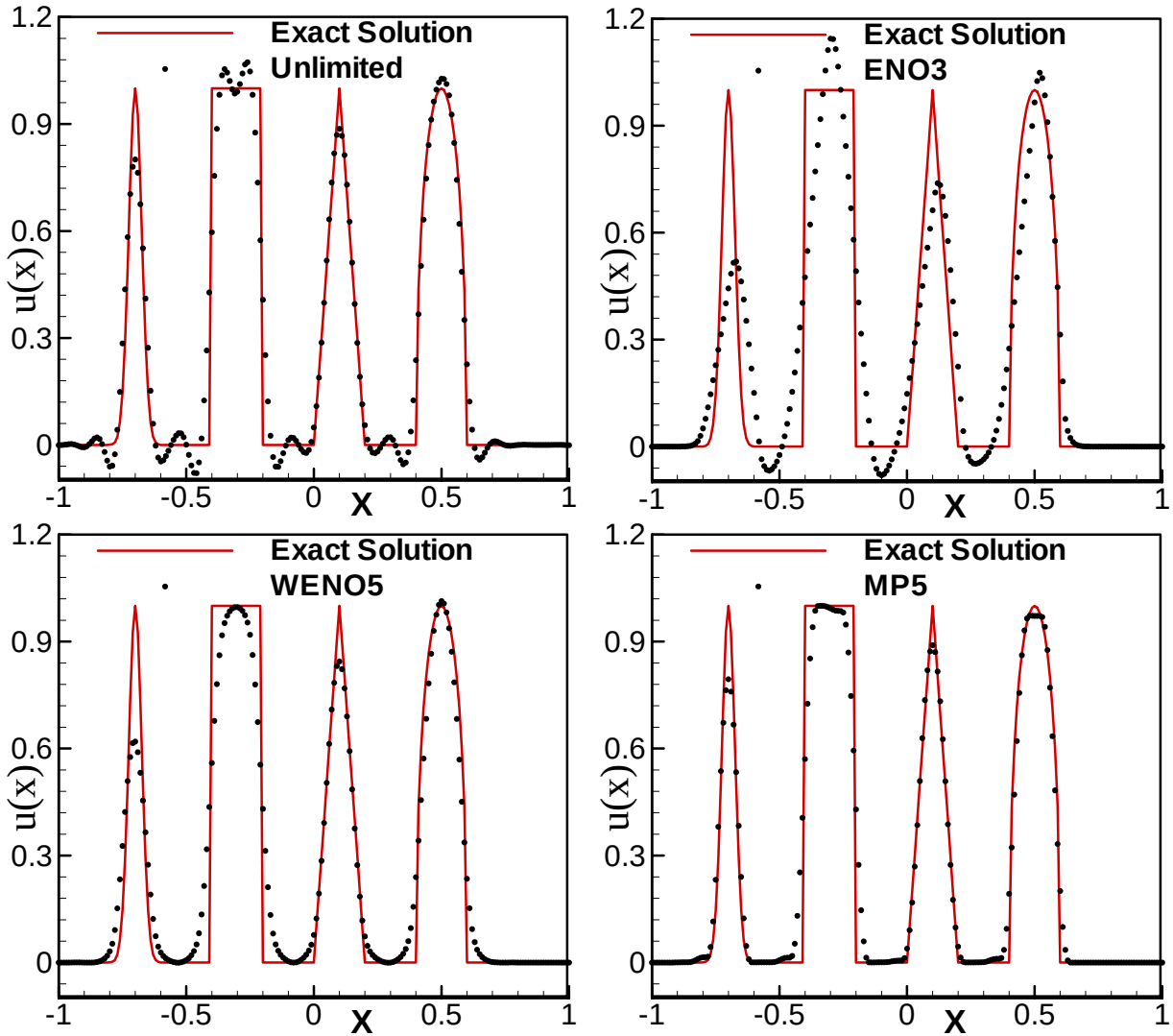
Temperature

Converging-Diverging Nozzle
3D calculations with Compact Scheme

High-Order Numerical Methods for LES of Supersonic Turbulent Flows

Solutions of 1D Advection Equation after 10 Periods with Compact, 3rd order ENO, 5th order WENO, and 5th order MP Schemes

NX=200
CFL=0.4

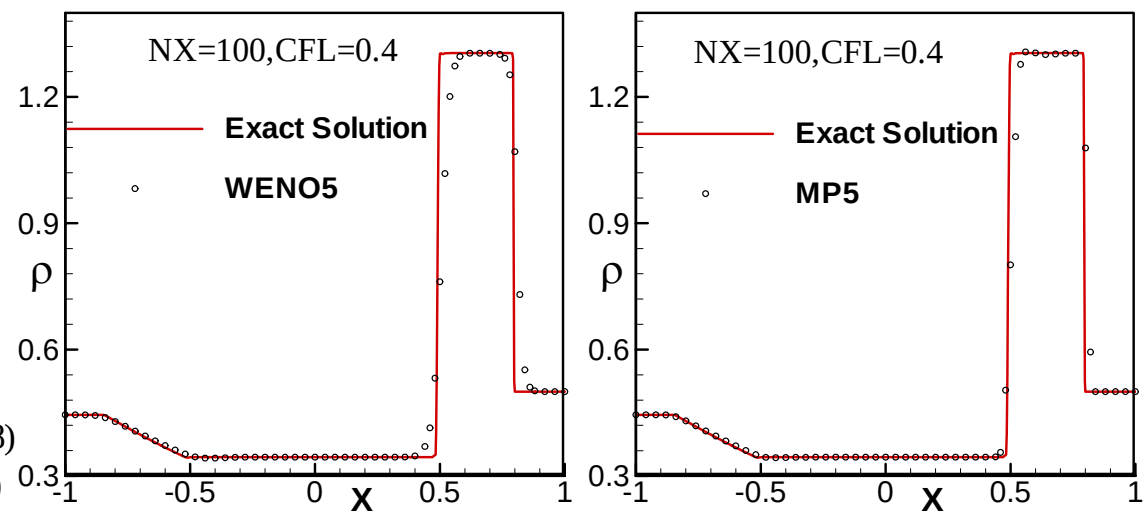


High-Order Numerical Methods for LES of Supersonic Turbulent Flows

Solutions of 1D Lax Problem with 5th order WENO and 5th order MP Schemes

Initial condition:

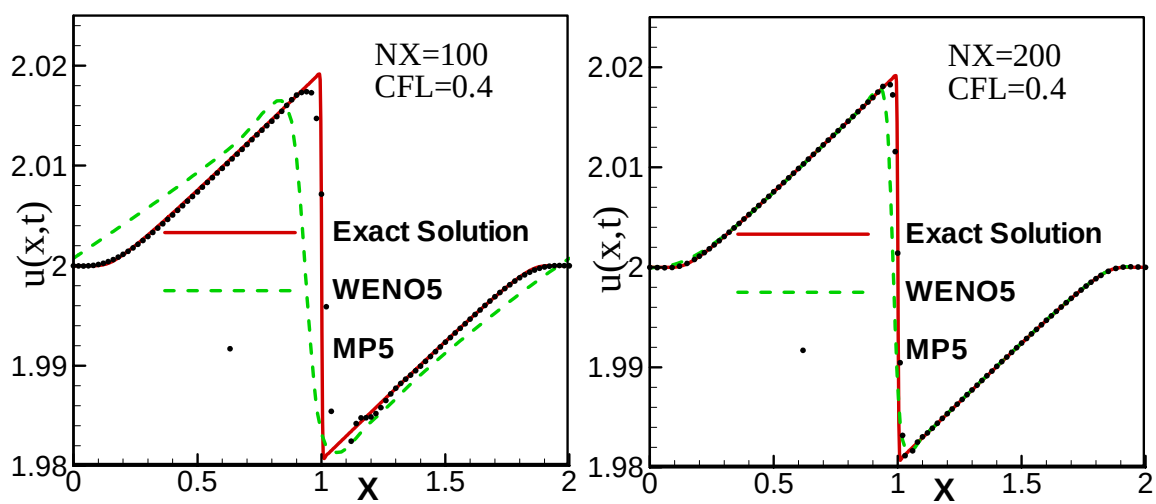
$$(\rho_L, u_L, p_L) = (0.445,\ 0.698,\ 3.528)$$
$$(\rho_R, u_R, p_R) = (0.5,\ 0.0,\ 0.571)$$



Solutions of 1D Burgers Equation with 5th order WENO and 5th order MP Schemes

Initial condition:

$$u(x,0) = 2 + \sin^9(\pi x)$$



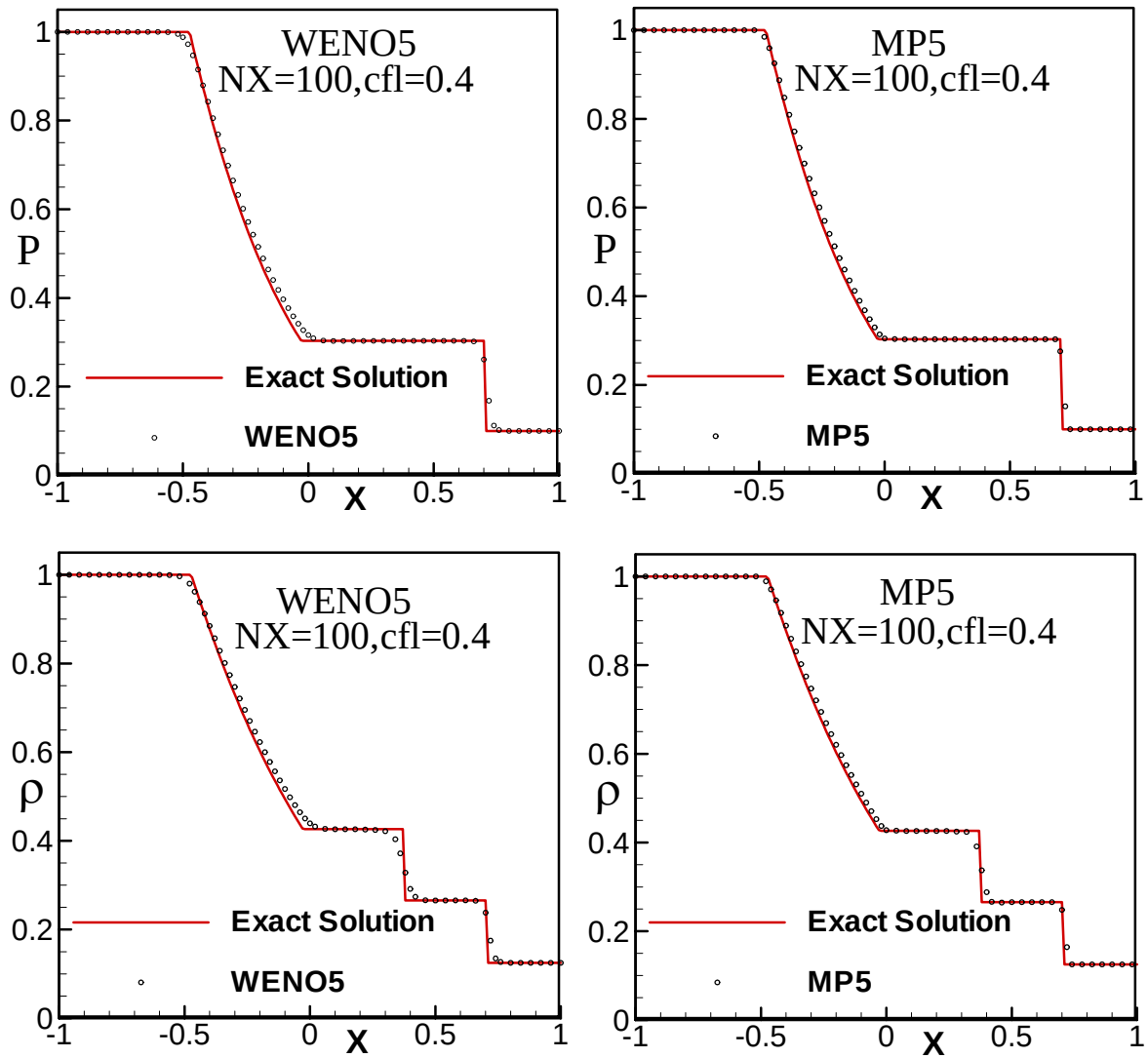
High-Order Numerical Methods for LES of Supersonic Turbulent Flows

Solutions of 1D Shock Tube Problem with 5th order WENO, and 5th order MP Schemes

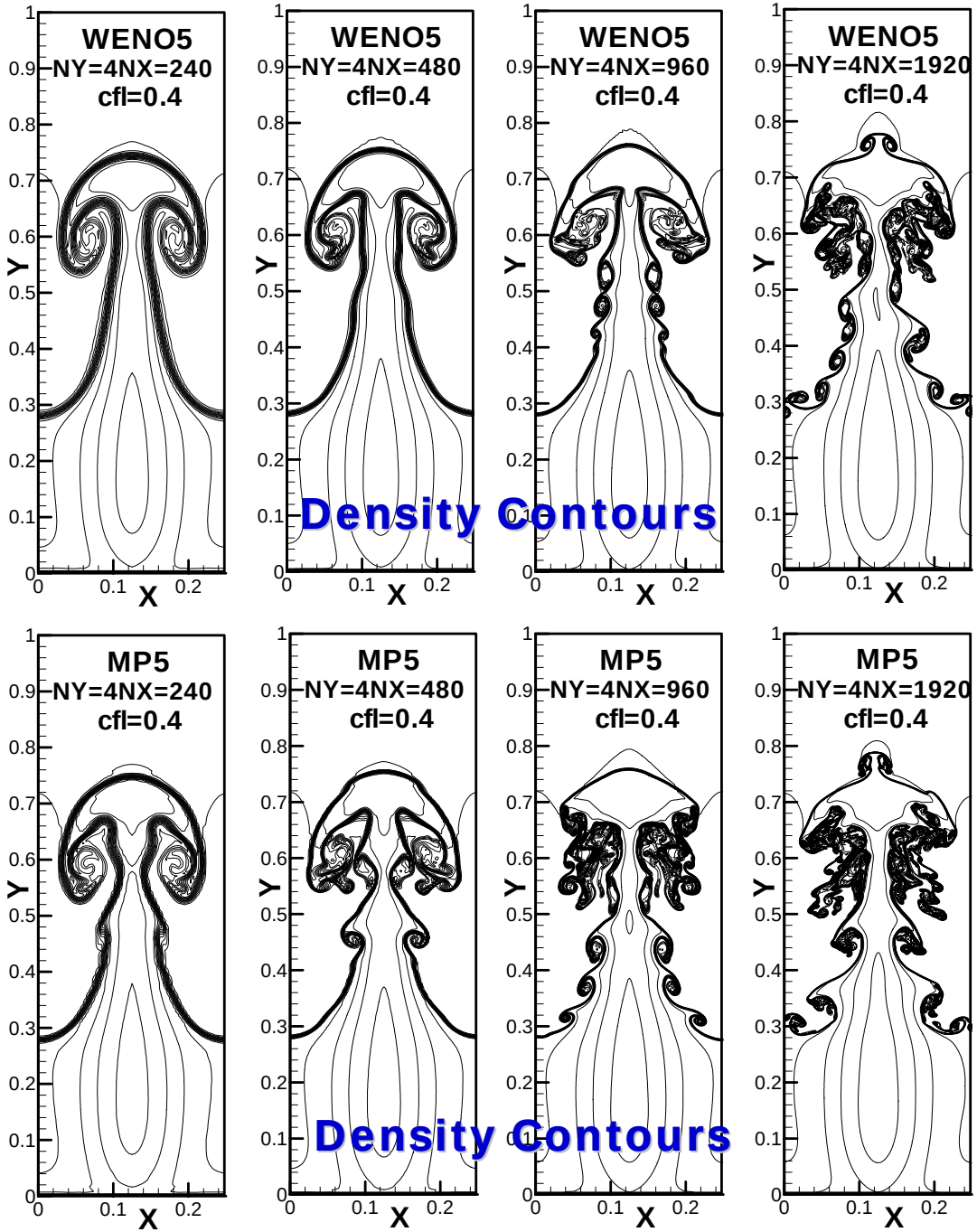
Initial Condition

$$(\rho_L, u_L, p_L) = (1.0,\ 0.0,\ 1.0)$$

$$(\rho_R, u_R, p_R) = (0.125,\ 0.0,\ 0.1)$$



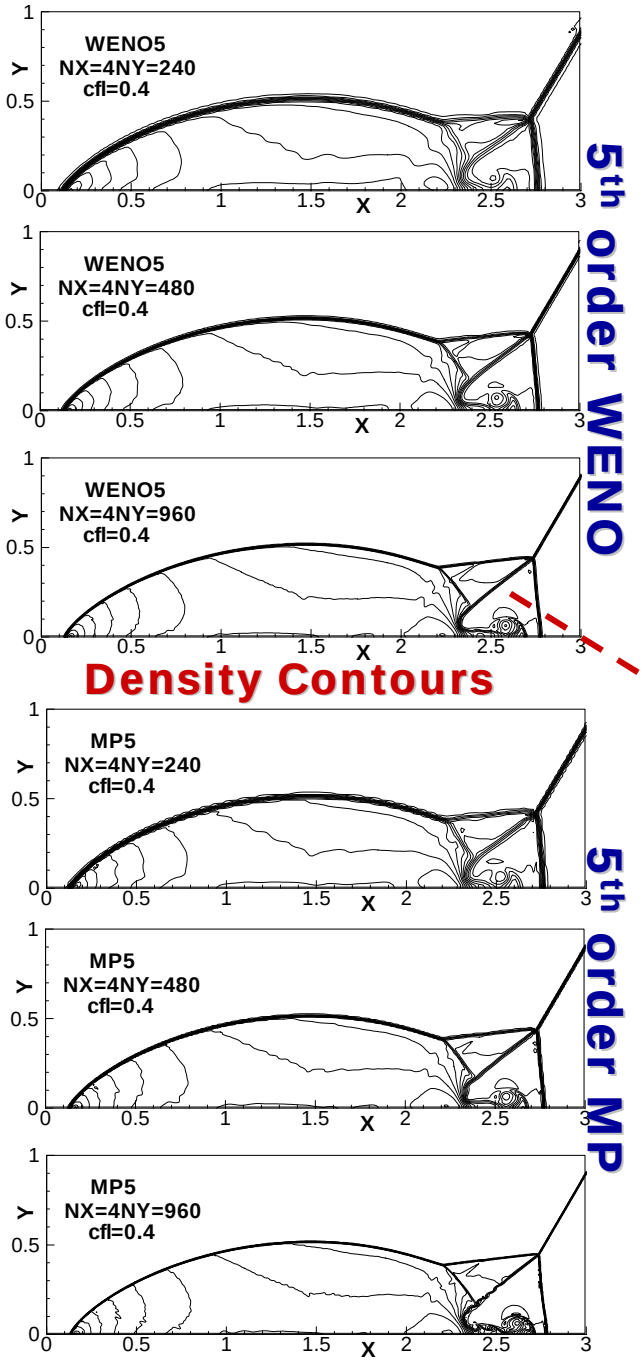
High-Order Numerical Methods for Supersonic Flows

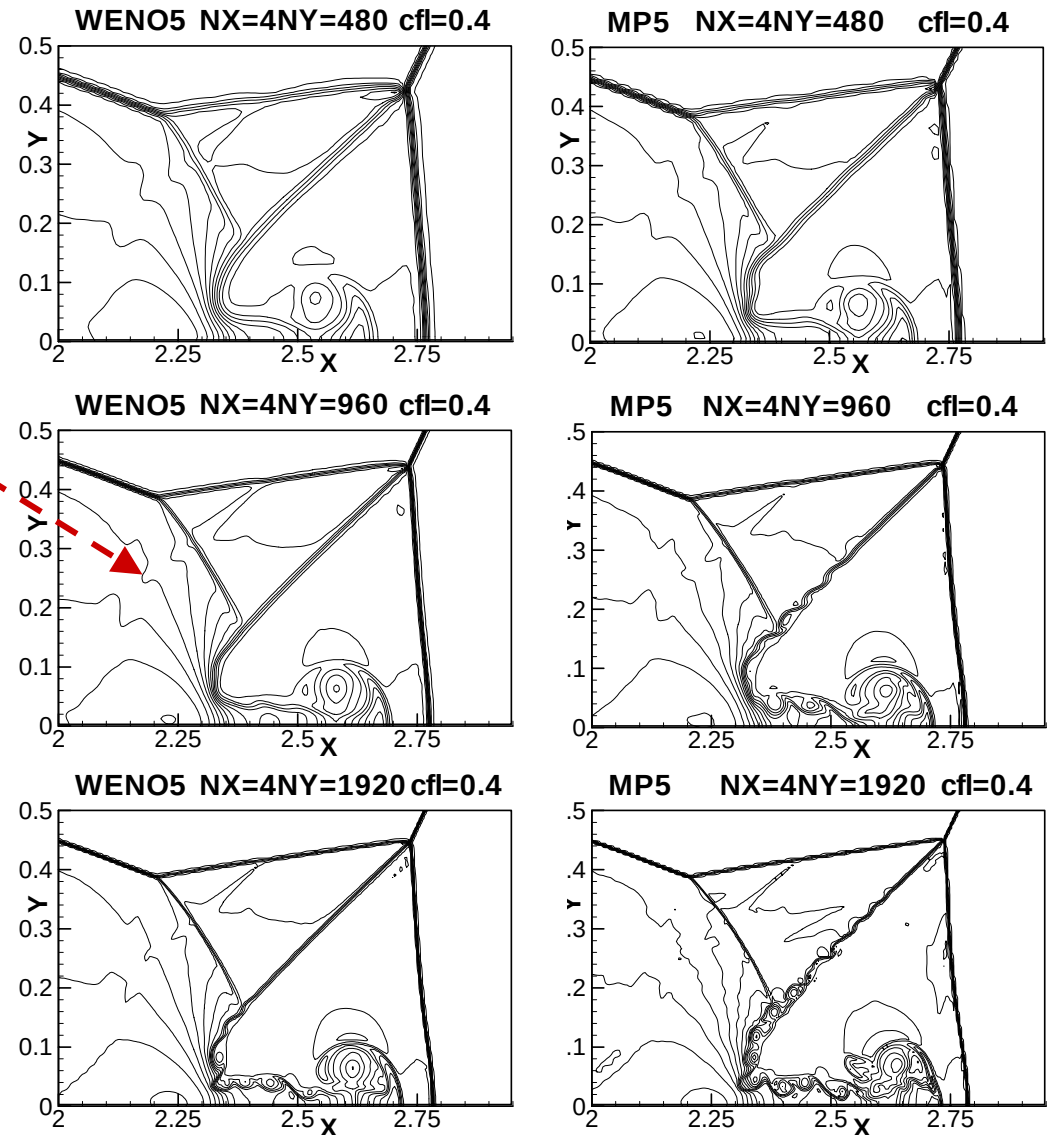


Solutions of 2D Inviscid Rayleigh-Taylor Instability Problem with 5th order WENO and 5th order MP Schemes

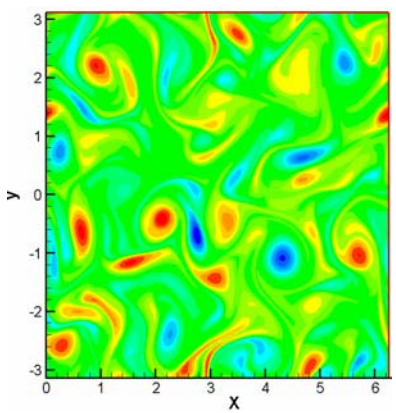
High-Order Numerical Methods for Supersonic Flows

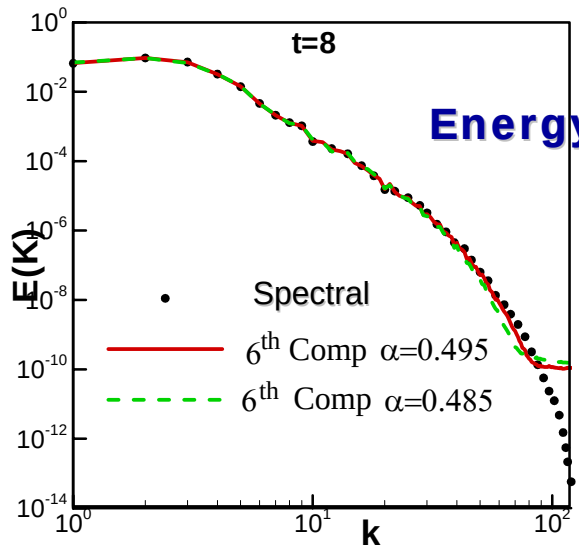
Double Mach Problem

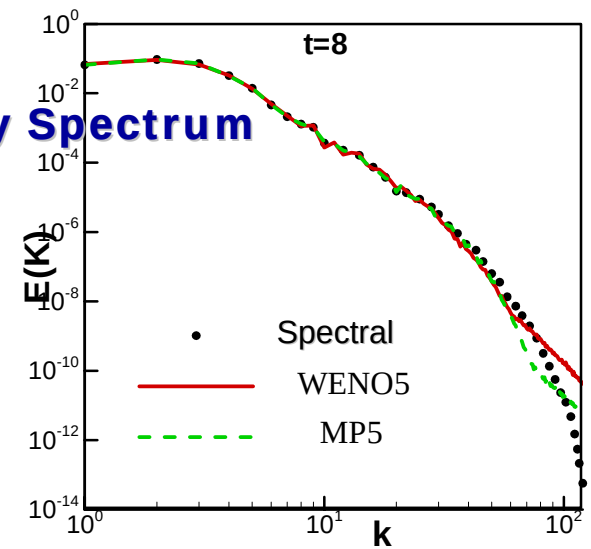




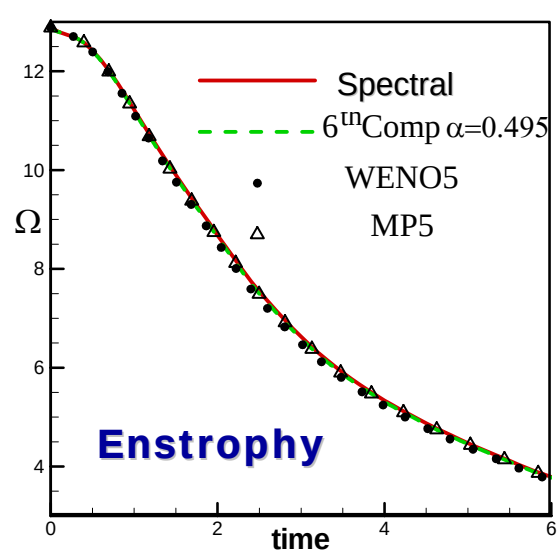
High-Order Numerical Methods for LES of Supersonic Turbulent Flows

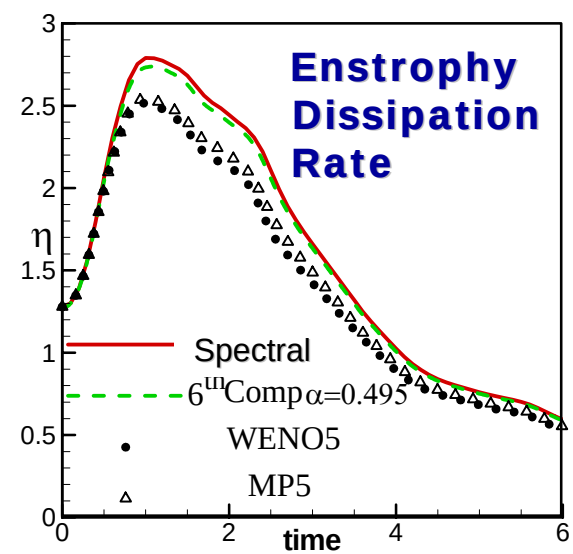






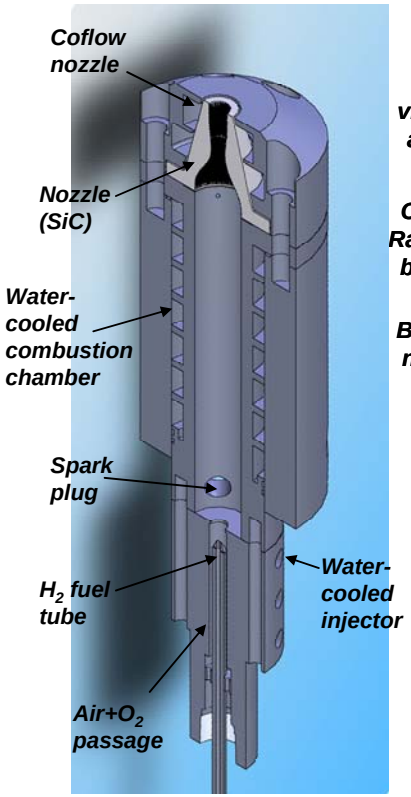
Solutions of 2D Isotropic Turbulence with Compact, Spectral, WENO and MP Schemes

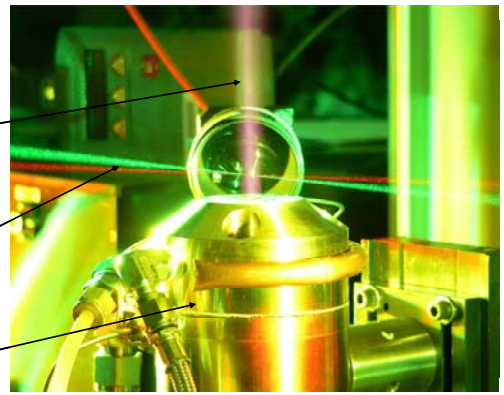




Supersonic Combustion - Free Jet Experimental Configurations (Laboratory and Full-Scale Models)

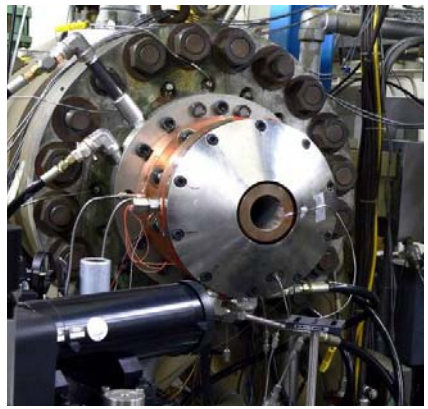
Small-scale facility

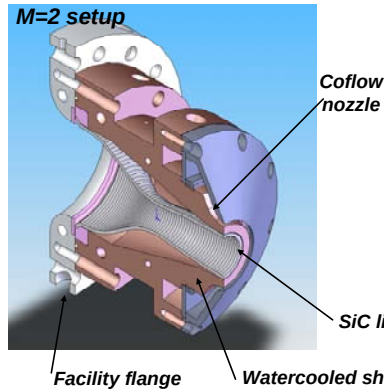




- **Operates in laser laboratory**
- **10 mm diameter Center jet**

Large-scale facility



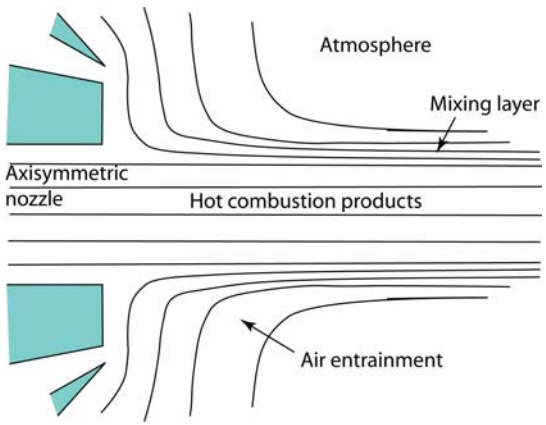


- **Nozzle connects to LaRC DCSCTF vitiated air heater**
- **63.5 mm dia. centerjet**

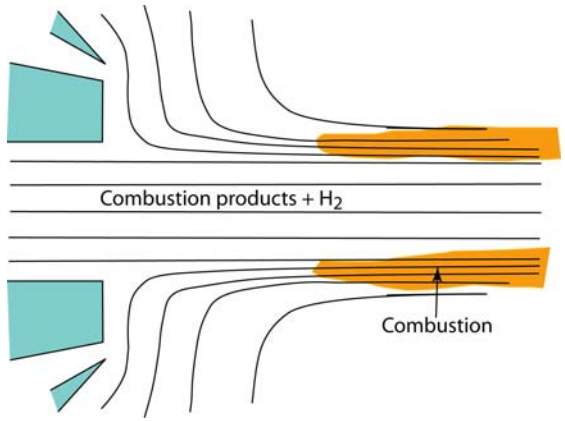
George Washington University and NASA LaRC

Supersonic Combustion Free Jet Experimental Configurations

Case 1: Mixing

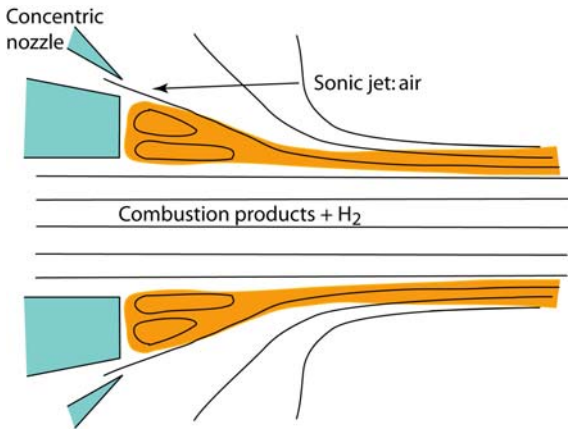


Case 2: Combustion

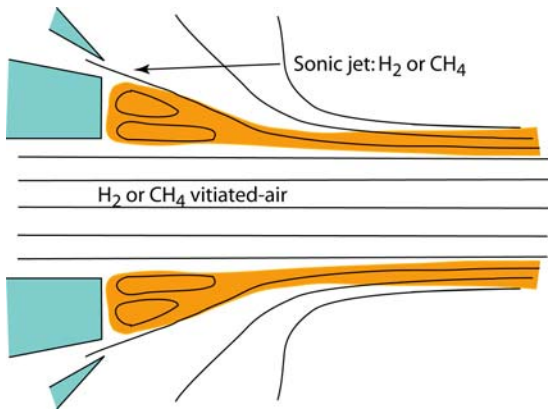


Case 3: Combustion with Flameholding:

(a) Center-jet fuel



(b) Coflow fuel



Ongoing and Near-Future Research

- In its present form, LES/FMDF is a robust and efficient methodology for single- and two-phase subsonic turbulent reacting flows in complex geometries
- Large-scale compressibility effects are explicitly calculated
- Robust high-order Eulerian finite difference methods (e.g. WENO, MP, Compact+MP) for LES of high speed turbulent flows have been developed
- Work is in progress to develop improved subgrid and wall (e.g. DES) models for supersonic and hypersonic flows
- Subgrid compressibility effects are being added to existent scalar FMDF model
- PDF-based subgrid compressible velocity-scalar stochastic models are being developed for supersonic flows
- Close collaborations with NASA scientists and other university investigators; continuously including their inputs into our work (flow configurations, experimental data, chemistry models,…….)