Entropy-Stabilized Discontinuous Galerkin Method for Gas-Dynamics Simulations

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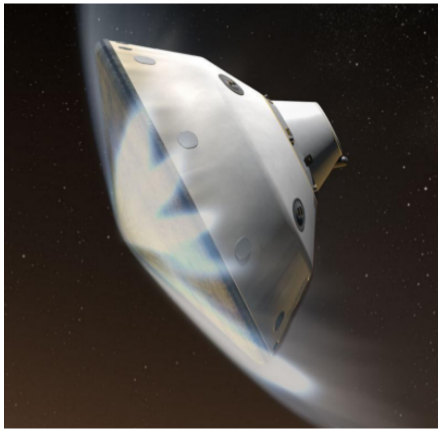
Motivation

Challenges in simulation of high-speed flows

- Turbulence and transition
- Shock-flow interaction
- Chemical reactions
  - › Gas-phase: dissociation, ionization, non-equilibrium flows
  - › Surface-reactions: pyrolysis, catalysis
- Radiation
- Coupling between turbulence, radiation, chemistry

Research issues

- Physical models
- Numerical and algorithmic developments
  - › High-order methods
  - › Shock-capturing
  - › High-performance computing



Credit: NASA

Gnoffo, Johnston, Kleb, Challenges to Computational Aerotherodynamic Simulation and Validation for Planetart Entry Vehicle Analysis”

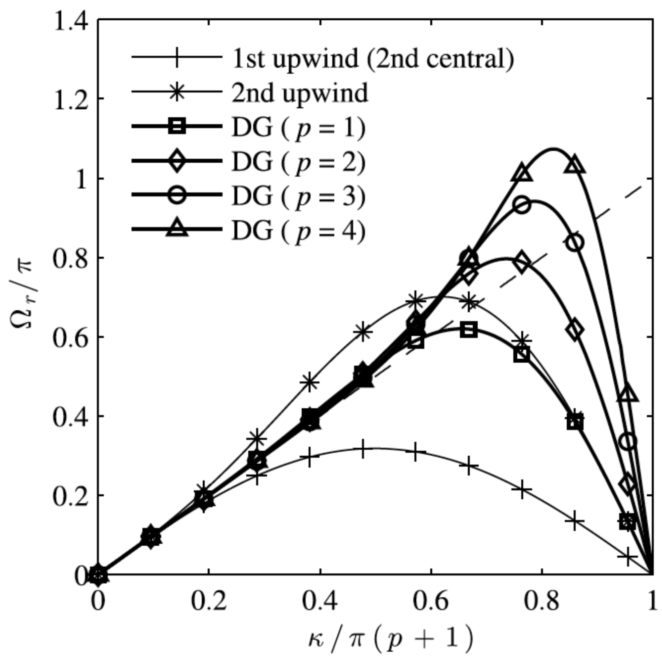
Motivation

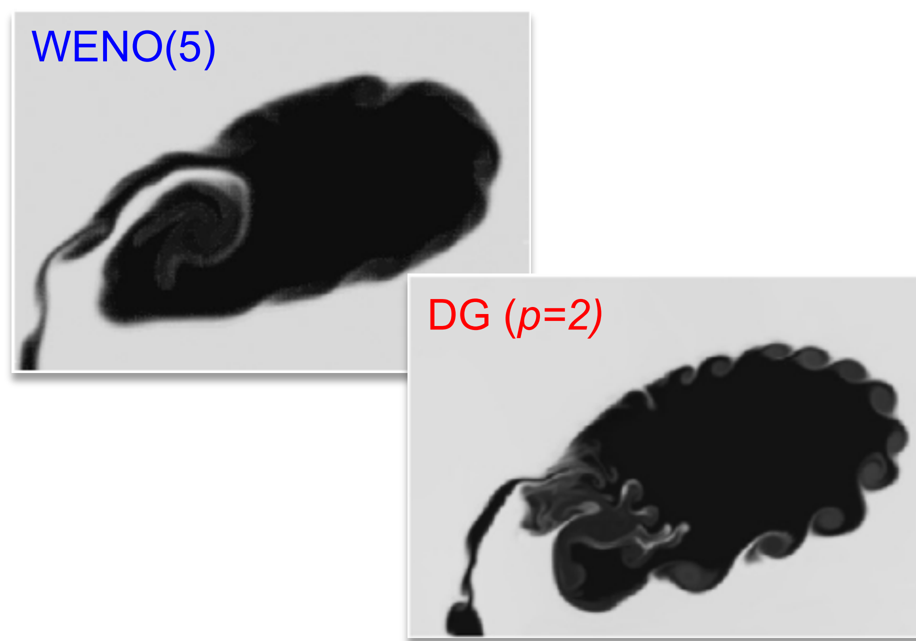
State-of-the-art in simulation of high-speed aerothermodynamic flows

- FD/FV formulations
- Lower-order or upwind-biased schemes

Potential of using discontinuous Galerkin method for reentry simulations

- Low dissipation and dispersion (compared to standard FV/FD-discret.)





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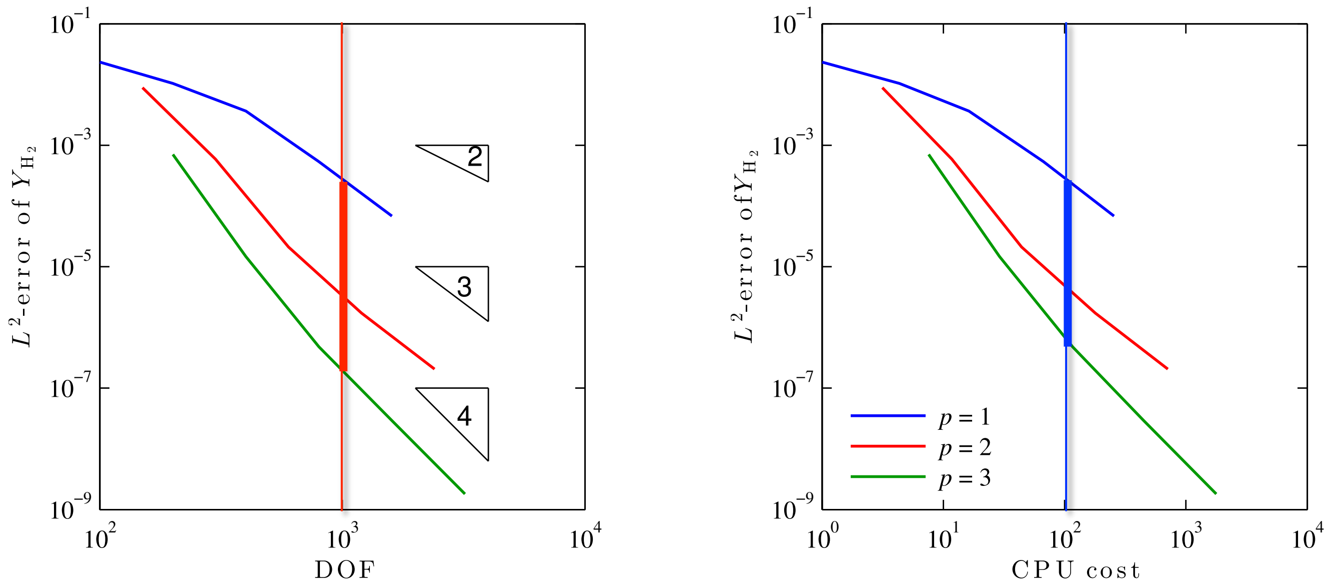
- High-order accuracy and optimal convergence properties (independent of mesh discretization)



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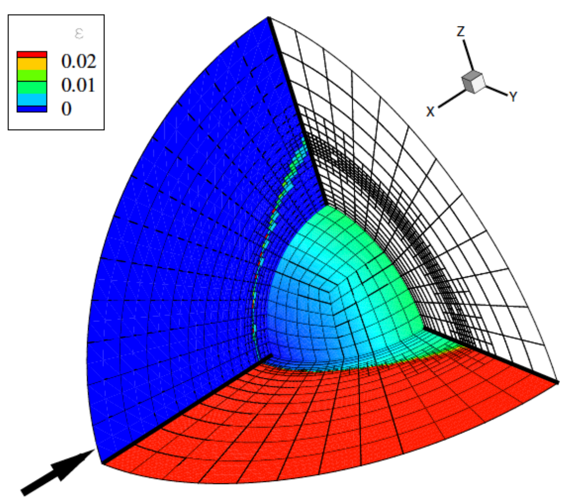
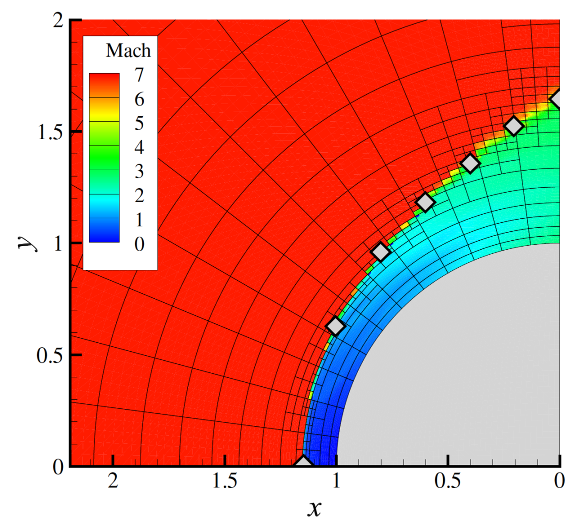
Potential of using discontinuous Galerkin method for reentry simulations

- Low dissipation and dispersion (compared to standard FV/FD-discret.)
- High-order accuracy and optimal convergence properties (independent of mesh discretization)
- Local mesh-adaptation (*h*) and refinement in polynomial order (*p*)





Objectives

Development of Discontinuous Galerkin (DG) method for high-speed aerothermodynamic simulations

- Physical modeling challenges
  - Treatment of transport properties
  - Reaction chemistry and chemical stiffness
  - Radiation
  - Coupling between turbulence, chemistry, and radiation

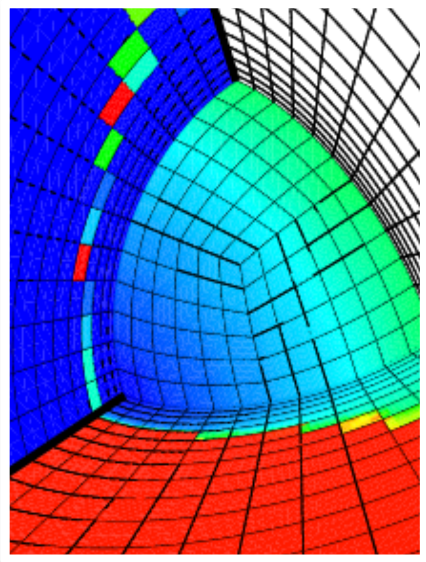
- Algorithmic aspects
  - Robustness of a high-order solver in present of underresolved features, shocks, and discontinuities
  - Localization of discontinuities (shocks, contacts)
  - Stabilization around discontinuities

Outline

- Motivation
- Objective
- Algorithmic developments: Entropy
  - Entropy-bounding for solution stabilization
  - Entropy-residual for shock detection and stabilization
- Multi-physics modeling
  - Transport, chemistry, flux formulation
- Applications
- Conclusions

Discontinuous Galerkin Method

ALGORITHMIC DEVELOPMENT



Methodology: Discontinuous Galerkin Discretization

Reacting Navier-Stokes equations

$$\partial U + \nabla \cdot (F^c - F^v) - S = 0$$

with

$$U = (\rho \boldsymbol{Y}, \rho \boldsymbol{u}, \rho e)^T$$

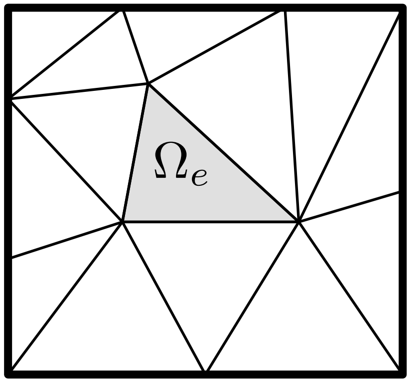
$$F^c = (\rho \boldsymbol{u} \boldsymbol{Y}, \rho \boldsymbol{u} \boldsymbol{u} + p\mathbf{I}, \rho \boldsymbol{u}(e + p/\rho))^T$$

$$F^v = (-\boldsymbol{j}, \boldsymbol{\tau}, -(q - \boldsymbol{u} \cdot \boldsymbol{\tau}))^T$$

$$S = (\dot{\boldsymbol{\omega}}, 0, 0)^T$$

Solution approximation (polynomial basis function)

$$U_h(t, x) = \sum_{e=1}^{N_e} \sum_{q=1}^{N_p} U_{eq}(t) \phi_{eq}(x)$$



Solve weak form of governing equations:

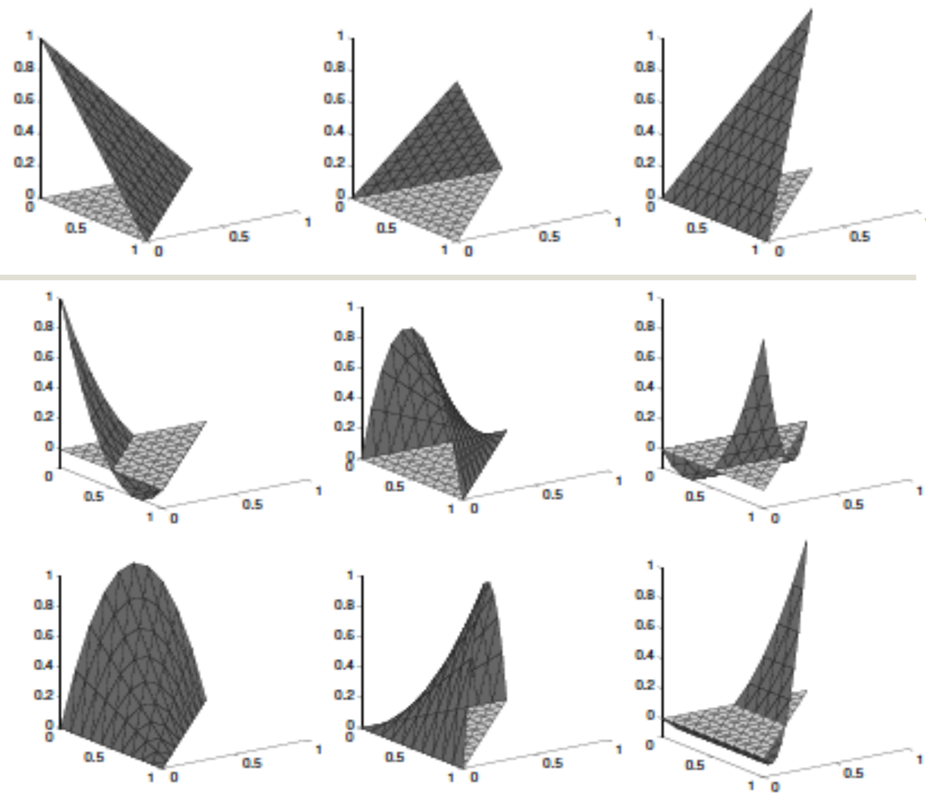
$$\left(\int_{\Omega_e} \phi_q \phi_p d\Omega_e \right) d_t U_q + \int_{\Omega_e} \phi_q \nabla \cdot (F^c - F^v) d\Omega_e - \int_{\Omega_e} \phi_q S d\Omega_e = 0$$

Methodology: Discontinuous Galerkin Discretization

- DG basis function:

P1DG

P2DG



Credit: K. J. Fidkowski, UM

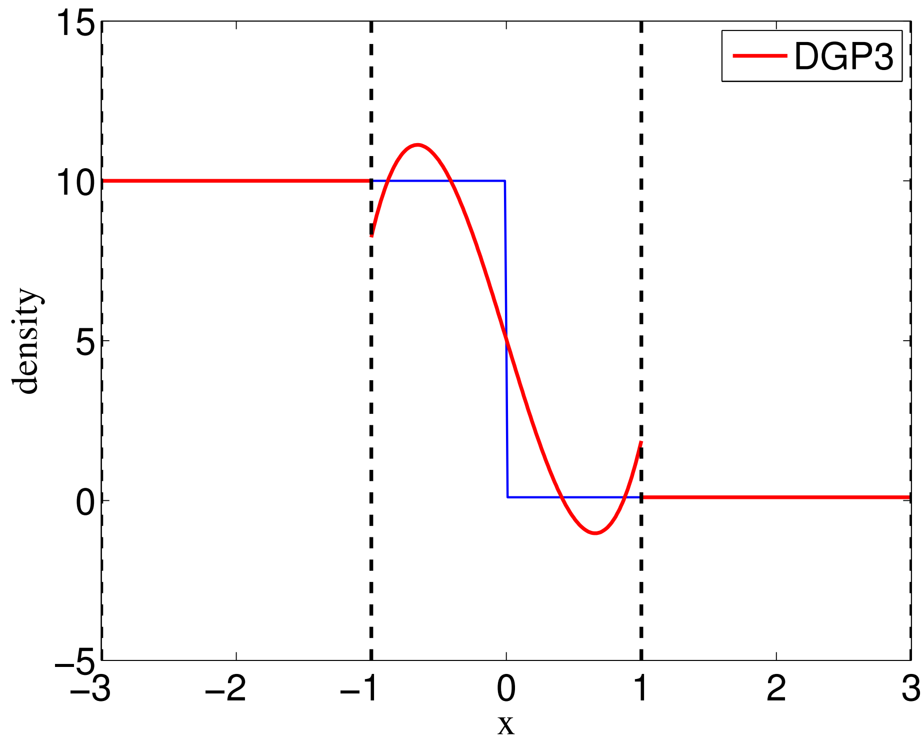
- Solution Approximation:

$$U_h(t,x) = \sum_{q=1}^{N_p} U_q(t)\phi_q(x)$$

Methodology: Discontinuous Galerkin Discretization

Realizability of high-order numerical scheme

$$U_h(t,x) = \sum_{q=1}^{N_p} U_q(t)\phi_q(x)$$



Discontinuous Galerkin Method

ALGORITHMIC DEVELOPMENT: ENTROPY-FUNCTION AND ENTROPY RESIDUAL

Algorithmic Developments for Entropy-Bounding DG

Introduce minimum entropy principle into DG-formulation for

- Robustness and constraining numerical solution
- Shock-detections
- Regularization
- Local solution adaptation and refinement

Entropy-bounded Discontinuous Galerkin (EBDG)
Local Entropy Constraint

Violation of entropy condition results in loss of robustness

- Constrain solution to obey embedded entropy law

$$\frac{\partial \mathcal{U}}{\partial t} + \nabla \cdot \mathcal{F} \leq 0\,,$$

$$(\mathcal{U}, \mathcal{F}) = (-\rho s, -\rho s u)$$

with entropy function

$$s(U) = \ln(p) - \gamma \ln(\rho) + s^0$$

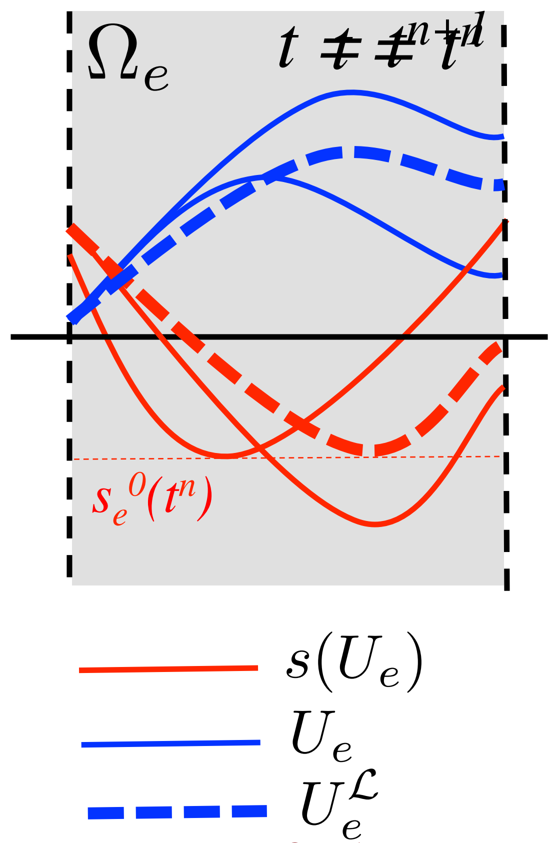
- Constrain solution to obey entropy bound

$$s(U_e^{\mathcal{L}}) \geq s_e^0(t)$$

with

$$U_e^{\mathcal{L}} = U_e + \epsilon(\overline{U}_e - U_e)$$

- Formulation of limiter introduces explicit CFL-stability condition



Zhang & Shu, JCP 2010, 2011; Numer. Math. 2012

Entropy-bounded Discontinuous Galerkin (EBDG)
Local Entropy Constraint

Limiting operator

- Derived and proved rigorous CFL condition for a variety of element types and polynomial order

Main benefits of EBDG

- Applicable to arbitrary types of elements on unstructured meshes
- Application of limiter requires only algebraic operations
- Implementation independent of specific quadrature rules
- Strictly local limiter (no neighboring information required) → no requirement for upwind-biased discretization
- Preserves high-order accuracy of scheme (on smooth solution)

Lv, Y. and Ihme, M., "Entropy-bounded Discontinuous Galerkin scheme for Euler equations." JCP, under review, arXiv:1411.5044

Entropy-bounded Discontinuous Galerkin (EBDG)
Shock Detection – Entropy Residual

- Use Entropy residual to detect shocks and spatial under-resolution

$$R(\mathcal{U}) = \frac{\partial \mathcal{U}}{\partial t} + \nabla \cdot \mathcal{F} \leq 0$$

- Physical interpretation of entropy residual
  - Physical entropy: shocks, discontinuities, dissipation, reaction, …
  - Numerical entropy: insufficient resolution, solution representation, oscillations, …

- Element-wise discretization of entropy residual

$$R_e = \frac{1}{V_e} \int_{\Omega_e} \left(\frac{\partial \mathcal{U}(U_e)}{\partial t} + \nabla \cdot \mathcal{F}(U_e) \right) d\Omega_e$$

- Use residual function for shock-detection

Lv, Y. and Ihme, M., “An Entropy-Residual Shock-Detector for Solving Conservation Laws Using RKDG.” JCP, submitted.

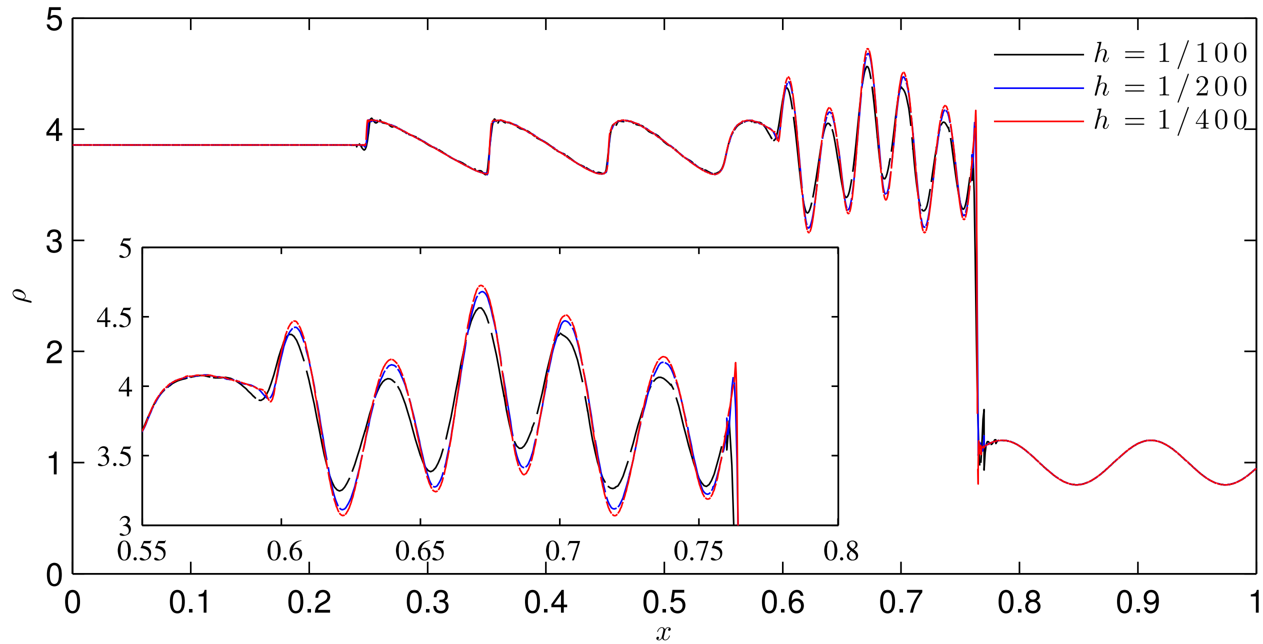
Lv, Y. and Ihme, M. “Taming nonlinear instability for Discontinuous Galerkin scheme with articficial viscosity.” CTR Annual Res. Briefs, 2014.

J.-L. Guermond, R. Pasquetti, and B. Popov. Entropy viscosity method for nonlinear conservation laws. JCP, 230, 2011.

Entropy-bounded Discontinuous Galerkin (EBDG)
Shock Detection – Entropy Residual

Shu-Osher Problem

- DG (p=4) solution: quartic polynomial function
- Interaction of Mach=3 shock with sinusoidal density wave



Entropy-bounded Discontinuous Galerkin (EBDG)
Shock Detection – Entropy Residual

Shu-Osher Problem

- DG (p=4) solution: quartic polynomial function
- Interaction of Mach=3 shock with sinusoidal density wave

Entropy-bounded Discontinuous Galerkin (EBDG)

Solution Adaptation – Entropy Residual

- Use Entropy residual for adaptation of solution and mesh refinement
- Adaptation indicator

$$R_e = \frac{1}{V_e} \int_{\Omega_e} \left(\frac{\partial \mathcal{U}(U_e)}{\partial t} + \nabla \cdot \mathcal{F}(U_e) \right) d\Omega_e$$

- Physical interpretation: Evaluate entropy-generation (physical and numerical contribution) and adapt solution in spatial and polynomial order

- Test case: Turbulent mixing layer
  - Re = δΔU/ν = 2000
  - $Ma_1 = 0.5$; $Ma_2 = 0.25$
  - Adaptation frequency: 0.5δ/ΔU
  - Ratio of adaptive cells: 0.08
  - Polynomial order: 1 (linear) … 4 (quartic)

K. J. Fidkowski, M. A. Ceze, P. L. Roe, "Entropy-based drag error estimation and mesh adaptation in two-dimensions." AIAA J. Aircraft, 49, 2012.
K. J. Fidkowski, P. L. Roe, "Entropy-adjoint approach to mesh refinement." SIAM J. on Sci. Comp. 32, 2010.

Entropy-bounded Discontinuous Galerkin (EBDG)
Solution Adaptation – Entropy Residual

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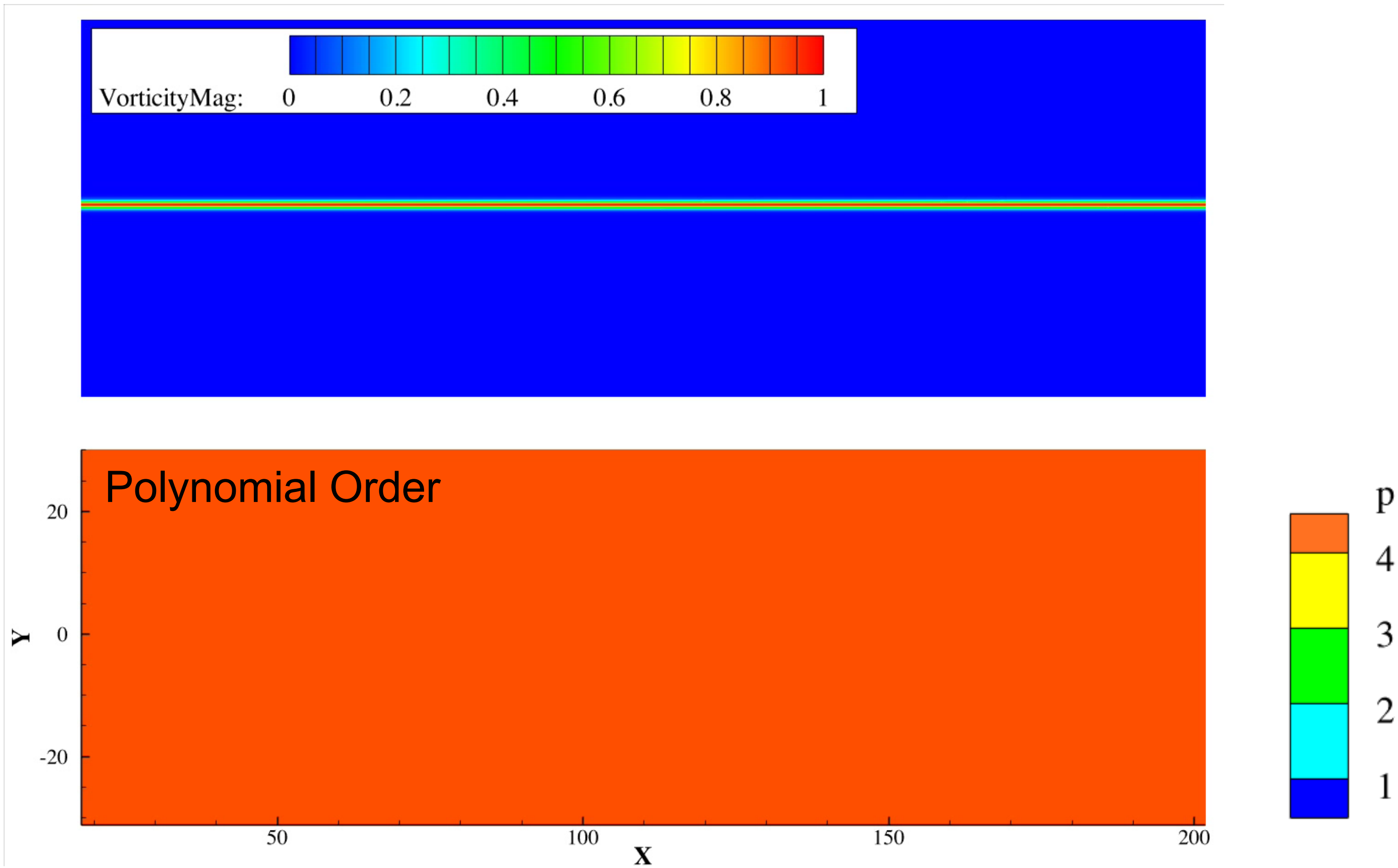


Entropy-bounded Discontinuous Galerkin (EBDG)

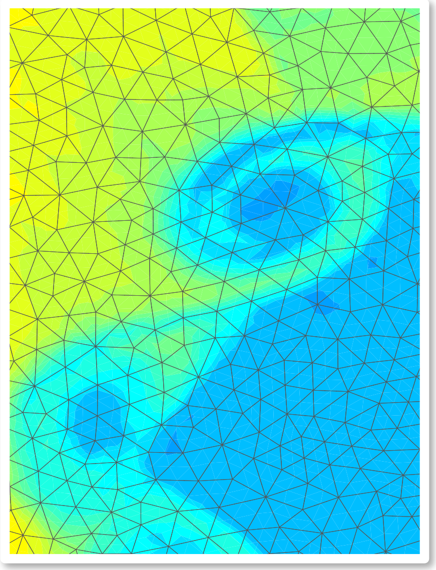
Summary

- Development of entropy-bounded Discontinuous Galerkin method for high-speed reacting flows

- Algorithmic attributes
  - Use entropy-function and entropy-residual for solution stabilization, shock detection, limiting, and adaptation
  - Strang splitting and stiff ODE-time integration
  - Order-adaptive artificial viscosity
  - Solution adaptation in spatial and polynomial order

- Physical modeling attributes
  - Reacting Navier-Stokes/Euler equation
  - Detailed chemistry
  - Complex thermo-viscous-diffusive transport
  - Heat-transfer and radiation

Applications



Applications and Test Cases

Shock/bubble interaction

Double Mach-reflection (M=10)

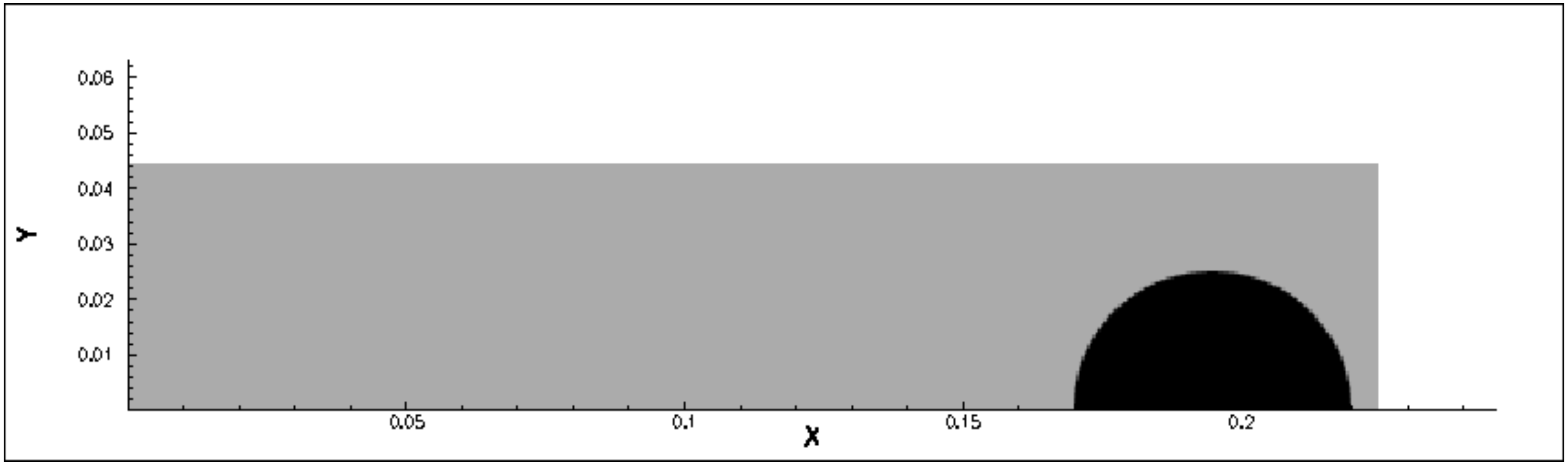
Shock over sphere (M=6.8)

Hydrogen combustion, detonation, and reignition

Applications and Test Cases
Shock/Bubble Interaction

Problem Description

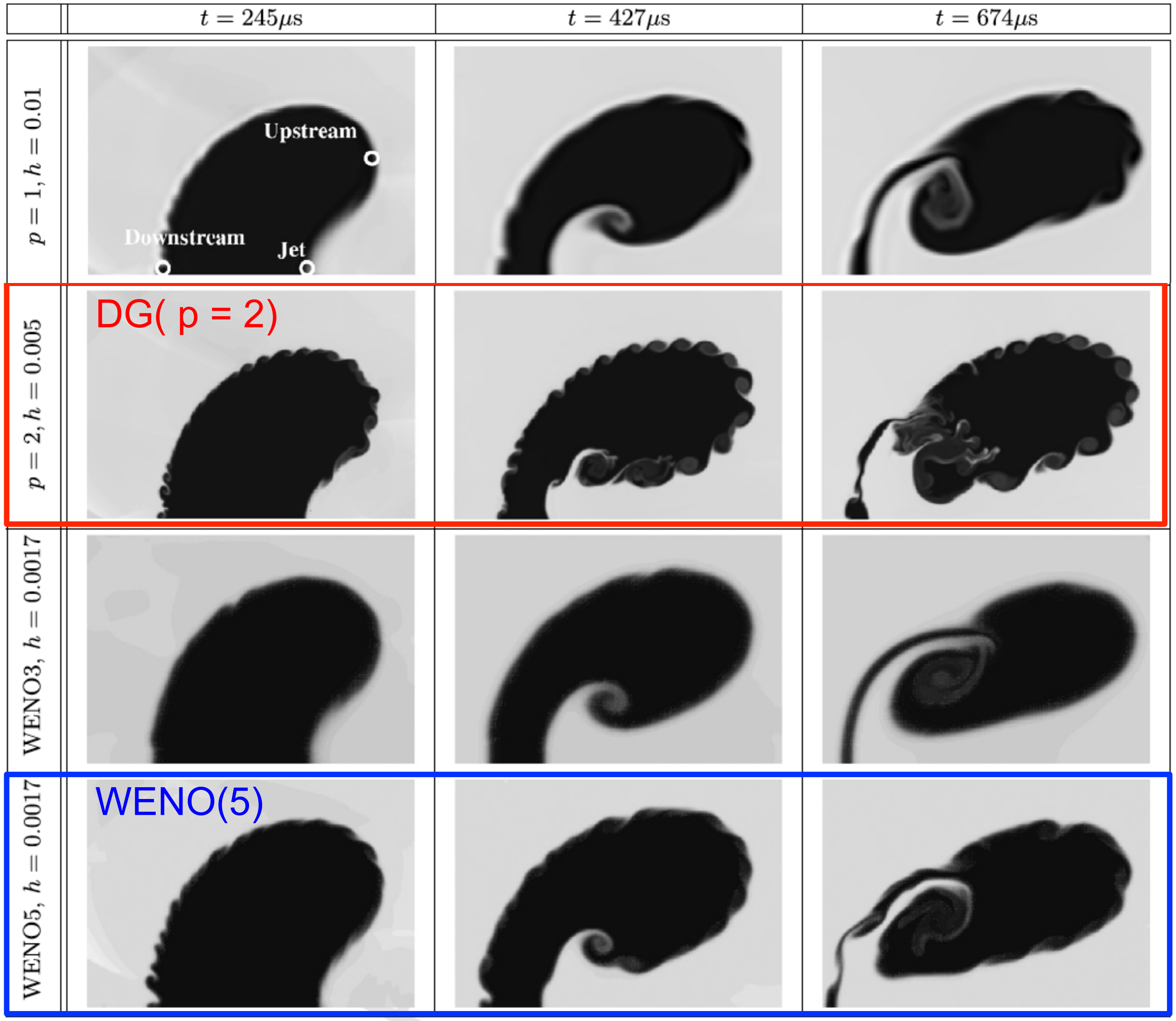
- Interaction of air shock at M=1.22 shock with helium bubble
- Variable thermodynamic properties: γ_{Air} =1.4; γ_{He} =1.67
- Non-diffusive interfacial flow



Lv, Y and Ihme, M., "Discontinuous Galerkin method for multicomponent chemically reacting flows." JCP 270, 2014

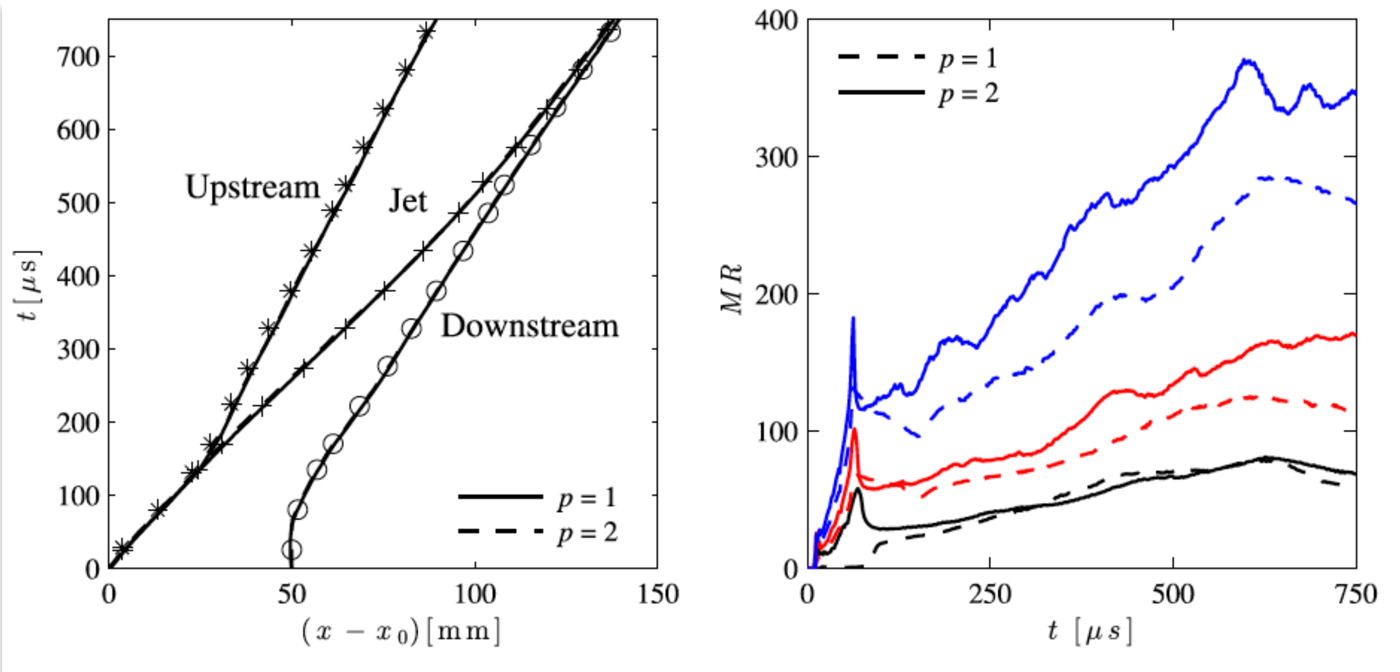
Applications and Test Cases

Shock/Bubble Interaction



Applications and Test Cases
Shock/Bubble Interaction

Quantitative results, showing spatio-temporal evolution of characteristic point along bubble interface, comparison with Terashima & Tryggvason

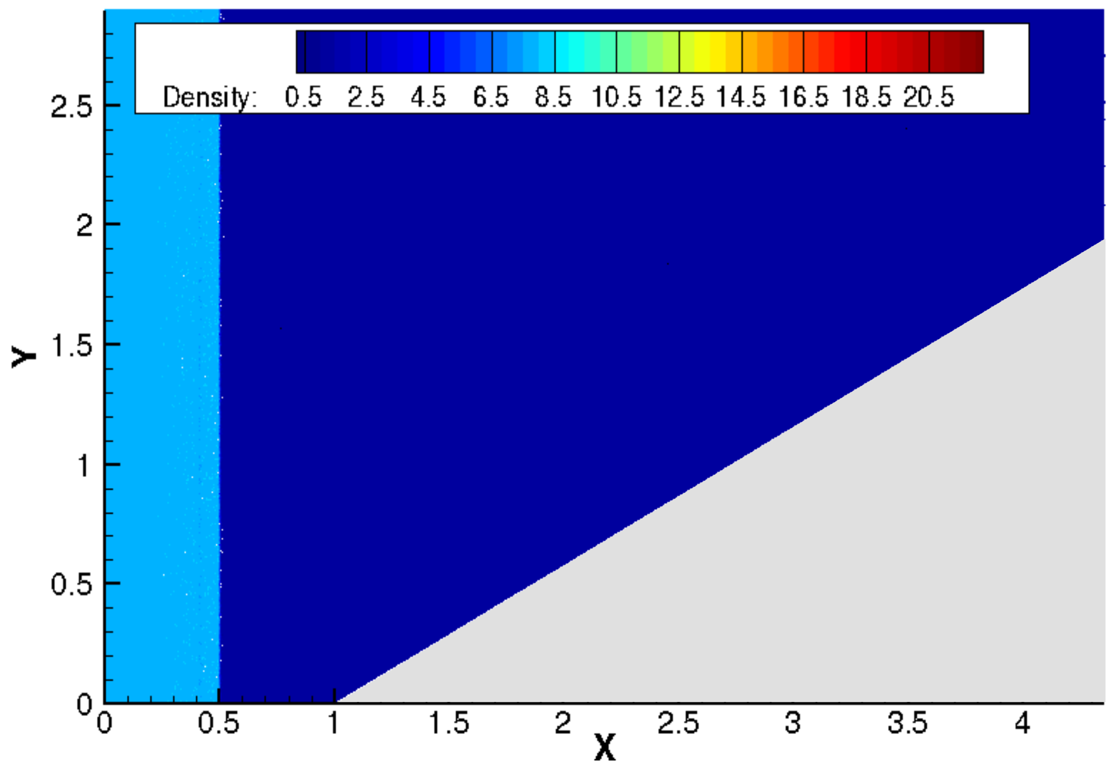


Terashima, H. and Tryggvason, G., "A front-tracking/ghost-fluid method for fluid interfaces in compressible flows." JCP, 228, 2009

Applications and Test Cases
Double Mach Reflection

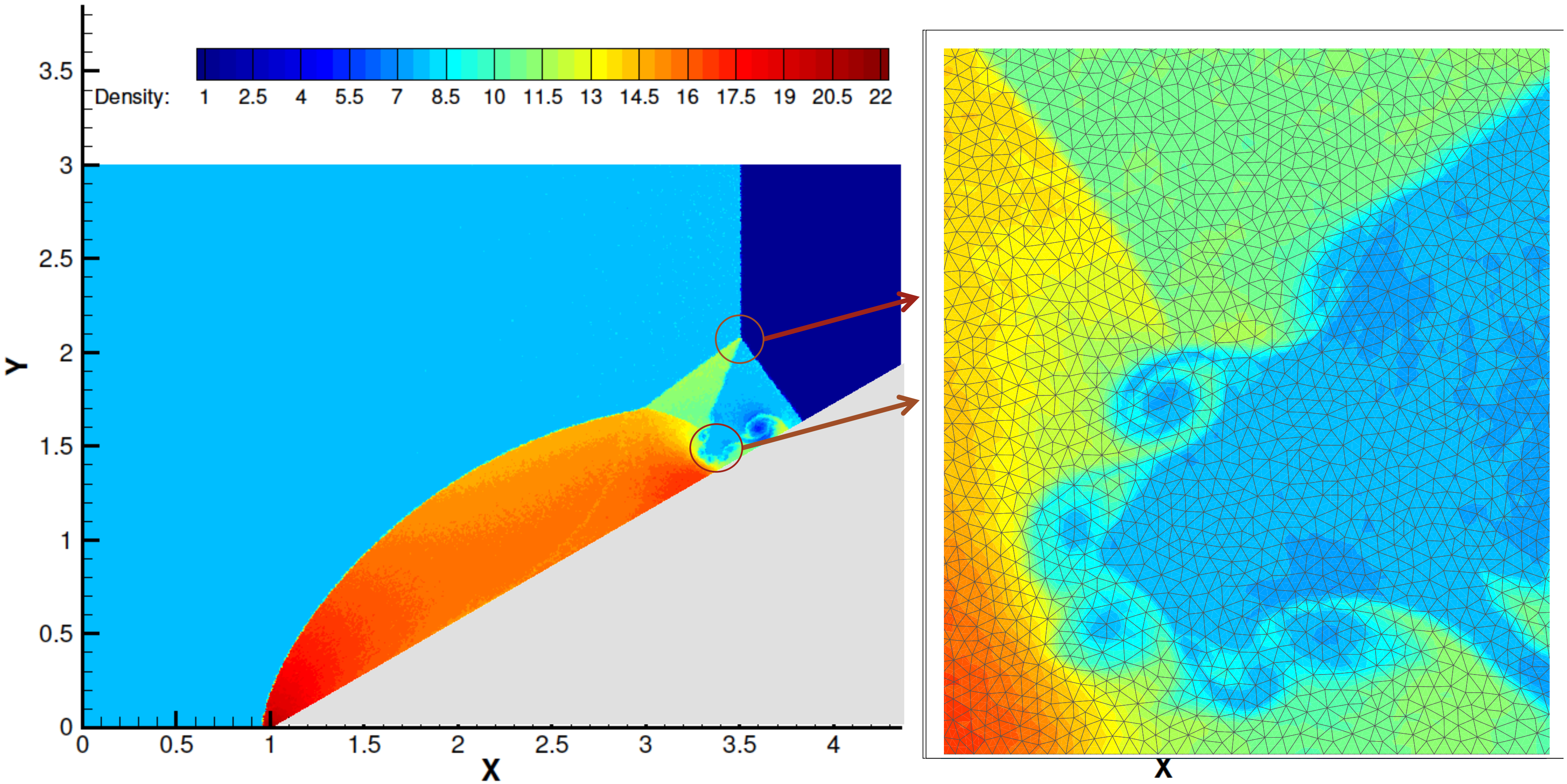
Problem Description

- Mach 10 shock attacks 30^o degree wedge
- Setting: DG (p=4) and *h* ≈1/100 on fully unstructured triangular mesh



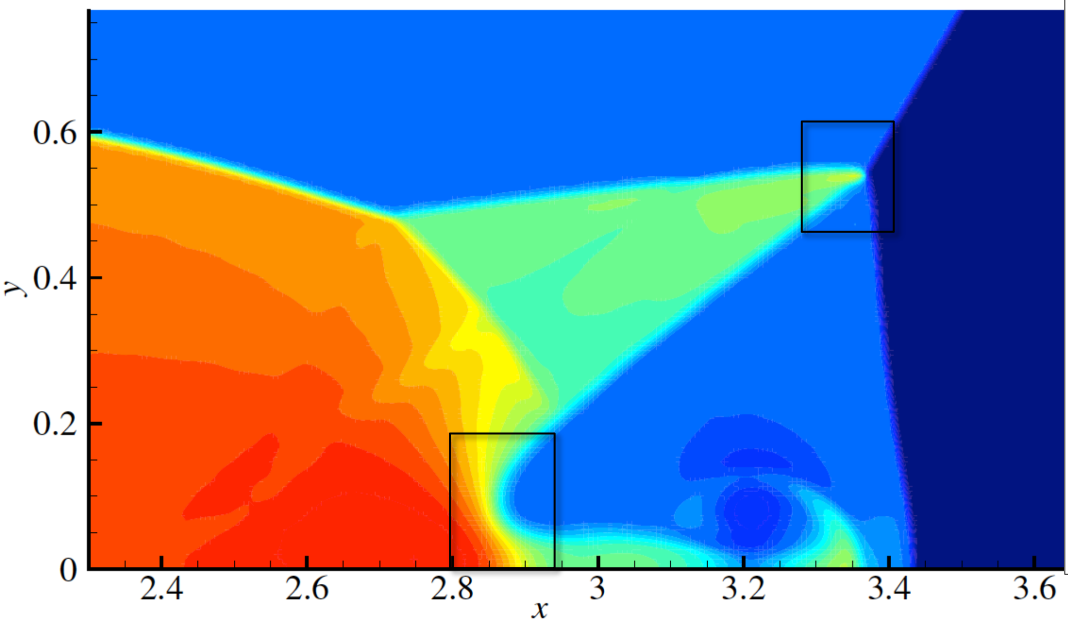
*Woodward, P. and Colella, P., JCP, 54, 1984.

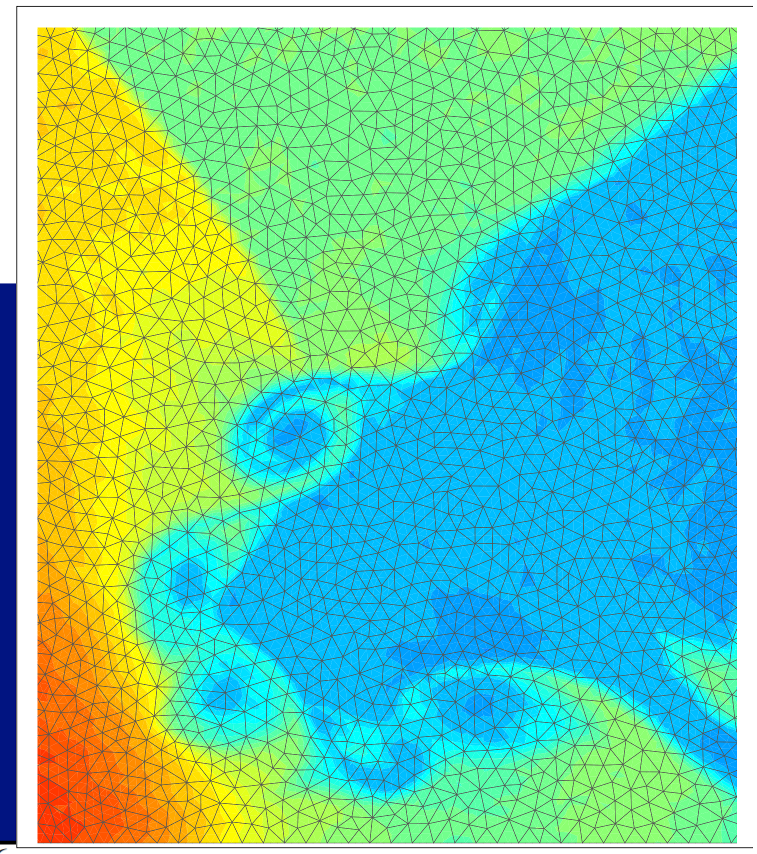
Applications and Test Cases
Double Mach Reflection



Applications and Test Cases
Double Mach Reflection

Comparison: WENO5 on quadrilateral mesh with h = 0.0067 (equiv DOFs)

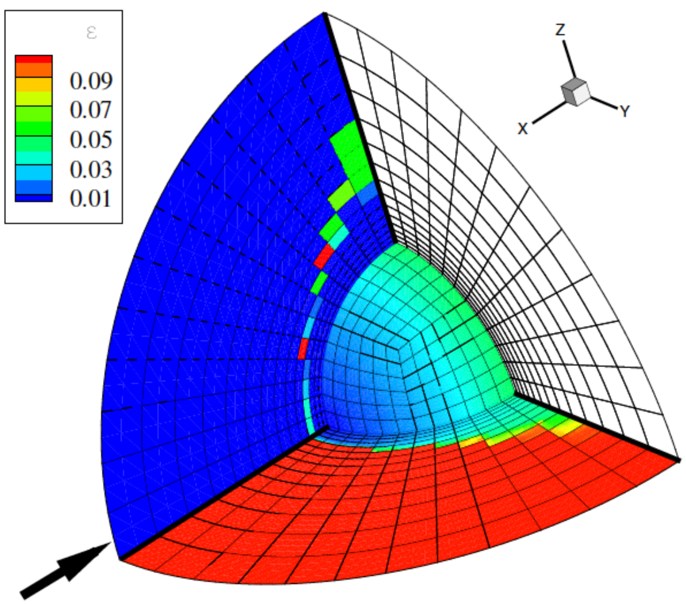




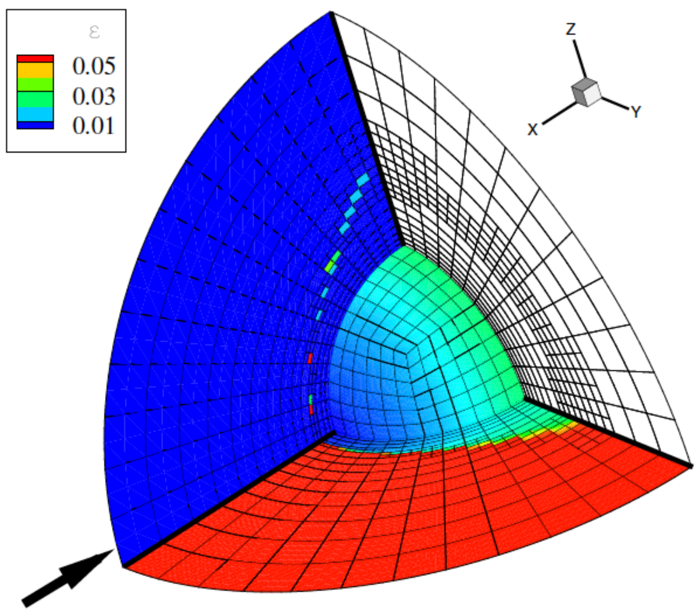
Applications and Test Cases
3D Supersonic Flow over Sphere

Problem Description

- Mach= 6.8 shock over sphere
- Radius: R = 1
- Setting: DG (p=2) on quadratically curved hexahedron elements
- Mesh adaptation using entropy residual



Baseline Mesh



Refinement level: 1

Applications and Test Cases
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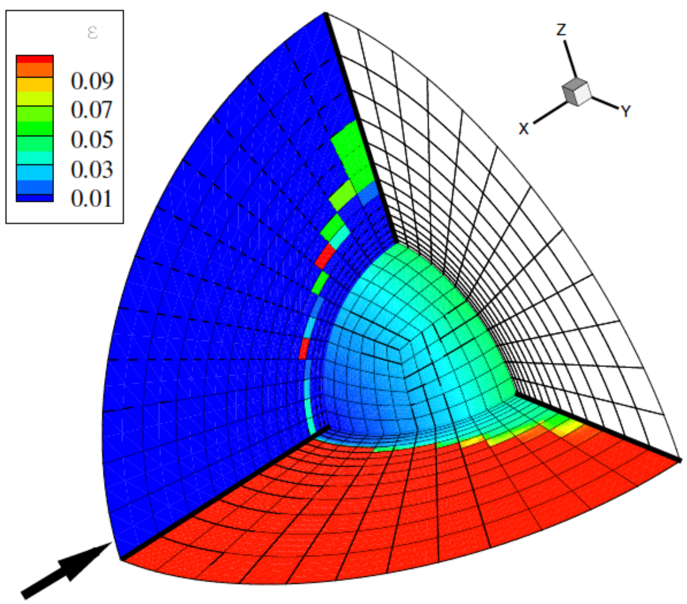

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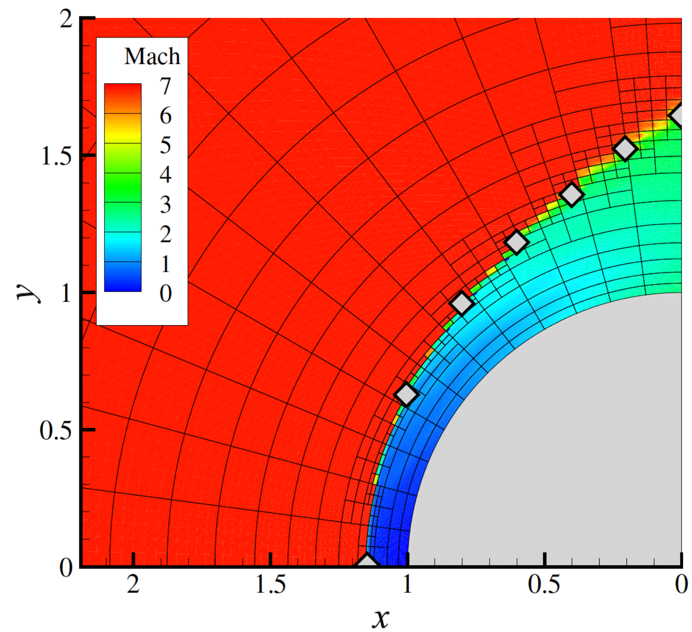
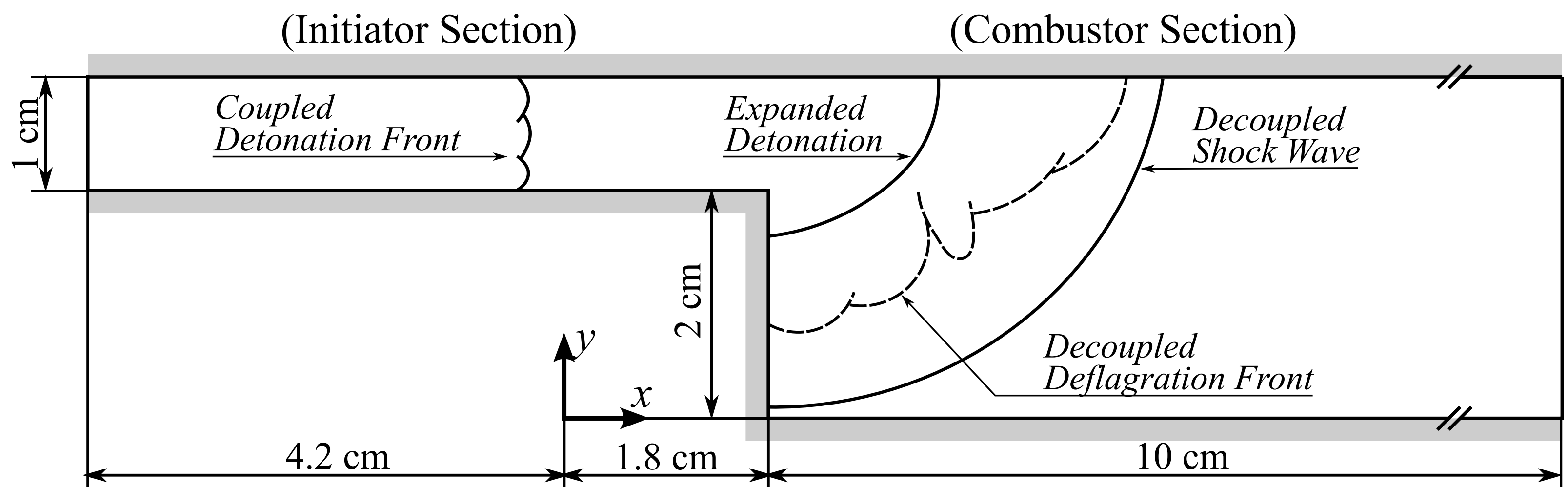


Refinement level: 2

F. S. Billig. Shock-wave shapes around spherical-and cylindrical-nosed bodies. J. Spacecraft Rockets, 4, 1967.

Applications and Test Cases
Physics of Detonation Reignition and Reinitiation



Mixture composition

$$2H_2 + O_2 + \beta Ar + (4 - \beta) N_2$$

Initial condition:

- p = 26.7kPa
- T = 293K
- M_{CJ} = 4.8 – 4.9

Reaction chemistry

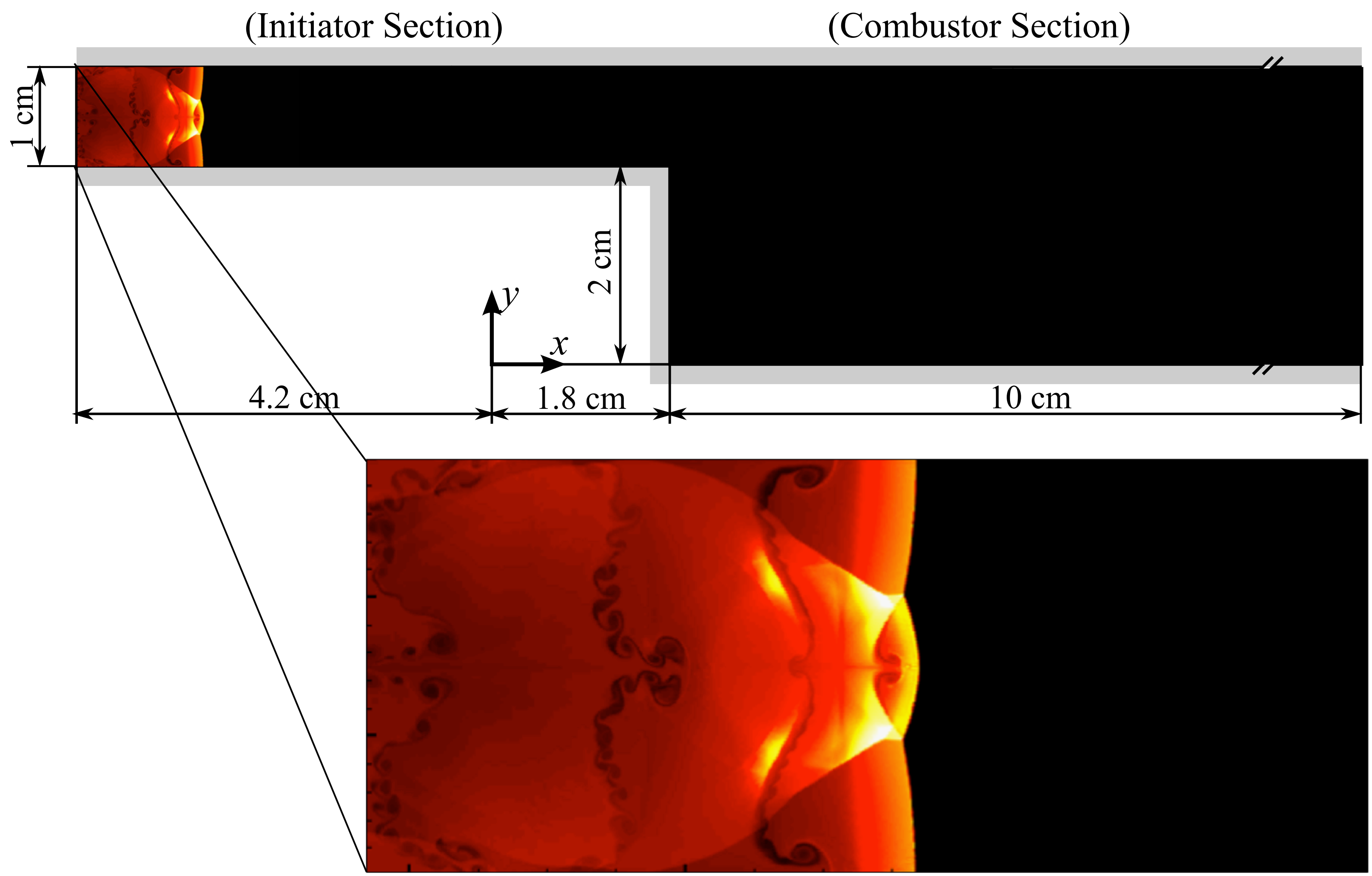
- Detailed chemical mechanisms for high-pressure H2/O2-systems: 8 Species, 24 reactions

Spatial Resolution

- > 22 DOFs to resolve induction length

Ohyagi et al. Shock Waves, 2002.

Applications and Test Cases
Physics of Reignition and Reinitiation

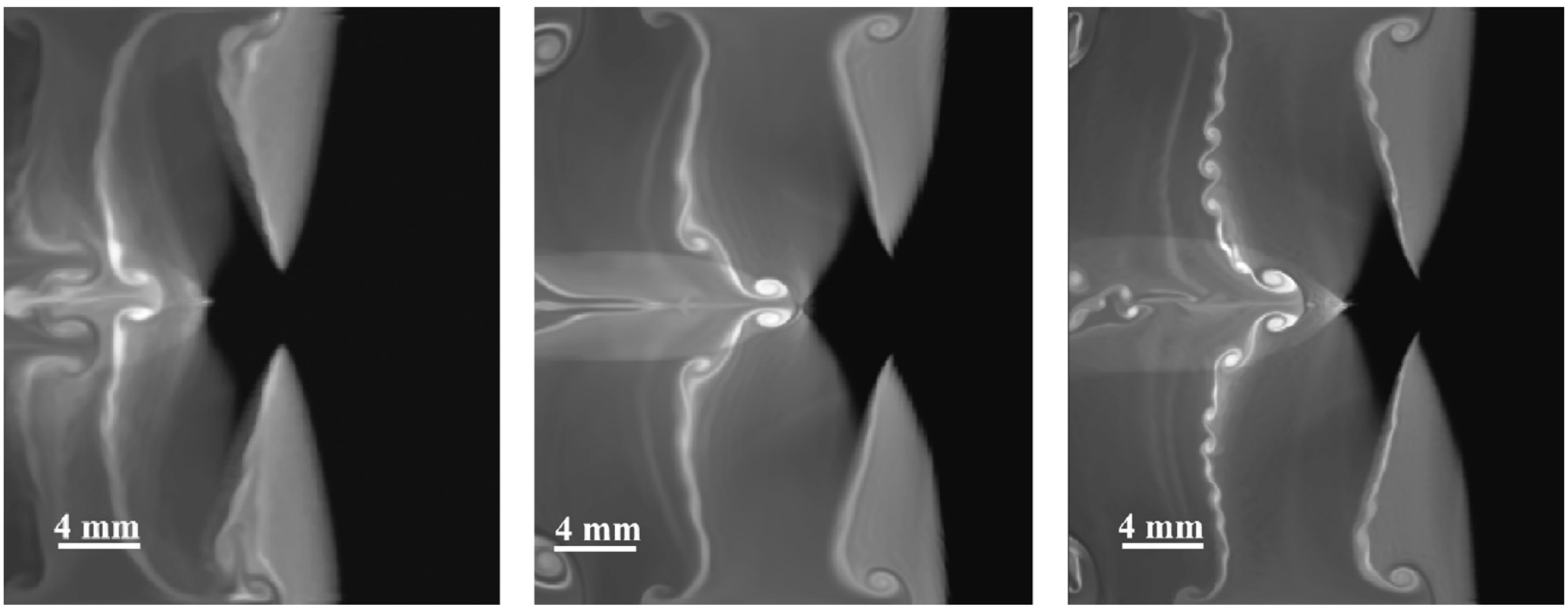


Lv, Y. and Ihme, M., "Computational analysis of re-ignition and re-initiation mechanisms of quenched detonation waves behind a backward facing step." Proc. Combust. Inst., 35, 2015.

Applications and Test Cases
Physics of Reignition and Reinitiation

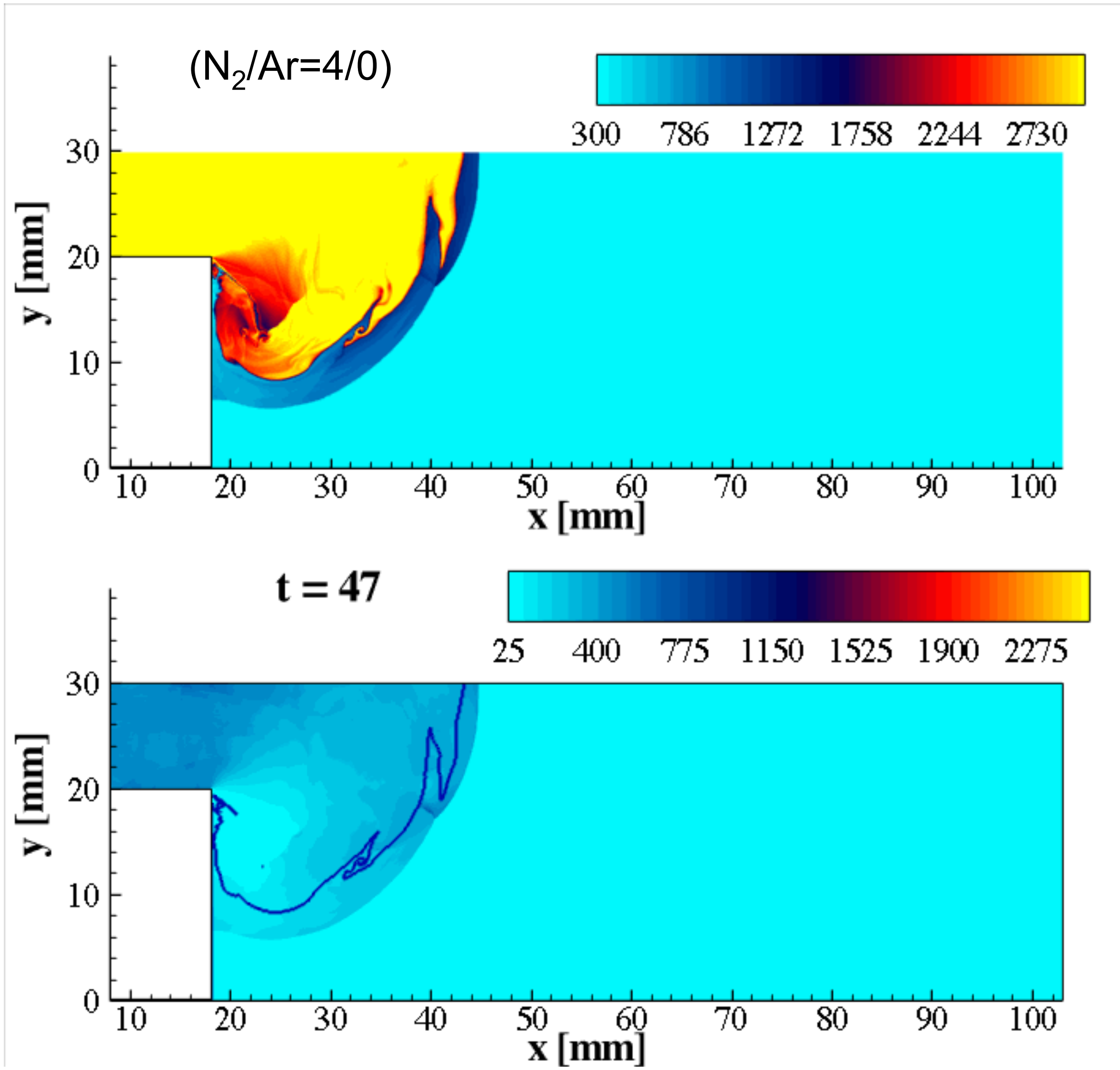
Model verification and benefit of high-order discretization

- Cellular structure of 2H2+O2+7Ar detonation at initial condition 6.7kPa and 298 K.

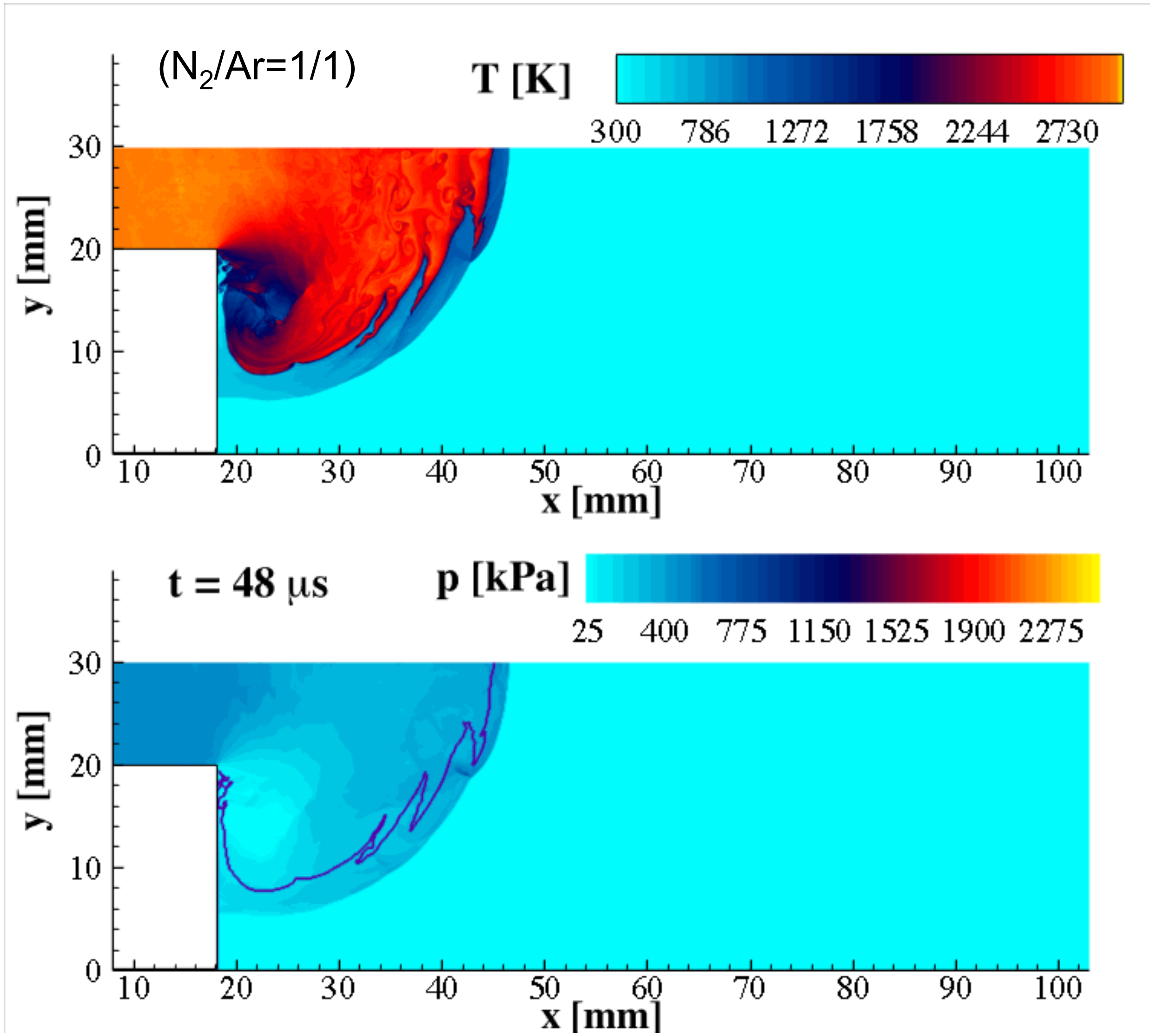


(a) $p = 2, h = 200\,\mu\text{m}$ (b) $p = 1, h = 100\,\mu\text{m}$ (c) $p = 2, h = 100\,\mu\text{m}$

Applications and Test Cases
Physics of Reignition and Reinitiation



Applications and Test Cases
Physics of Reignition and Reinitiation

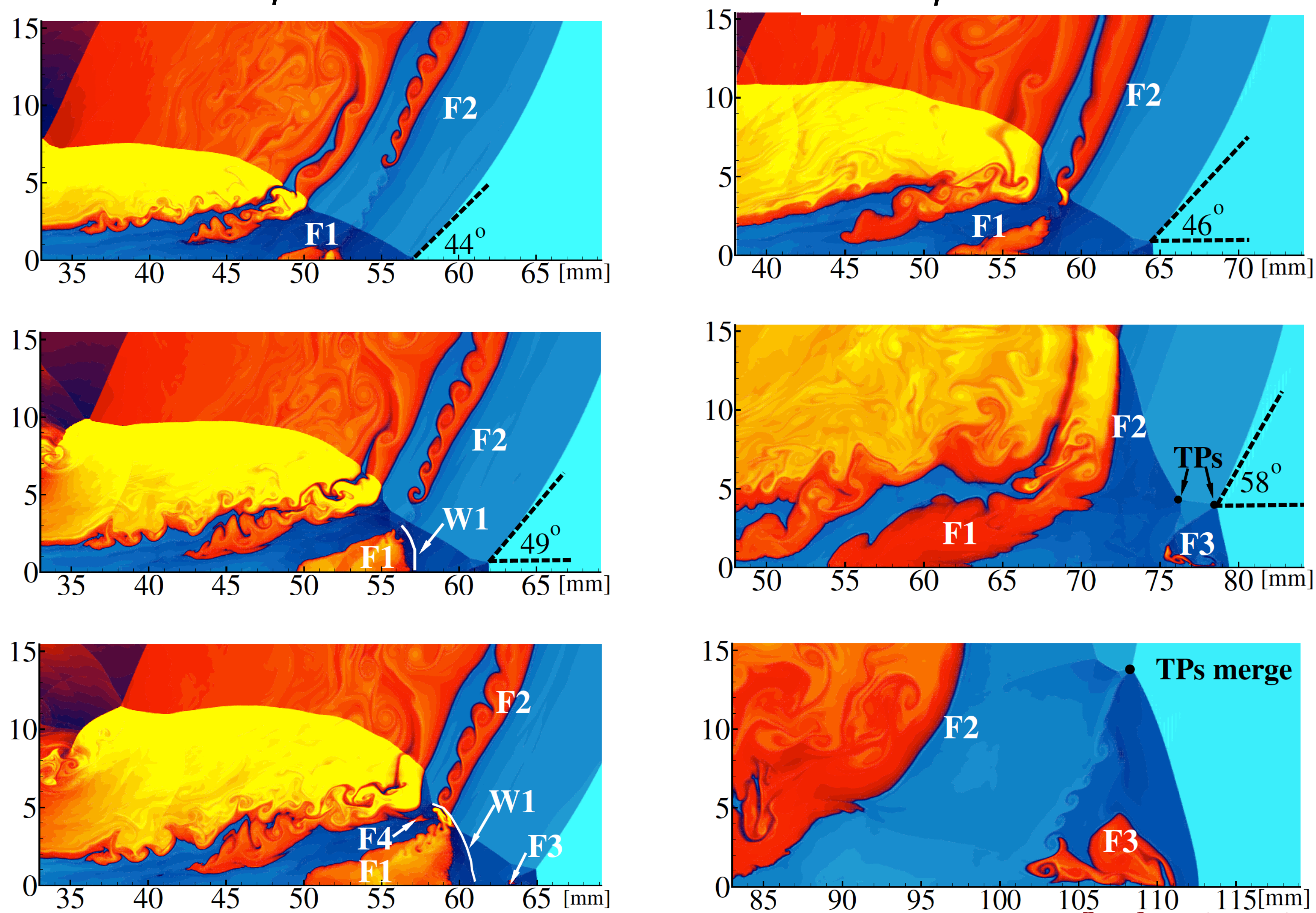


Applications and Test Cases

Physics of Reignition and Reinitiation

Case: β = 2

Case: β = 1.5



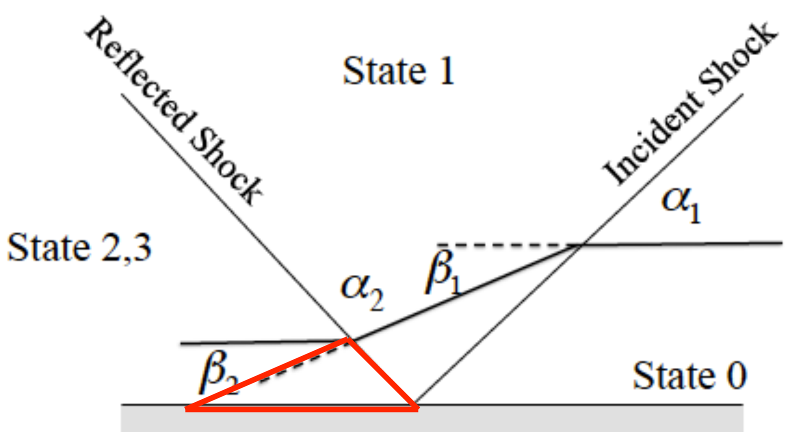
F – flame front; W – pressure wave

Applications and Test Cases
Physics of Reignition and Reinitiation

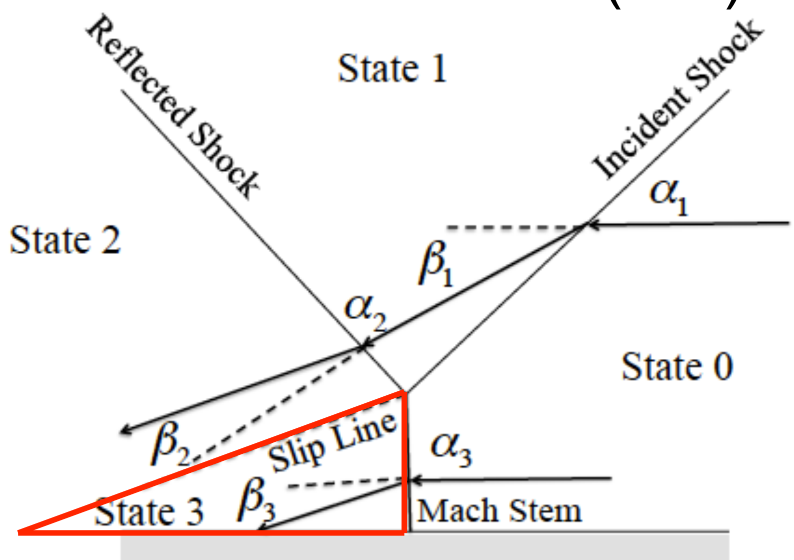
Theoretical analysis:

- Consider shock theory to develop theoretical model[1] to reconcile reignition behavior

Regular Reflection (RR)



Mach Reflection (MR)



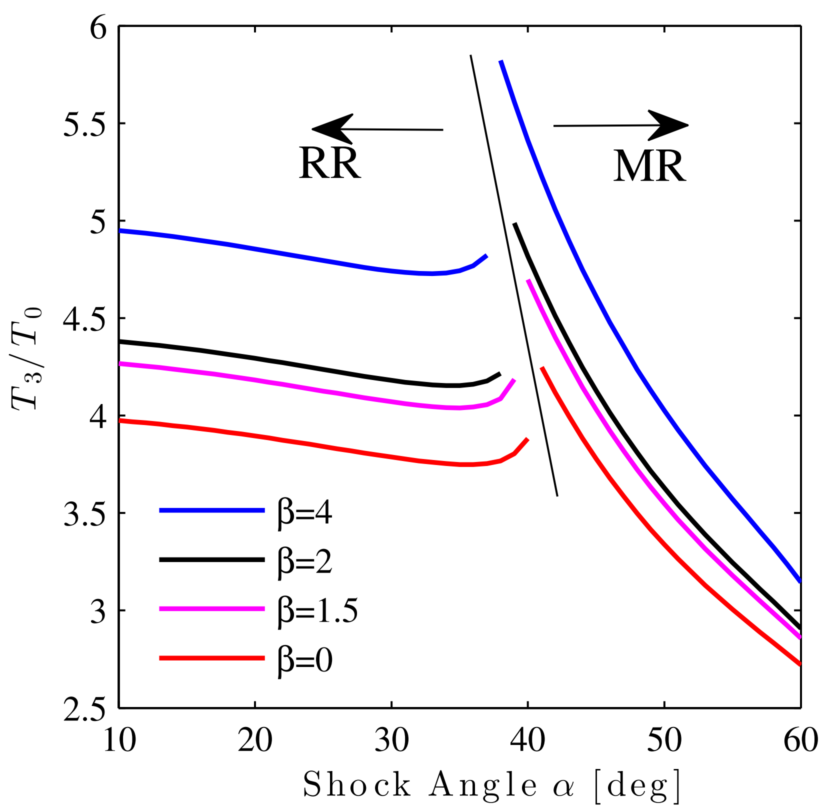
Problem formulation

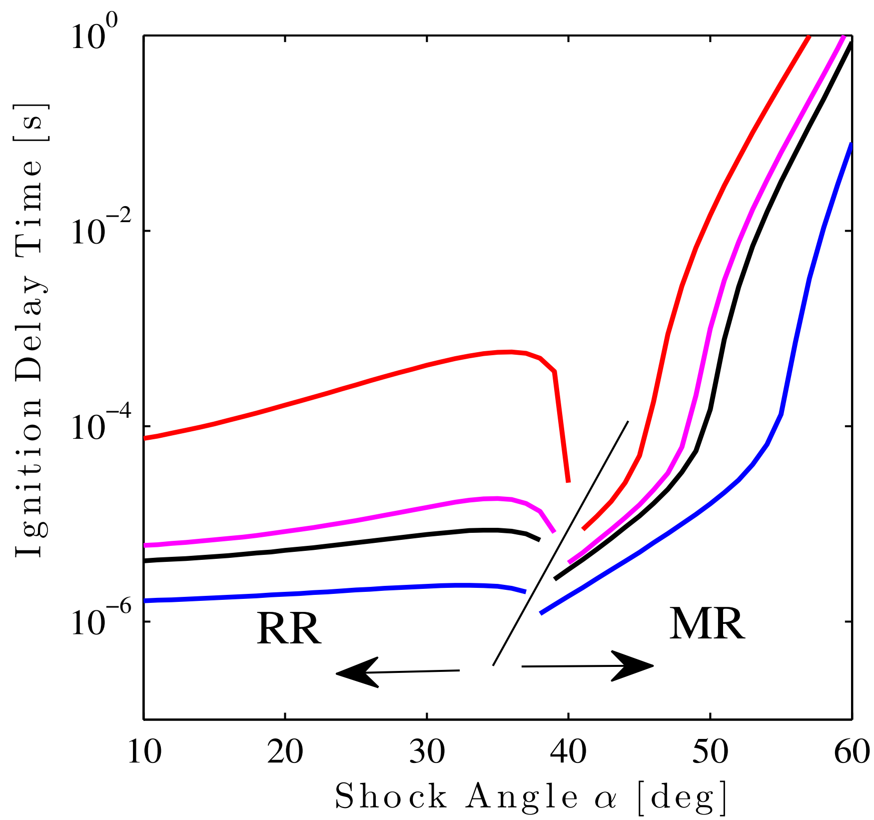
- Given State 0 and shock angle α, determine State 3

[1] G. Ben-Dor, Shock Wave Reflection Phenomena, Springer, 2007.

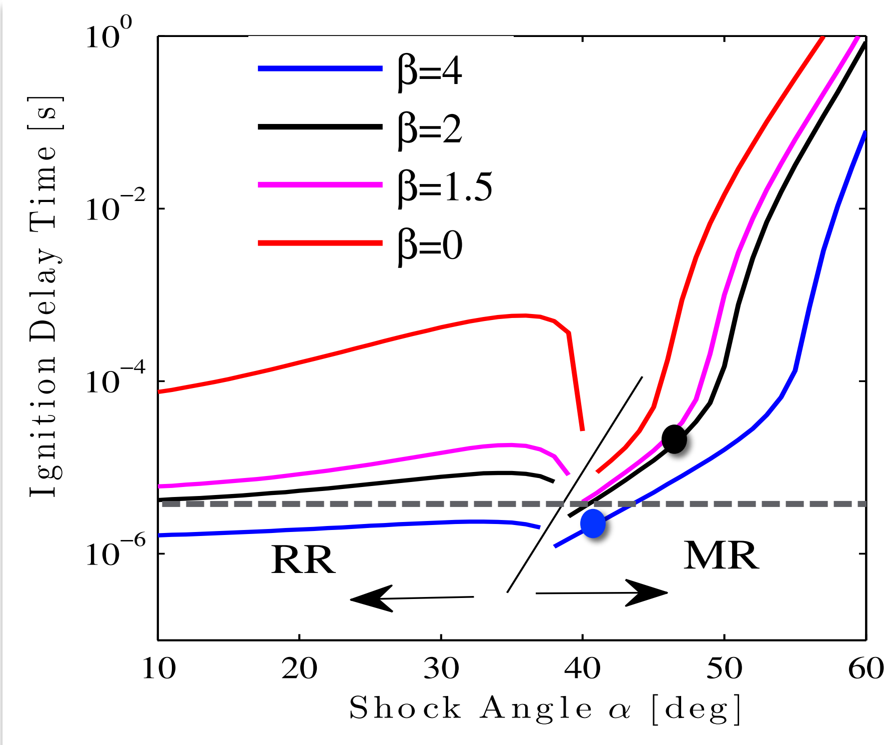
Theoretical Analysis

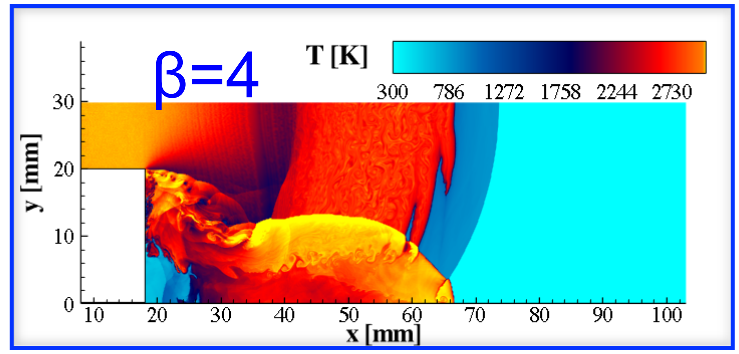
Ignition conditions computed from shock-theory

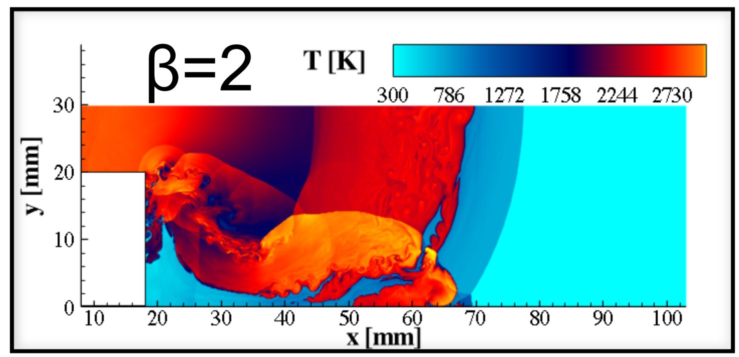




Theoretical Analysis







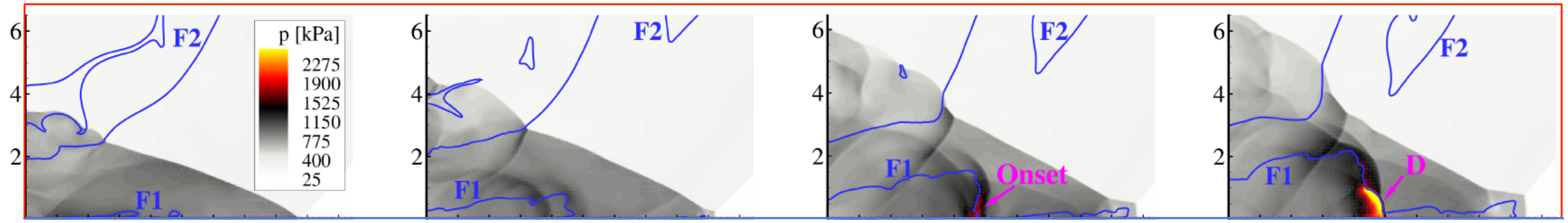
Applications and Test Cases
Physics of Reignition and Reinitiation

Analysis

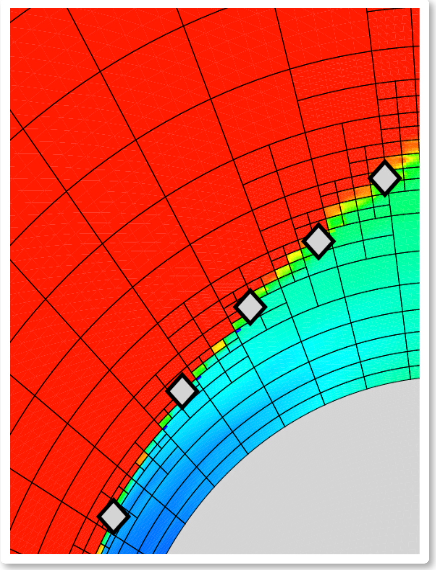
Effect of viscous heating

time

Viscous calculation



Summary and Conclusions



Summary and Conclusions

Development of shock-capturing framework for high-order schemes, integrating entropy-bounding, shock detection and artificial viscosity

- Algorithmic developments and capabilities
  - Generality: applicable to arbitrary elements, discretization orders, and spatial dimensions
  - Robustness: entropy-constrain enables the description of shock discontinuities with any strength
  - Simplicity: code extensions are restricted to algebraic modifications
  - Multiphysics
    - Detailed transport
    - Complex chemistry, radiation
    - Turbulence and shock/detonation transition

Summary and Conclusions

Development of shock-capturing framework for high-order schemes, integrating entropy-bounding, shock detection and artificial viscosity

Potential of DG-method for hypersonic aerothermodynamic flows

- High-order accuracy and optimal convergence properties
- Intrinsic minimum entropy-principle ensures stability
- Local discretization and subcell shock capturing
- Applicable to arbitrary meshes and spatial discretization
- Local mesh-adaptation (*h*) and refinement in polynomial order (*p*)
- Ideally suitable for bandwidth-limited HPC-architectures

Thank you!

QUESTIONS