Shock-Capturing Methods for High-Order Discontinuous Galerkin Schemes

YU LV, ERIC CHING, MATTHIAS IHME

CENTER FOR TURBULENCE RESEARCH
DEPARTMENT OF MECHANICAL ENGINEERING
STANFORD UNIVERSITY

AMS Seminar Series,
NASA Ames Research Center, September 1, 2016

Funding: NASA ECF
Acknowledgement: Dr. Barnhardt, Dr. Gnoffo

Outline

1. Background
2. DG and entropy-bounded DG schemes
3. Entropy-residual detector – Localization of discontinuities
4. Artificial-viscosity method for explicit time-integration
5. Artificial-viscosity method for implicit time-integration
6. Conclusions & Outlook

Background

Target applications:

- High-speed propulsion and reacting flows
- Hypersonic reentry aerothermodynamics
- Astrophysics

Challenges:

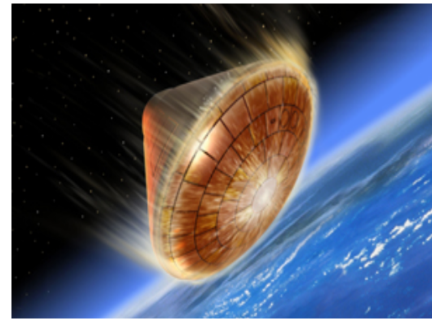
- Multi-scale characteristics (turbulence, flame)
- Shock-capturing
- Real-world geometry
- Physical realizability (solver robustness)
- Stiff chemical source term
- Complex gas models

Objective:

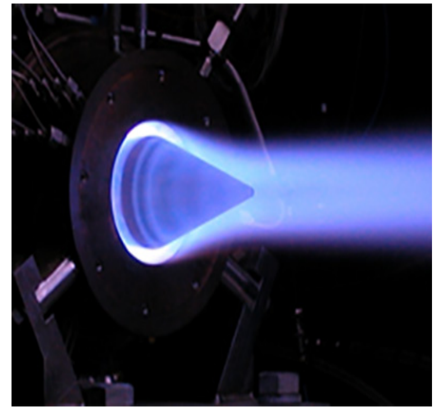
- Development of a flow solver capable of handling these challenges

Figure credits: DOE/NASA

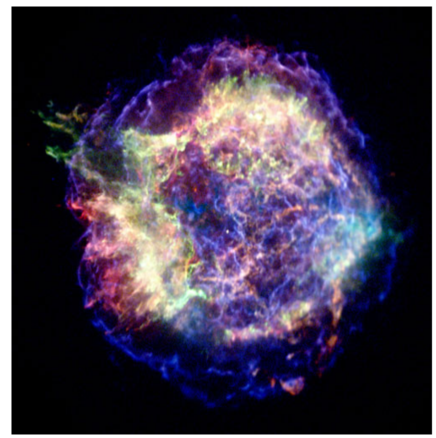
Hypersonic reentry



Detonation engine



Supernova explosion



Discontinuous Galerkin discretization scheme

- Basis/test functions:

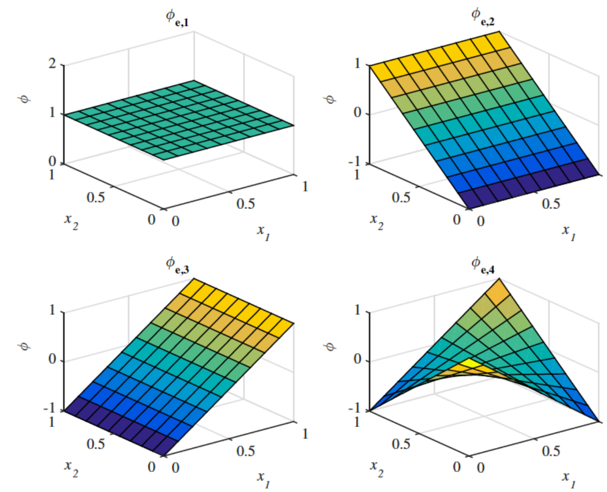
$$\mathbb{V}_h^p = \{\phi \in L^2(\Omega) : \phi_e \equiv \phi|_{\Omega_e} \in \mathbb{P}^p, \forall \Omega_e \in \Omega\}$$

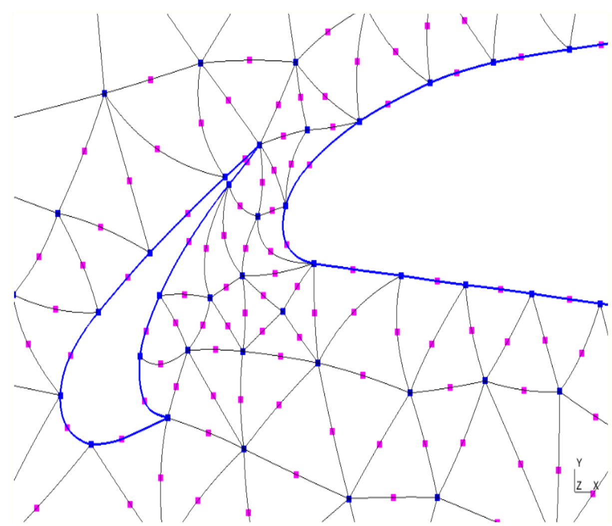
- Solution approximation:

$$U_e(t,x) = \sum_{i=1}^{N_p} \boxed{\widetilde{U}_{e,i}(t)} \phi_{e,i}(x), \quad x \in \Omega_e$$

- Strengths of DG scheme:
  1. High-order accuracy
  2. Compactness
  3. Energy stability
  4. Adaptation
  5. High-order geometry representation

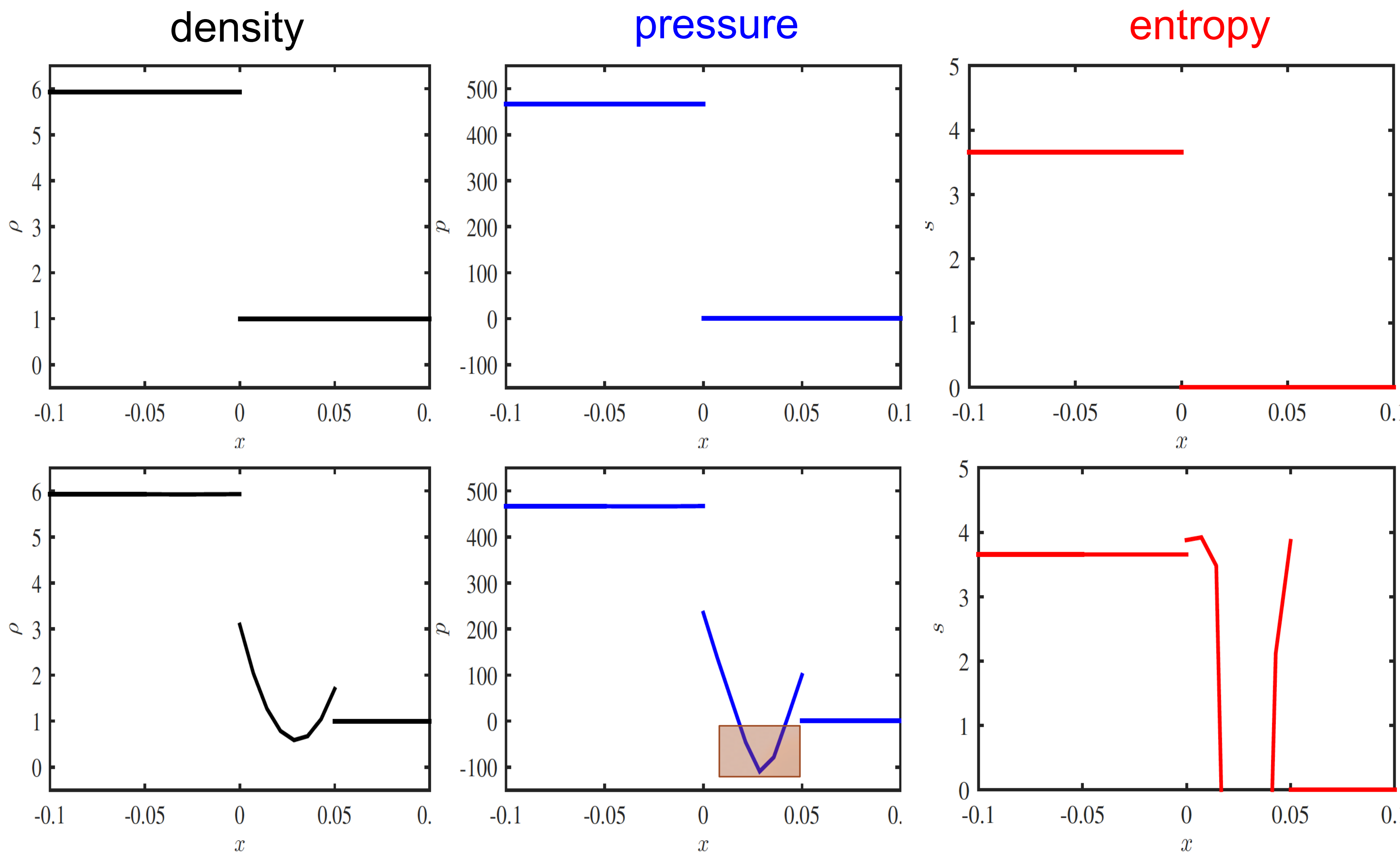
DGP1/p=1 with legendre polynomial in 2D



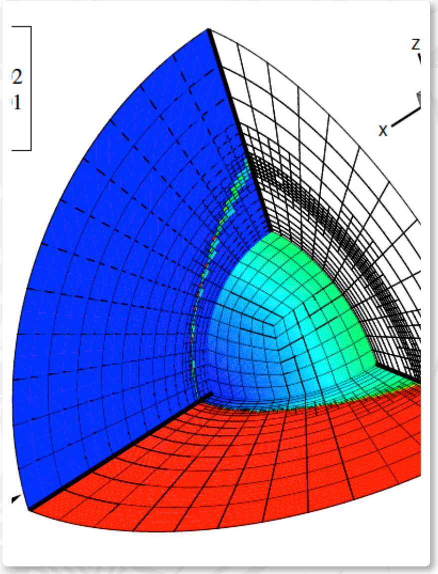


Stanford University

Nonlinear instability of DG scheme



Entropy-bounded DG scheme (EBDG)



Flow models

Compressible Navier-Stokes equations:

$$\underbrace{\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) &= 0 \\ \partial_t (\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I}) &= \nabla \cdot \boldsymbol{\tau} \\ \partial_t (\rho e) + \nabla \cdot (\boldsymbol{u}(\rho e + p)) &= \nabla \cdot (\boldsymbol{u} \cdot \boldsymbol{\tau} - \boldsymbol{q}) \end{aligned}}_{\partial_t \mathbf{U} + \nabla \cdot \mathbf{F} = \nabla \cdot \mathbf{Q}}$$

Law of entropy:

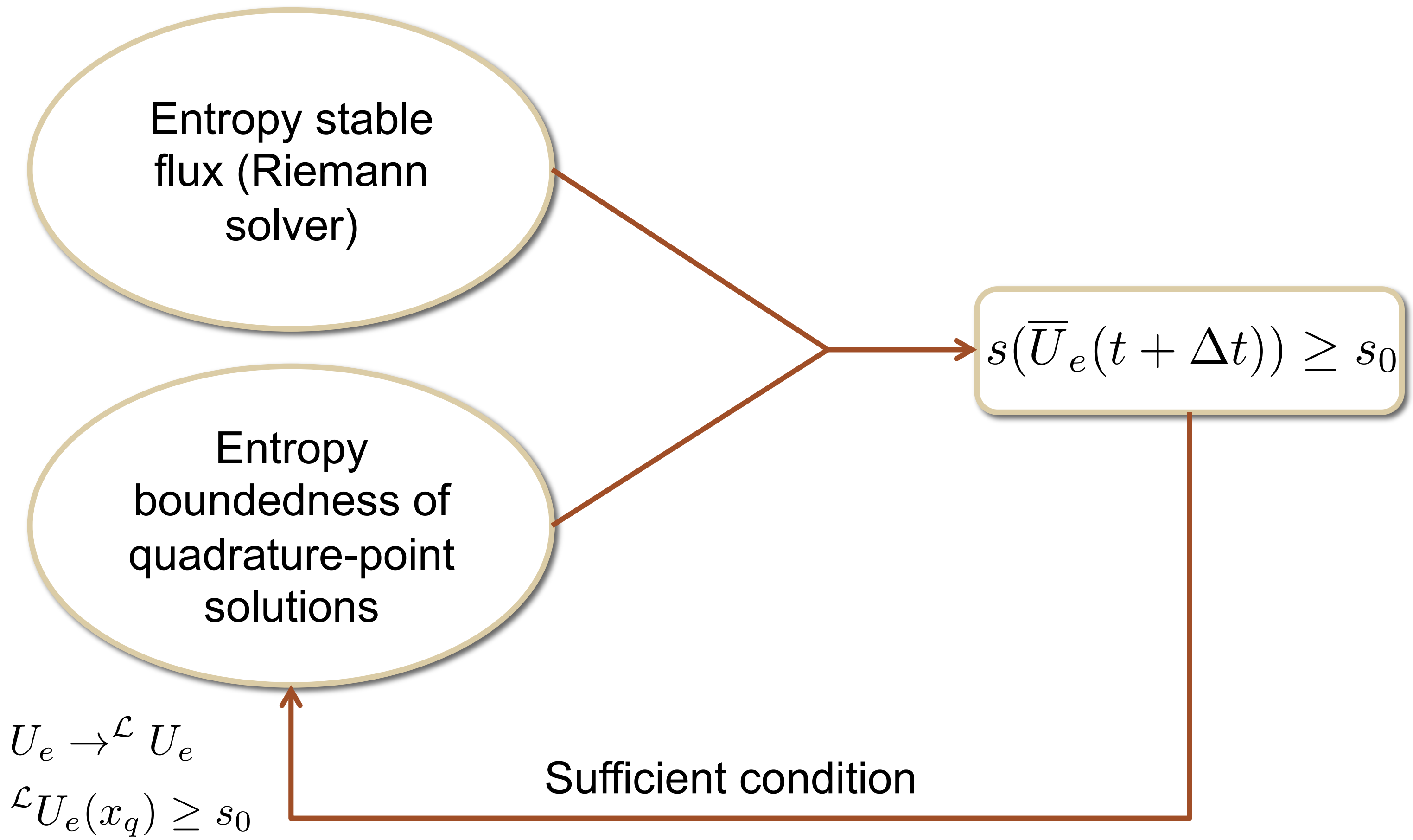
- Entropy residual $\mathcal{R} = \partial_t \mathcal{U} + \nabla \cdot \mathcal{F} \leq 0$ is true for any convex function $\mathcal{U}$ with respect to $\mathbf{U}$.
- Common choice of $\mathcal{U}$:

$$\mathcal{U} = -\rho s \qquad s = \log(p \rho^{-\gamma})$$

- Discrete minimum entropy principle (Tadmor, 1986)

$$s(U(x_i, t + \Delta t)) \geq \min_{i-1 \leq j \leq i+1} s(U(x_j, t))$$

Functioning mechanism of EBDG scheme



[1] Lv & Ihme, JCP, 2015.
[2] Zhang & Shu, JCP, 2010-2011.

Functioning mechanism of EBDG scheme

- Solution constraining implemented using a scaling operator:

Find

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

such that

$$s(^{\mathcal{L}}U_e(x_q)) \geq s_0$$

$$\frac{p(^{\mathcal{L}}U_e)}{\rho^{\gamma}(^{\mathcal{L}}U_e)} \geq \exp(s_0)$$

where s_0 is the minimum entropy, x_q denotes quadrature points.

- s is nonlinear function, but the problem can be solved using algebra relations:

$$p(^{\mathcal{L}}U_e) \geq (1-\varepsilon)p(U_e) + \varepsilon p(\overline{U}_e) \qquad (1)$$

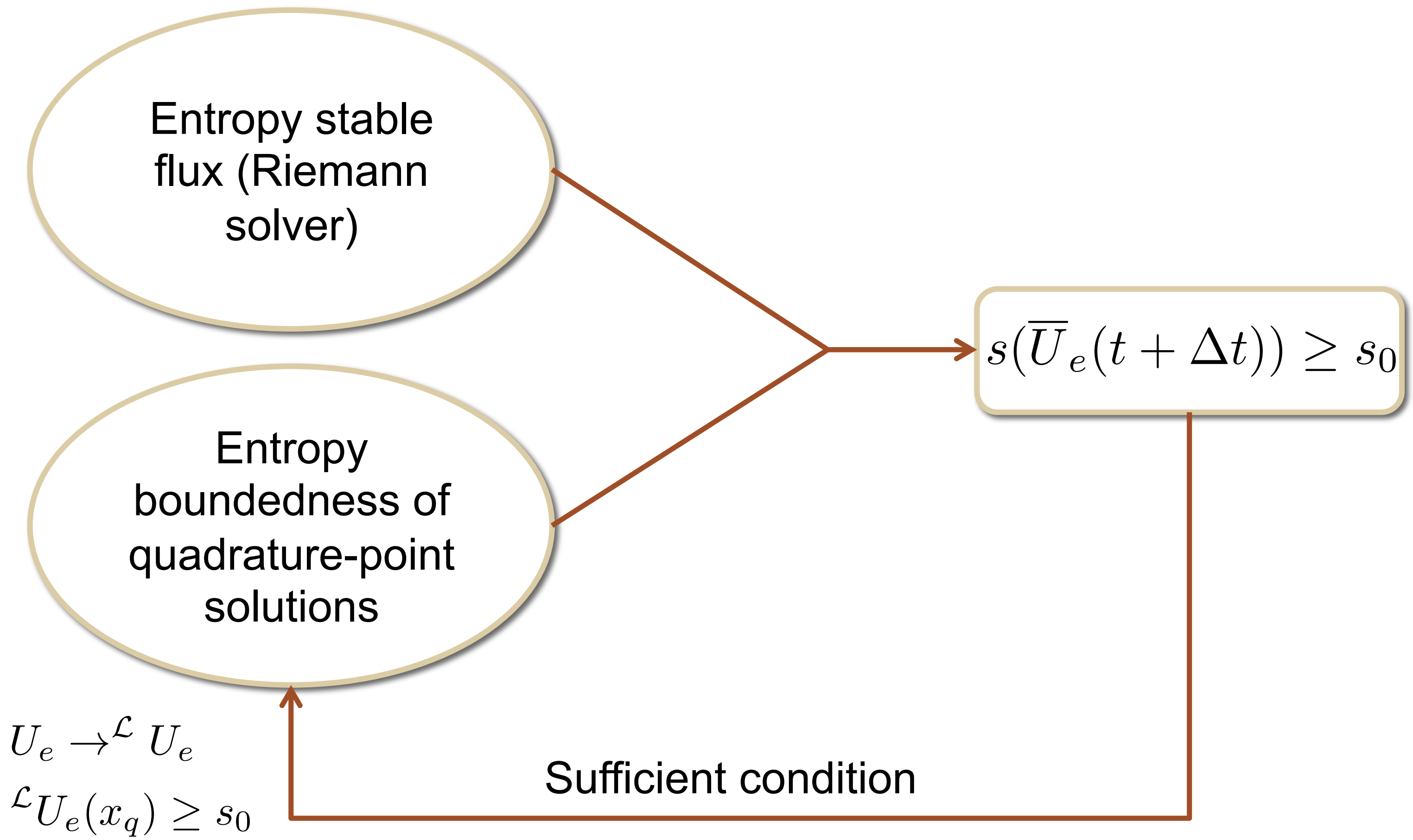
$$(1-\varepsilon)\rho^{\gamma}(U_e) + \varepsilon\rho^{\gamma}(\overline{U}_e) \geq \rho^{\gamma}(^{\mathcal{L}}U_e) \qquad (2)$$

- Find ε by setting

$$(1) \geq (2) \times \exp(s_0)$$

[#] Zhang & Shu, *JCP*, 2010-2011.

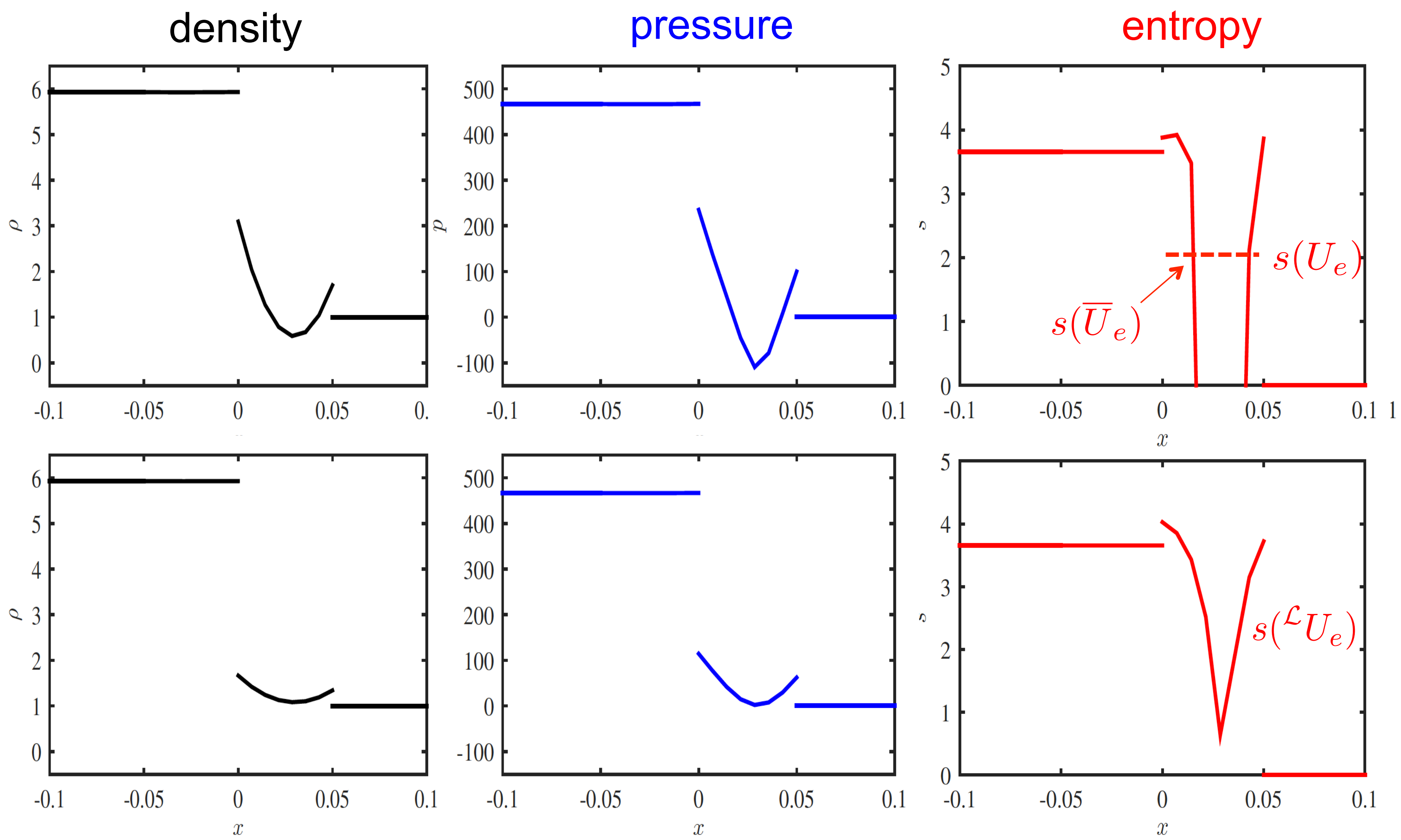
Functioning mechanism of EBDG scheme



[1] Lv & Ihme, JCP, 2015.
[2] Zhang & Shu, JCP, 2010-2011.

Elimination of failure modes using EBDG

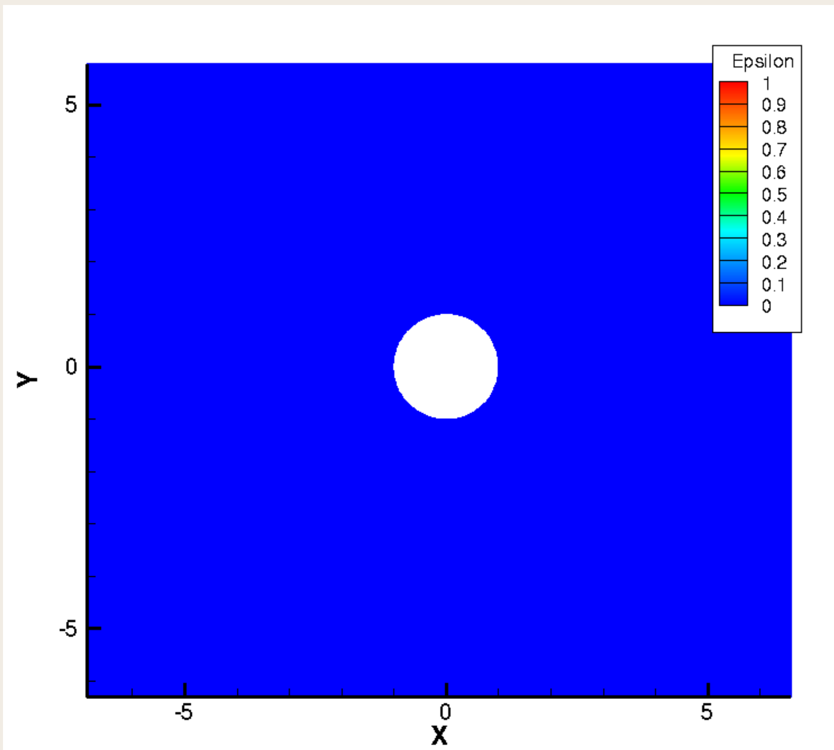
Demonstration of solution constraining $U_e \to^{\mathcal{L}} U_e$ with a Mach-20 moving shock



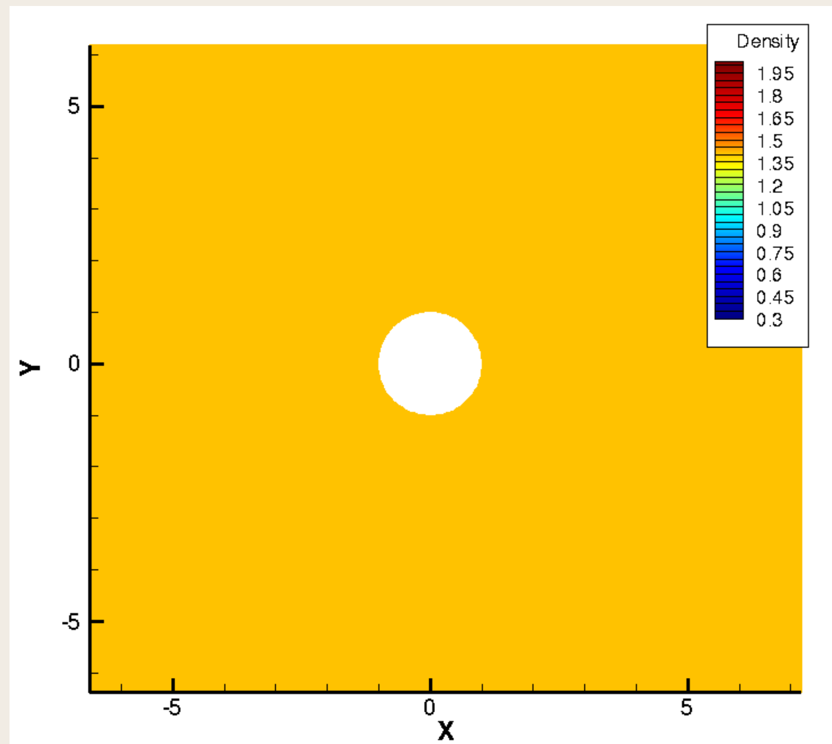
Elimination of failure modes using EBDG

“Vanilla”-version DG

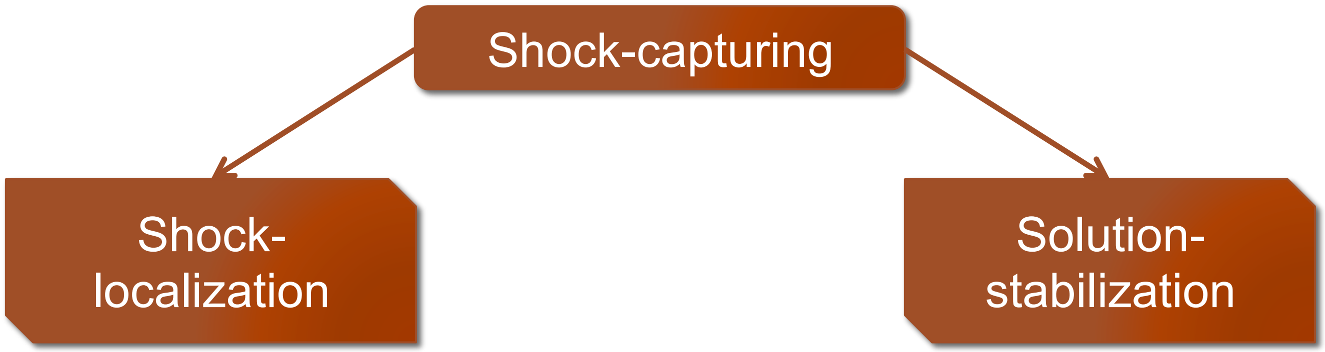
Entropy-bounded DG



Entropy-bounded DG



Overview of shock-capturing methods for DG



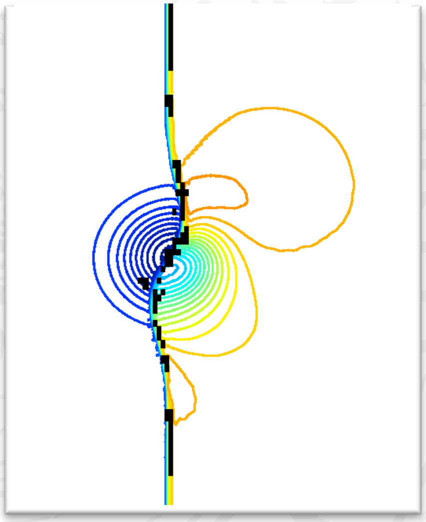
Shock-localization

- **Minmod functions (Cockburn & Shu, 1989)**
- **Local moments (Biswas et al., 1994; Burbeau et al., 2001)**
- **Inter-element solution jump (Krivodonova, 2004)**
- **Local modal decomposition (Persson & Peraire, 2006)**

Solution-stabilization

- **Limiter (TVB, WENO, Moments …) (Cockburn & Shu, 1989; Biswas et al., 1994; Krivodonova, 2007 Luo, 2007; …)**
- **Artificial viscosity (Persson & Peraire, 2006; Barter & Darmofal, 2010, …)**
- **Filtering (Sheshadri & Jameson; Lopez-Morales & Jameson, 2015; 2016)**
- **Posterior solution updating (Dumbser, 2016)**

Entropy-residual shock detector



Entropy residual

- Physical definition: $\mathcal{R} = \partial_t \mathcal{U} + \nabla \cdot \mathcal{F}$

- Interpretation: (1) $\mathcal{R} = 0$: smooth solution
  (2) $\mathcal{R} < 0$: discontinuous solution

- Discrete entropy residual:

$$R_{\mathcal{U}}(U_e) = \frac{1}{|\Omega_e|} \int_{\Omega_e} \left[\frac{\mathcal{U}(U_e(t+\Delta t)) - \mathcal{U}(U_e(t))}{\Delta t} + \frac{1}{2} \nabla \cdot \left(\mathcal{F}(U_e(t)) + \mathcal{F}(U_e(t+\Delta t)) \right) \right] d\Omega$$

- Convergence property of entropy-residual for smooth solution*

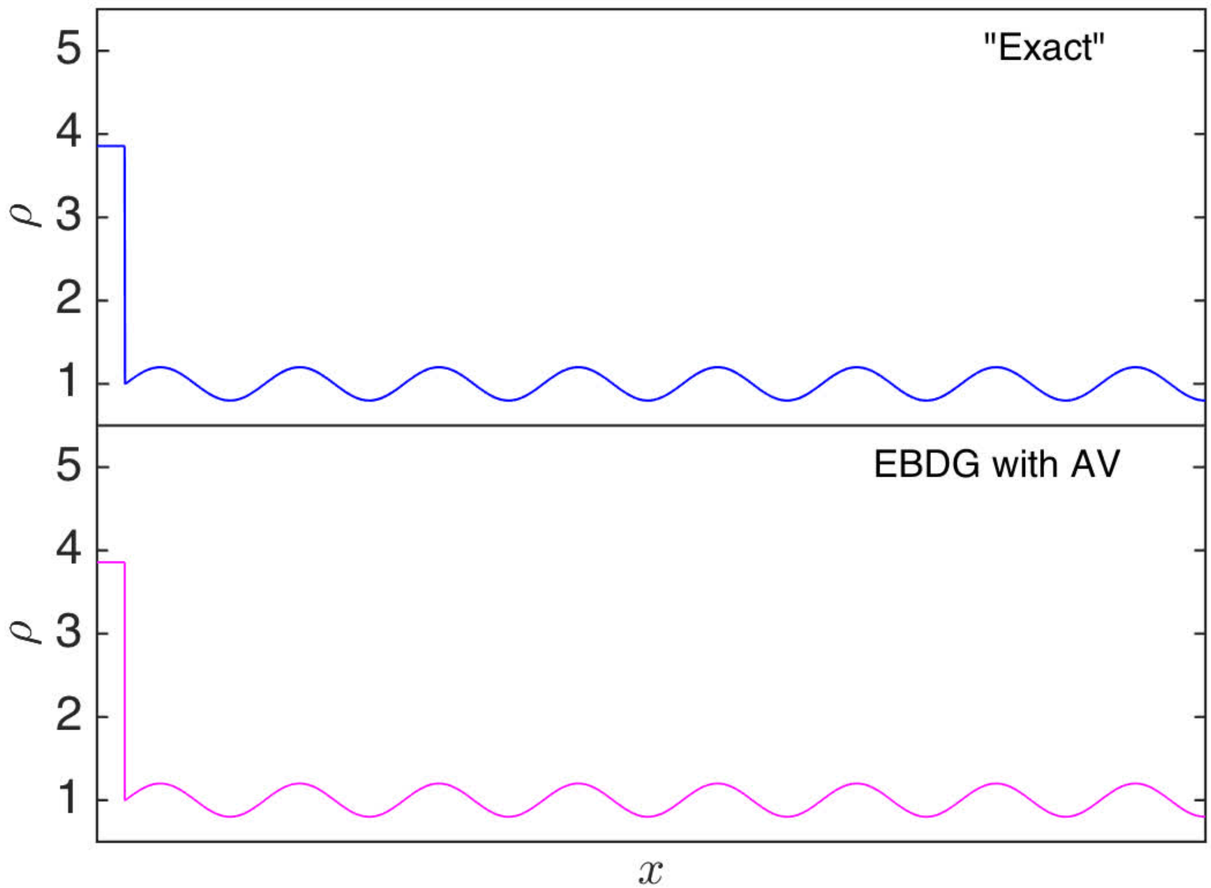
$$|R_{\mathcal{U}}(U_e)| \le b h^r, \qquad r = \min\left\{ p - \frac{dim}{2}, 1 \right\}$$

- Related studies: entropy-residual in the context of FEM and Fourier approximation (Guermond & Pasquetti, 2008; Guermond et al., 2011)

* Lv & Ihme, JCP, 2016.

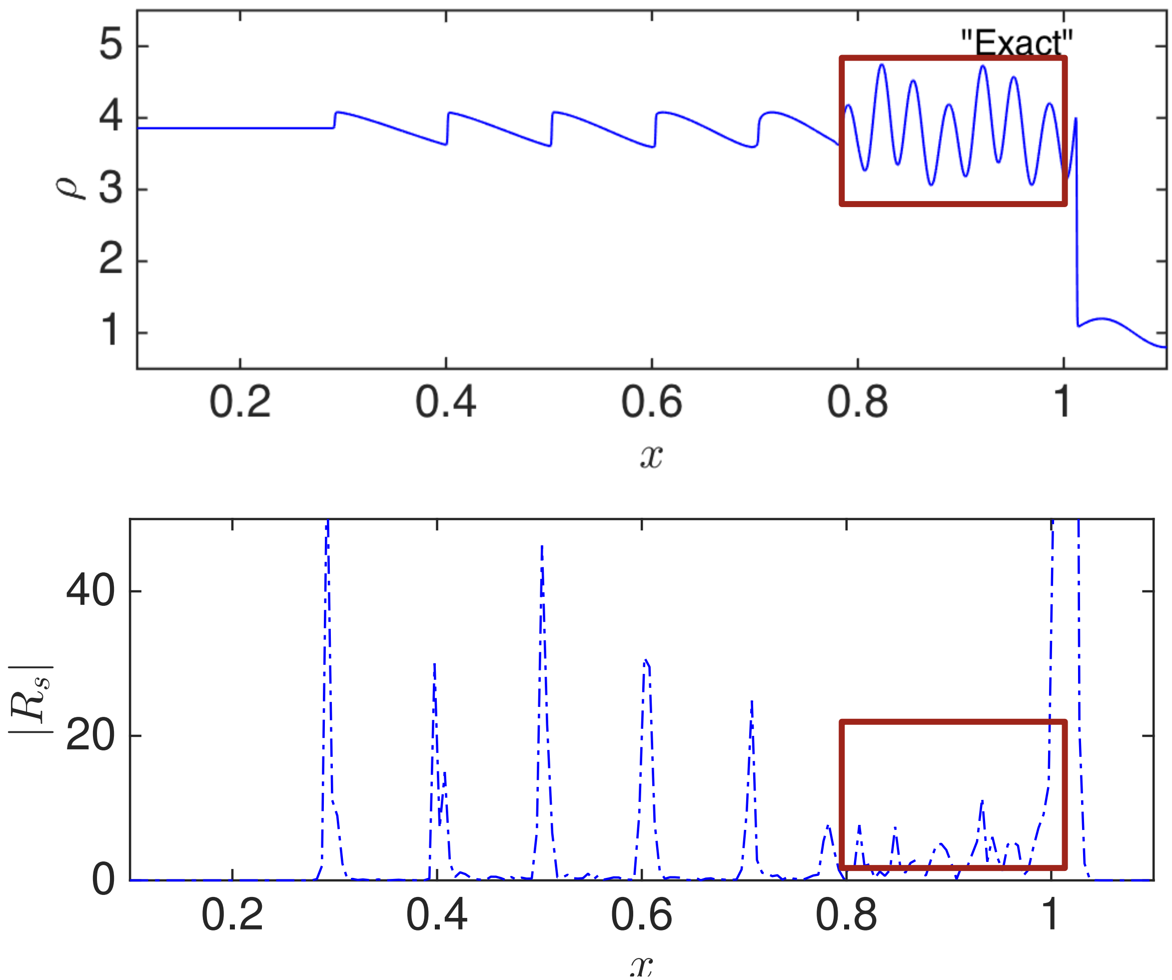
Numerical test and demonstration

Shu-Osher problem: Mach3 shock interacts with a sinusoidal density wave



Numerical test and demonstration

Shu-Osher problem: Mach3 shock interacts with a sinusoidal density wave



Threshold setting for $|\mathcal{R}_{\mathcal{U}}(U_e)|$

- Troubled-cell detection criterion:

$$|\mathcal{R}_{\mathcal{U}}(U_e)| > \varepsilon$$

- How to set ε ?

For smooth solutions, no effect when *h* is sufficiently small.

- Local and dynamic estimate for ε

$$|R_{\mathcal{U}}| \sim \frac{1}{|\Omega_e|}\int_{\Omega_e} \frac{\partial(\rho u s)}{\partial x_1} dx \ ,$$

Assume that entropy flux mostly varies along x_1

$$\sim \frac{1}{h_e}(\bar{\rho}^*\bar{u}^*\bar{s}^* - \bar{\rho}\bar{u}\bar{s}) \ ,$$

Approximate sub-cell using neighbors' informatio

$$\sim \frac{\bar{s}}{h_e}(\bar{\rho}^*\bar{u}^* - \bar{\rho}\bar{u}) \ ,$$

Entropy variation is a third-order term

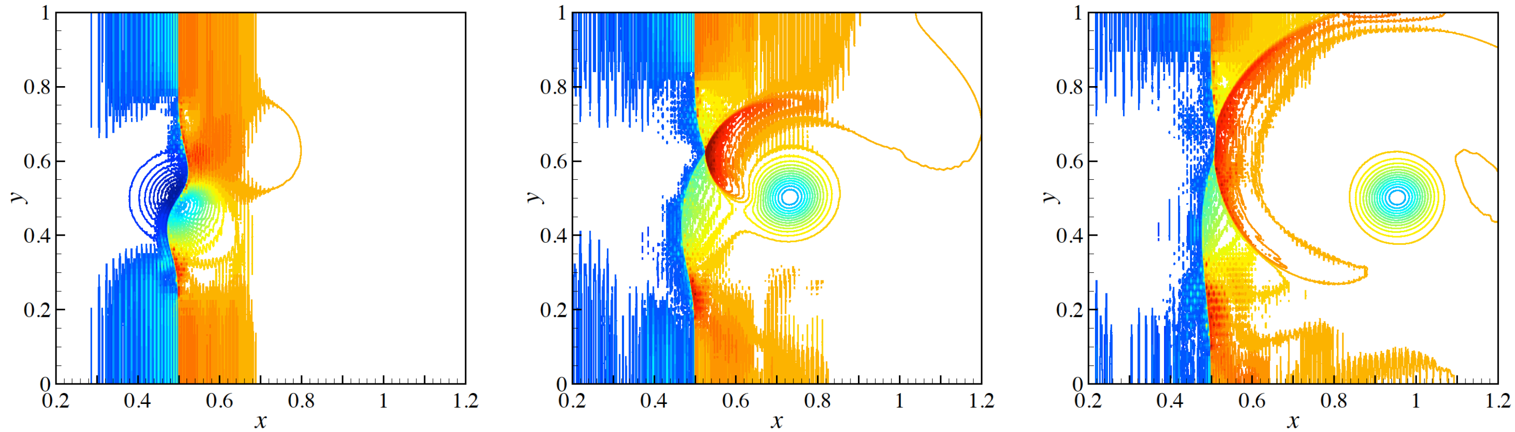
$$\sim \frac{\bar{s}\bar{\rho}v_s}{h_e}\left(\frac{\bar{\rho}^*}{\bar{\rho}} - 1\right) \ ,$$

Introduce v_s as shock velocity

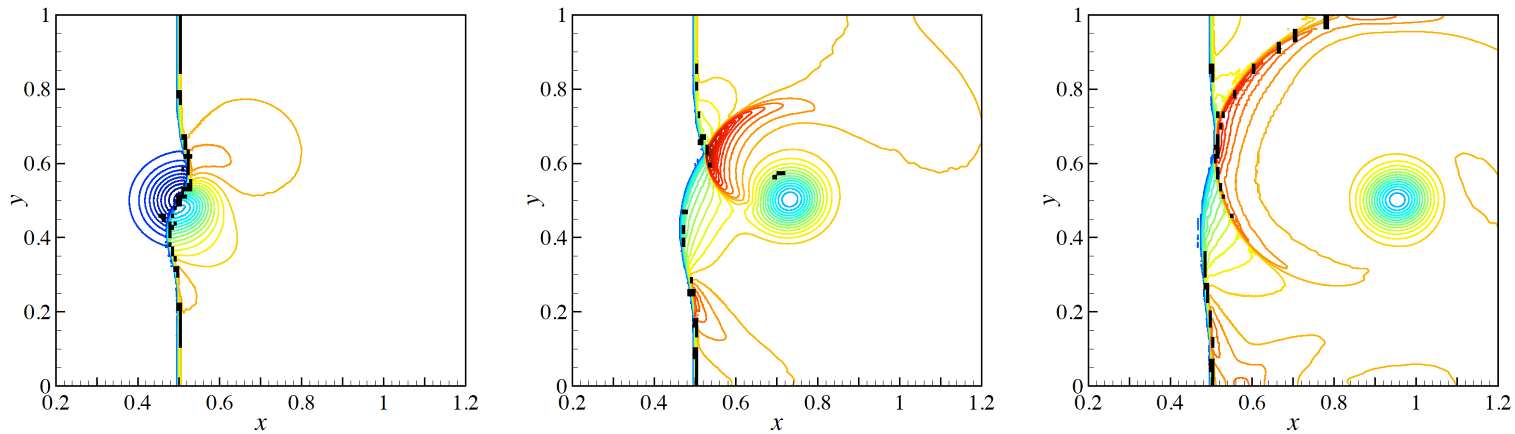
$$\sim \frac{1}{h_e}\left(|\bar{u}| + \bar{c}\sqrt{\frac{\gamma-1}{2\gamma} + \frac{\gamma+1}{2\gamma}\frac{\bar{p}^*}{\bar{p}}}\right)\frac{\frac{2}{\gamma-1}\left(\frac{\bar{p}^*}{\bar{p}} - 1\right)\bar{s}\bar{\rho}}{\frac{\gamma+1}{\gamma-1} + \frac{\bar{p}^*}{\bar{p}}} \ .$$

Effect of threshold setting on detector performance

Example: Shock-vortex interaction (Ma = 1.1)*



(a) $t = 0.20$, constant threshold $\varepsilon = 1$ (b) $t = 0.40$, constant threshold $\varepsilon = 1$ (c) $t = 0.60$, constant threshold $\varepsilon = 1$



(d) $t = 0.20$, DTS (e) $t = 0.40$, DTS (f) $t = 0.60$, DTS

* Jiang & Shu, JCP, 1996.

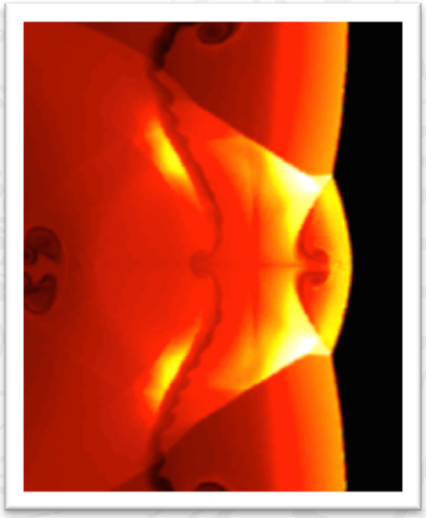
Numerical test – Shu-Osher problem

Simulation setting:
1) EBDGP4
2) h = 1/200
3) Entropy-residual shock indicator
4) Artificial viscosity

Krivodonova, et al. *Appl. Numel. Math.*, 2004.
Persson P.-O. and Peraire J., 2006.

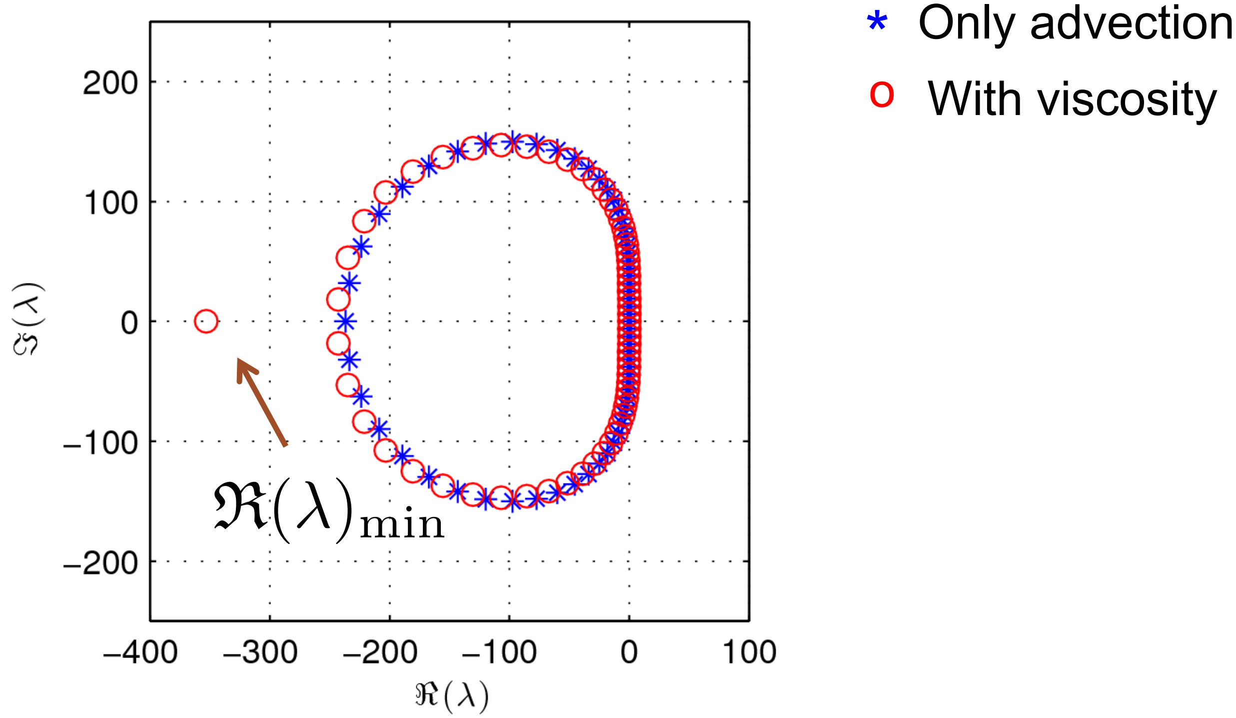
Artificial-viscosity method for unsteady & explicit calculations

HOW MUCH AV SHOULD BE INTRODUCED?



Determination of AV magnitude by Fourier Analysis

- Equation: $\partial_t U = -a\partial_x U + \mu_0 \partial_{xx} U$
- Assumption: μ_0 is locally added to only one cell of the domain
- Eigen-spectrum:

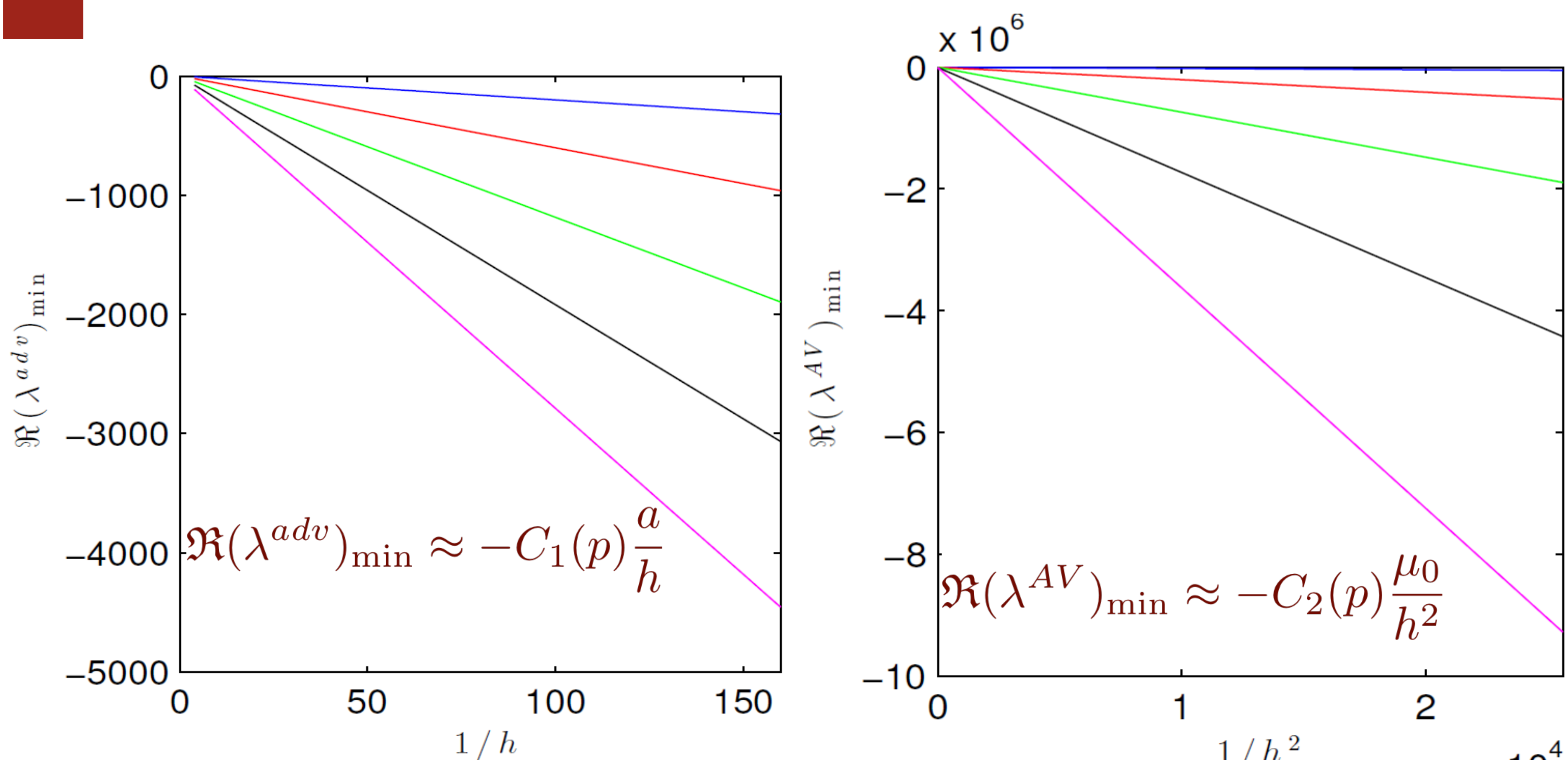


Settings: DGP2, BR2 scheme, 20 elements, $\mu_0 = 0.1$

Eigenvalue magnitude scaling

- Approximate the behavior of $\Re(\lambda)_{\min}$

$$\Re(\lambda)_{\min} \approx \Re(\lambda^{AV})_{\min} + \Re(\lambda^{adv})_{\min}$$



Determination of AV magnitude

Impose a constraint on $\Re(\lambda)_{\min}$ for efficient time-stepping

$$|\Re(\lambda)_{\min}| \approx |\Re(\lambda^{AV})_{\min}| + |\Re(\lambda^{adv})_{\min}| \leq \beta|\Re(\lambda^{adv})_{\min}|$$

The range of β should be in (1, 2)

- $\beta = 1$ means that no AV is added
- $\beta = 2$ means that diffusion mode become dominating locally

The suggested values for

- for nonlinear problems $\beta = 1.5$
- for linear problems $\beta = 1.15$

AV is determined as $\mu_0 = (\beta - 1)\dfrac{C_1(p)}{C_2(p)}ah$

where the scaling is consistent to the Persson's formula.*

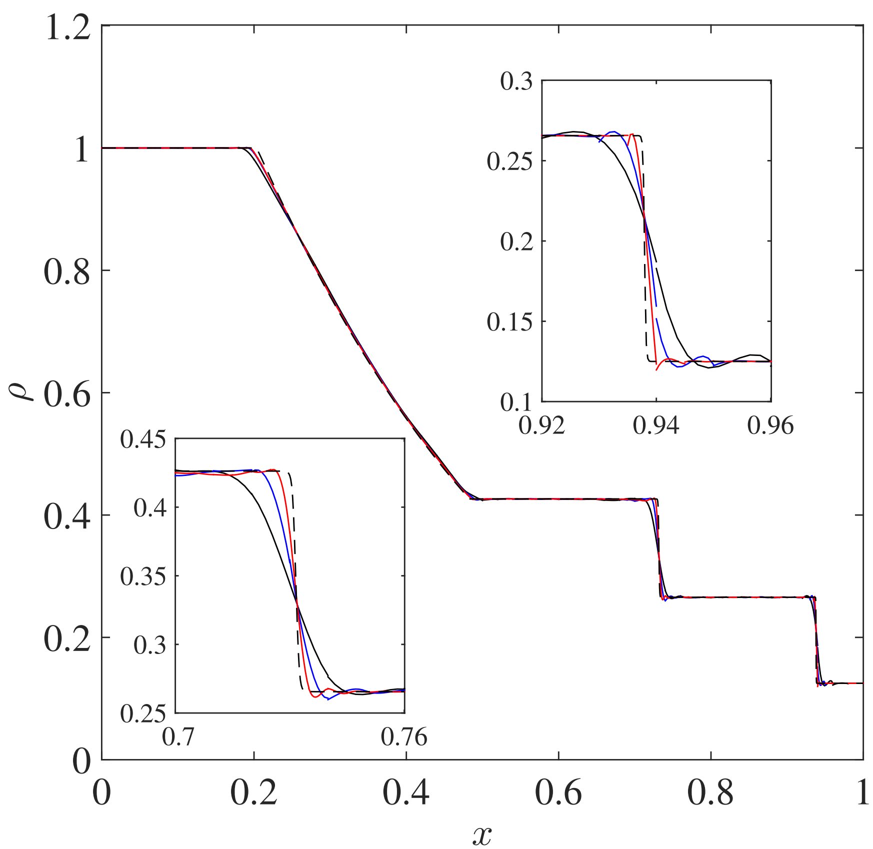
*Persson P.-O. and Peraire J., 2006.

Numerical test – Sod shock-tube problem

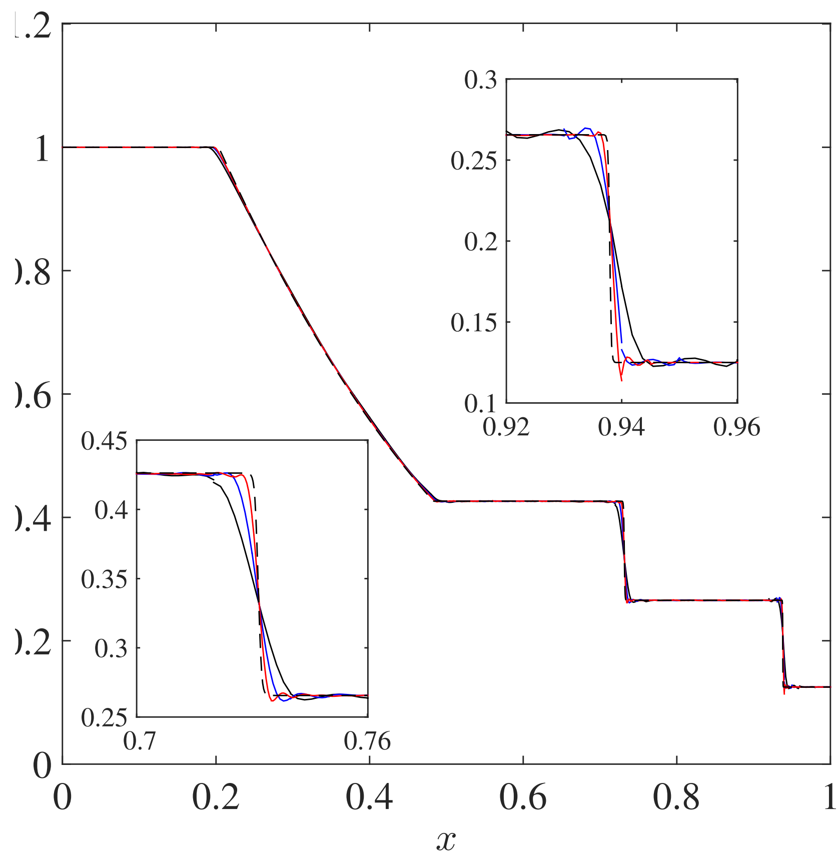
Refinement study:

$h = 1/50$
$h = 1/100$
$h = 1/200$

EBDGP3

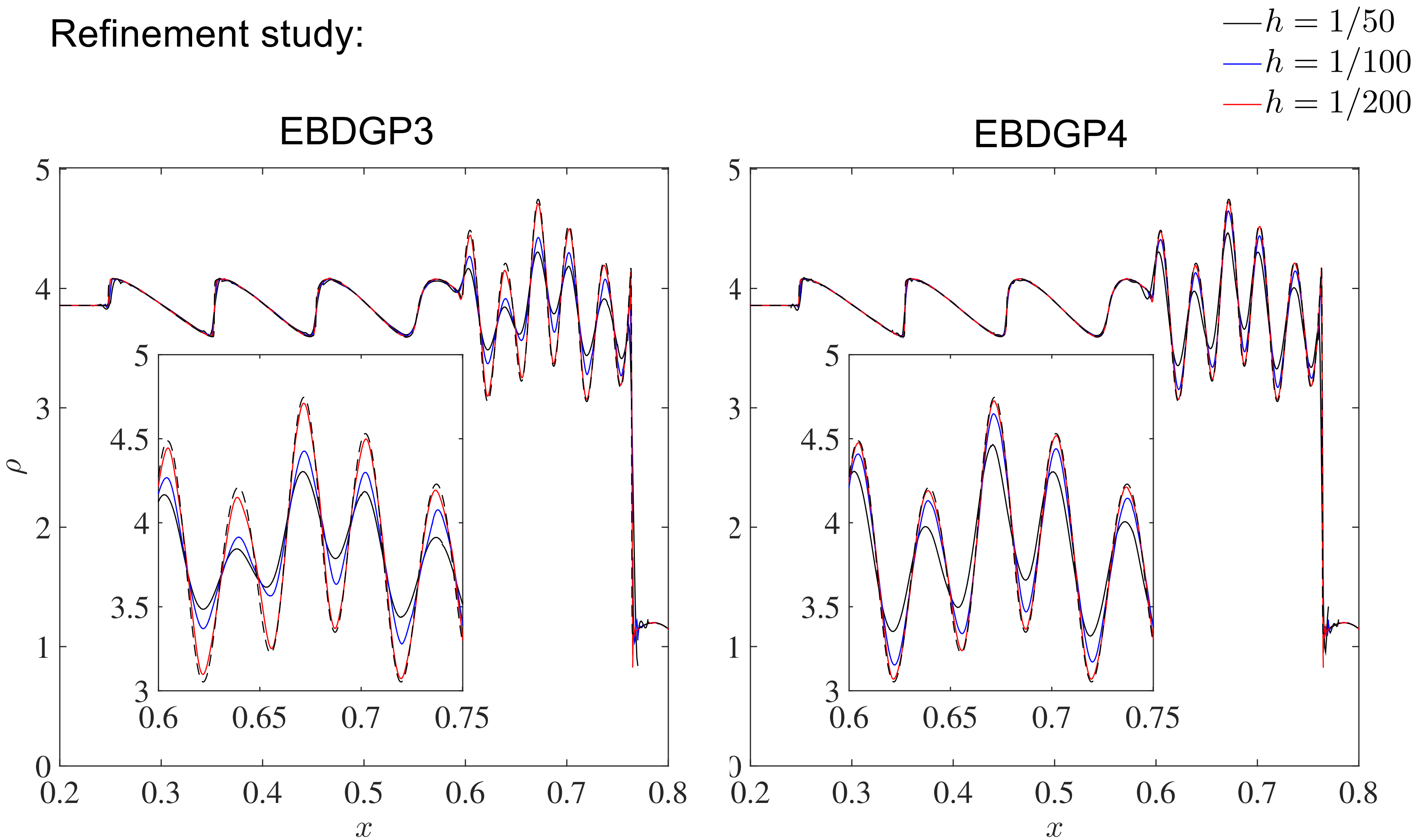


EBDGP4



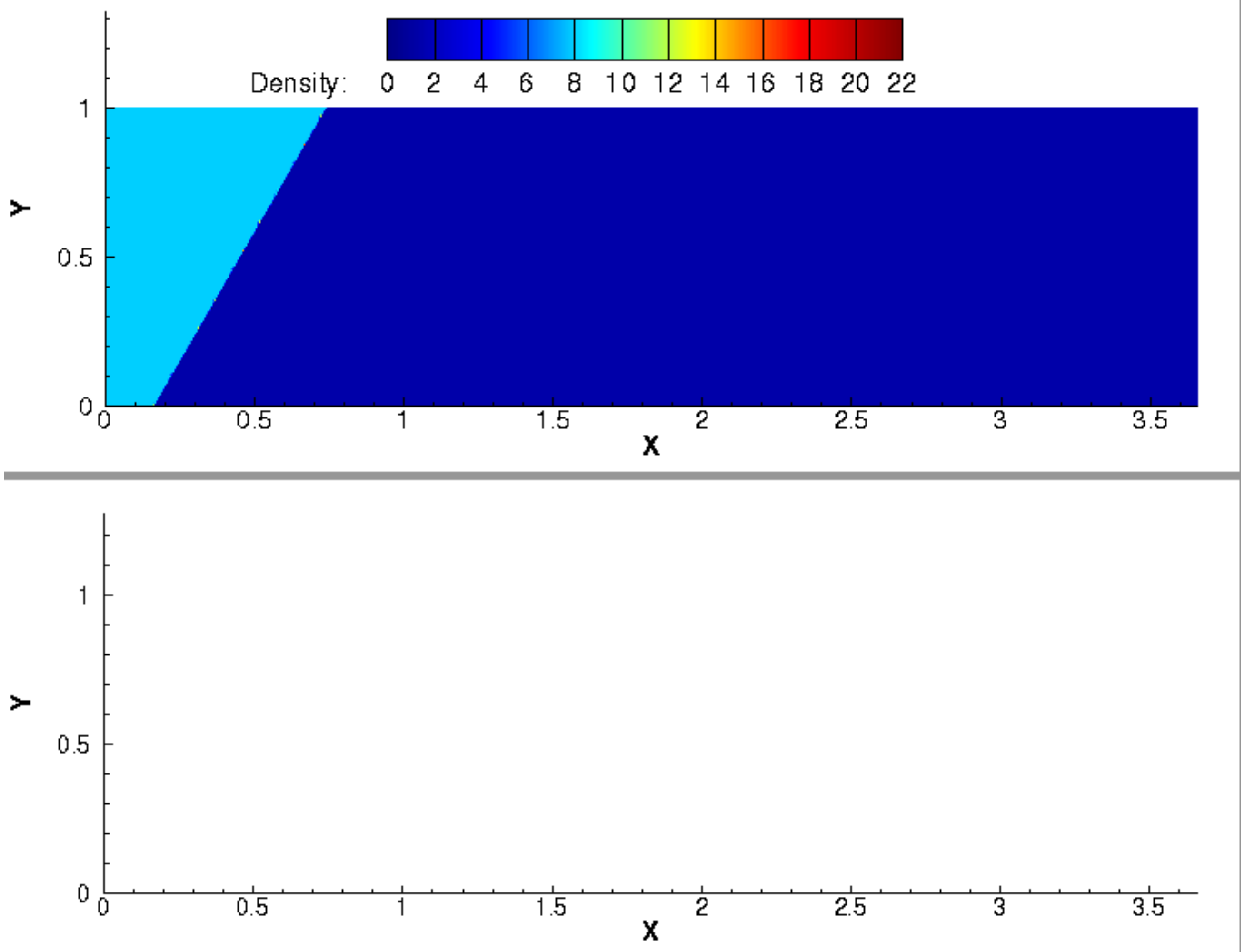
Numerical test – Shu-Osher problem

Refinement study:



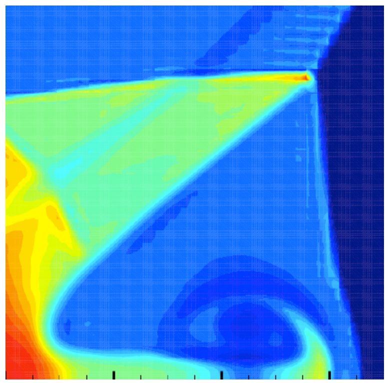
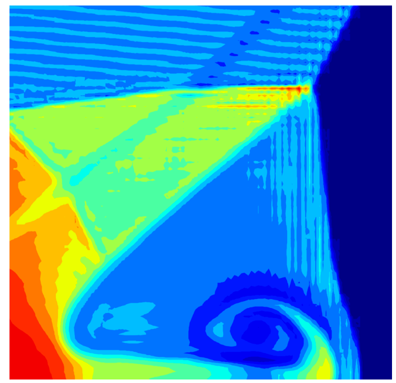
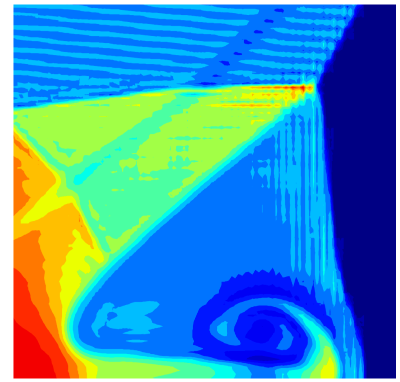
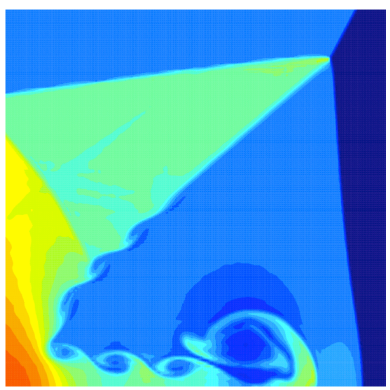
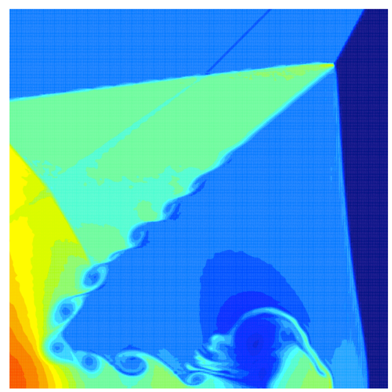
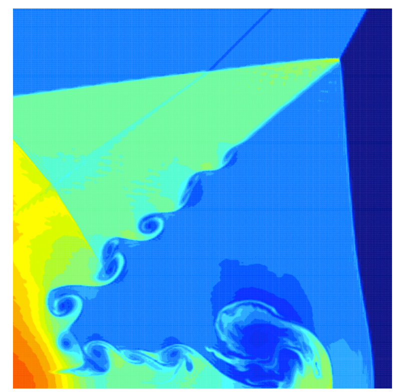
Numerical test – double Mach reflection

Double Mach reflections: Mach 10 shock impinges on a wall with 60^{o}



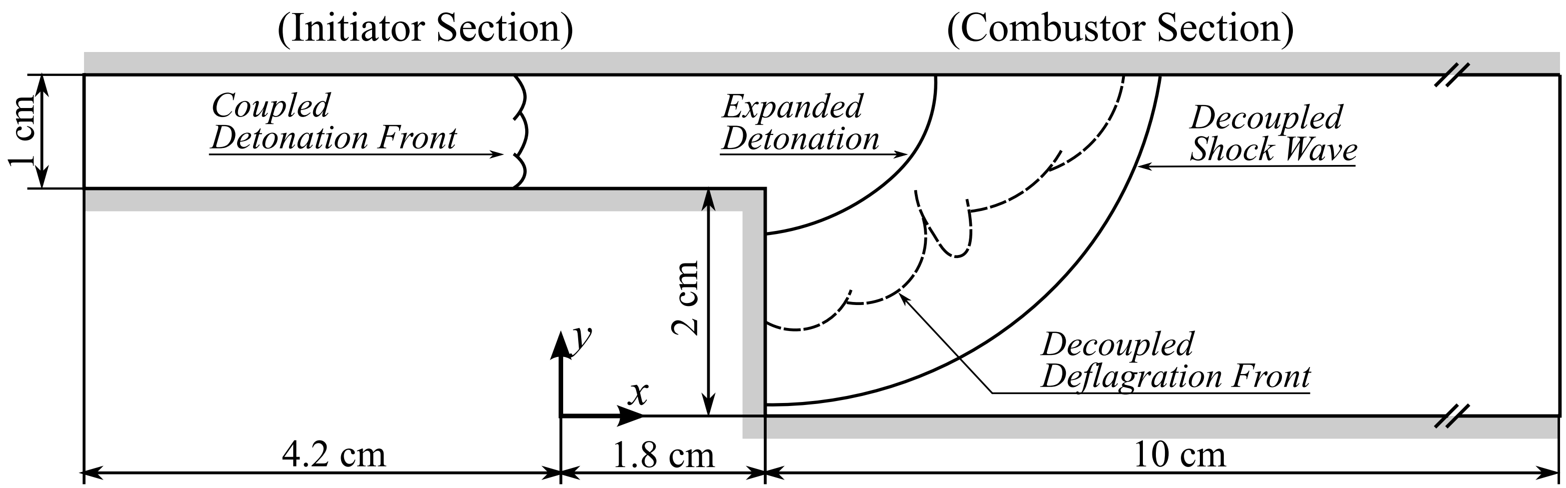
Simulation setting:
1) EBDGP4
2) h = 1/200
3) Entropy-residual shock indicator
4) Artificial viscosity

Numerical test – double Mach reflection

	DGP2	DGP3	DGP4
Predictions by EBDG			
EBDG + entropy-residual detector + artificial viscosity			

Stanford University

Application: Detonation diffraction and re-initiation



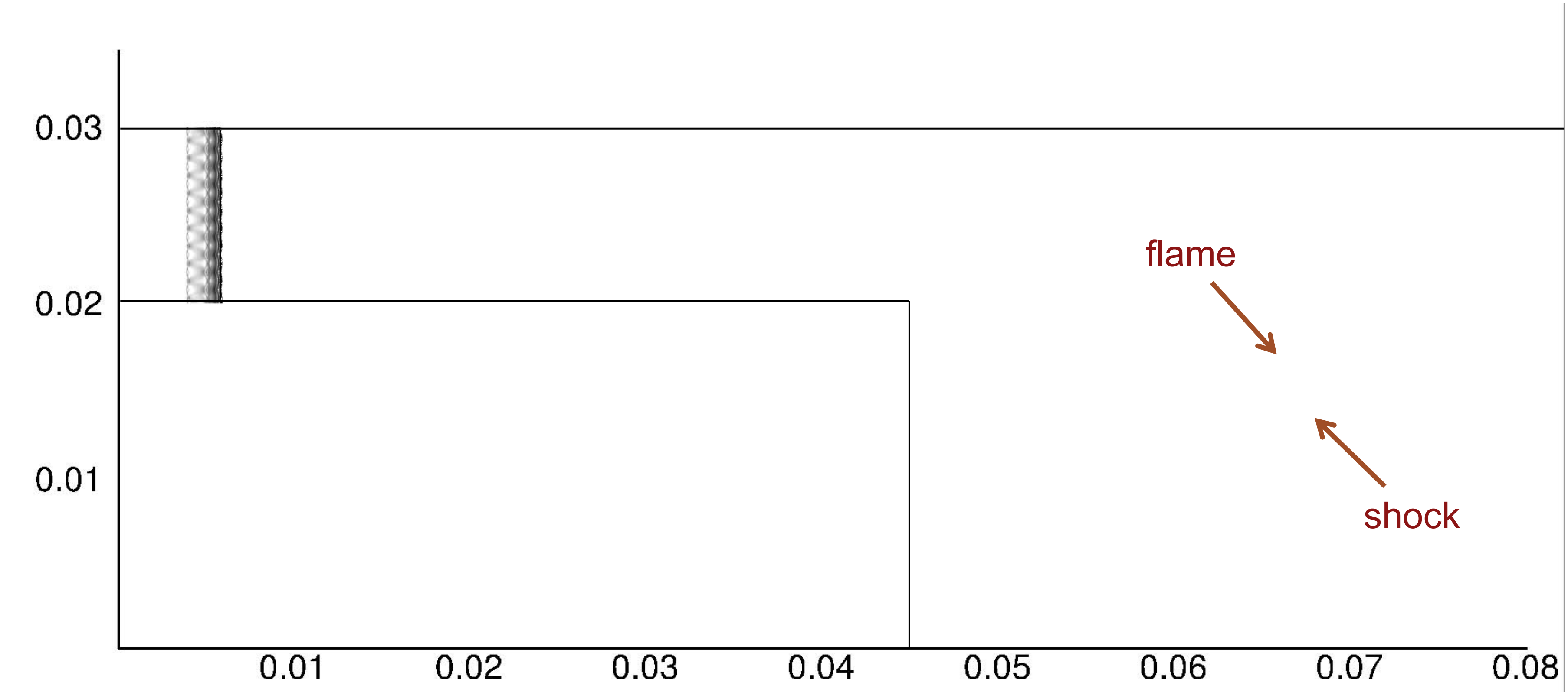
Operating condition and parameters

- mixture composition $2\mathrm{H}_2 + \mathrm{O}_2 + \beta\mathrm{Ar} + (4-\beta)\mathrm{N}_2$
- pressure: 26.7 kPa
- temperature: 293 K
- thermochemical model: 11 species / 19 elementary reactions*
- h = 1/200 reactive zone length / EBDG / shock-capturing capability

*Burke et al. *Int. J. Chem. Kinet.*, 2012.

Detonation diffraction and re-initiation

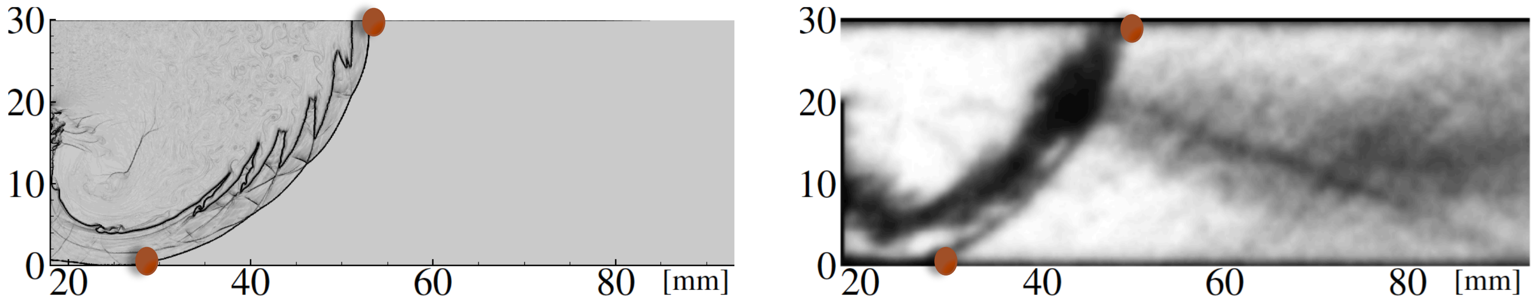
Detonation dynamics before shock-wall interaction



Numerical Schlieren image (density gradients)

Detonation diffraction and re-initiation

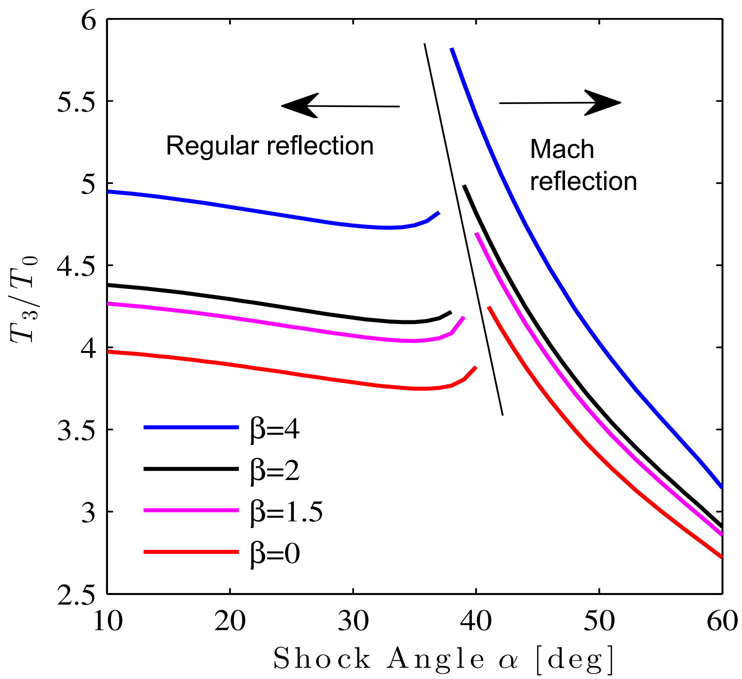
Comparison of simulation to measurement*

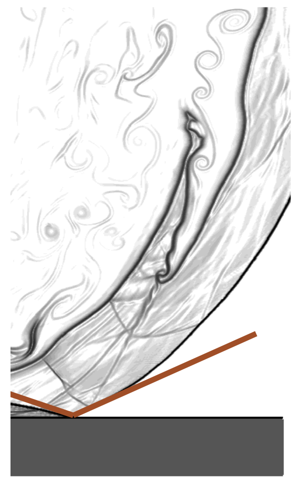


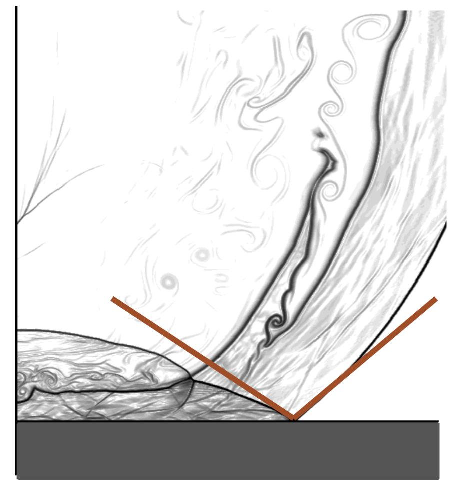
*Ohyagi, et al., Shock Waves, 2002.

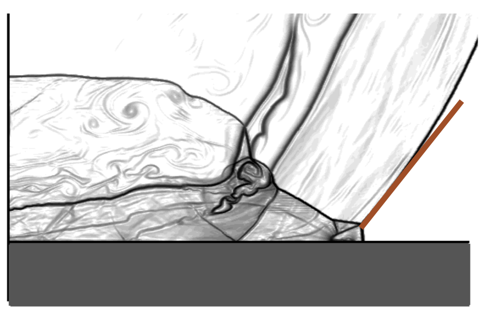
Re-initiation through shock-wall interactions

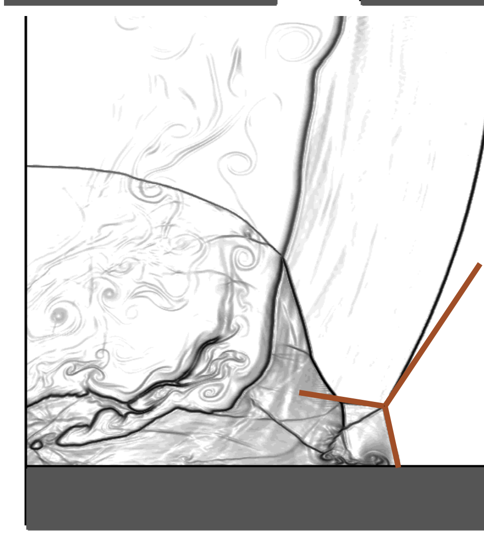
Dynamics of shock-wall interaction (case with $2\mathrm{H}_2 + \mathrm{O}_2 + 4\mathrm{N}_2/\beta = 0$)





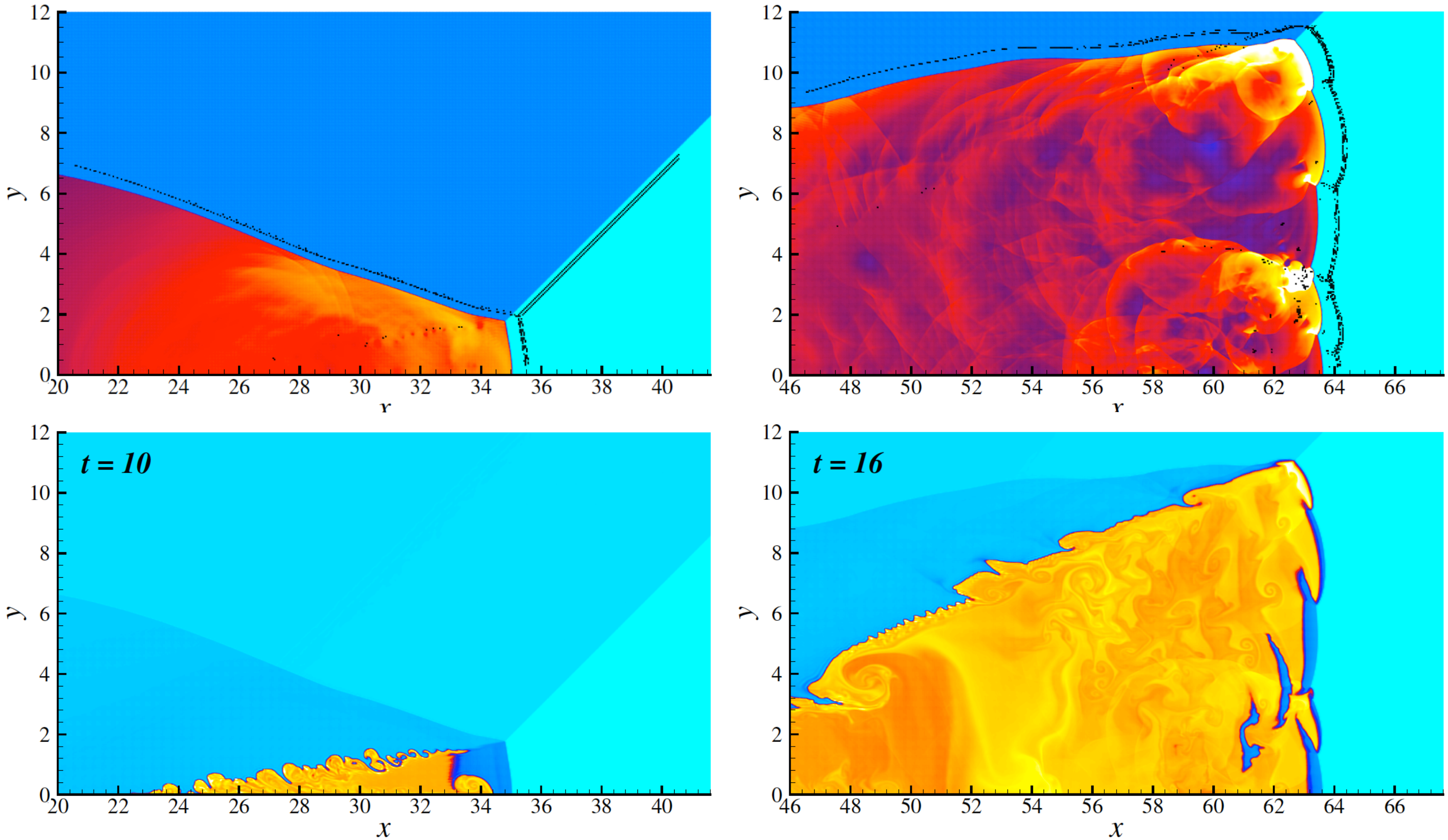




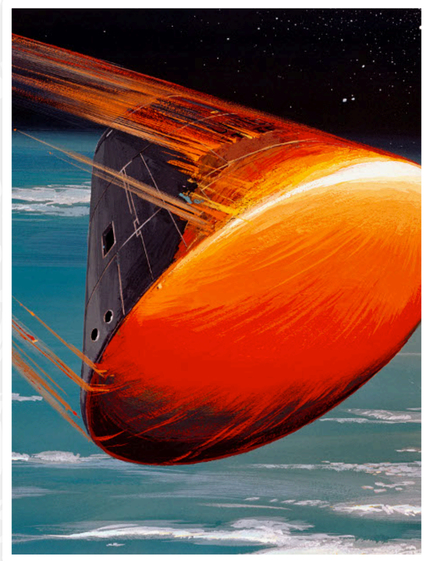


Re-initiation through shock-wall interactions

Modeled mixture and one-step simplified chemistry

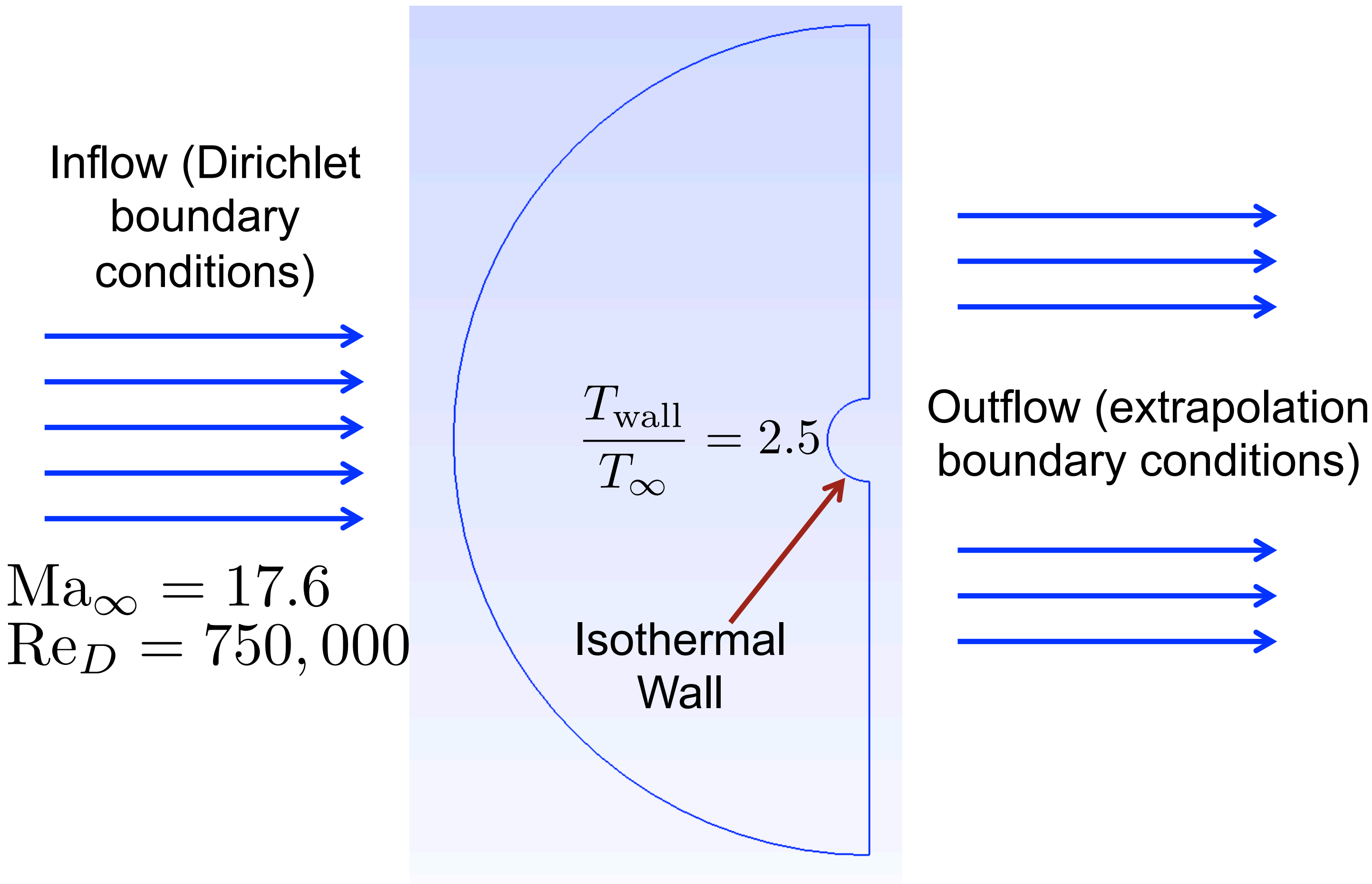


Artificial-viscosity method for steady-flow predictions



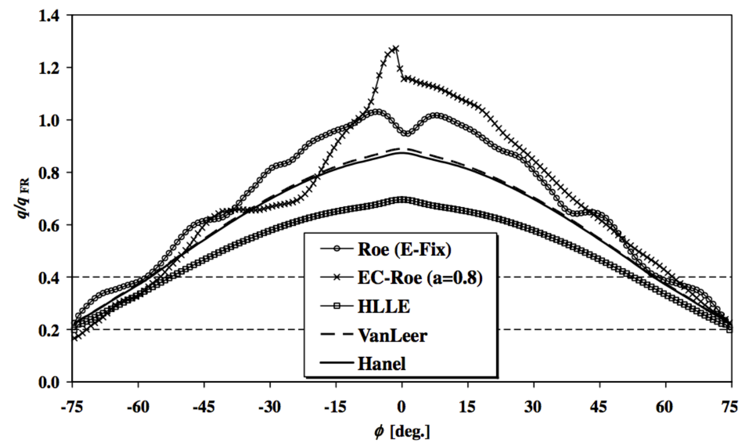
Target flow configuration

Quantity of interest: surface heating rate of hypersonic blunt body



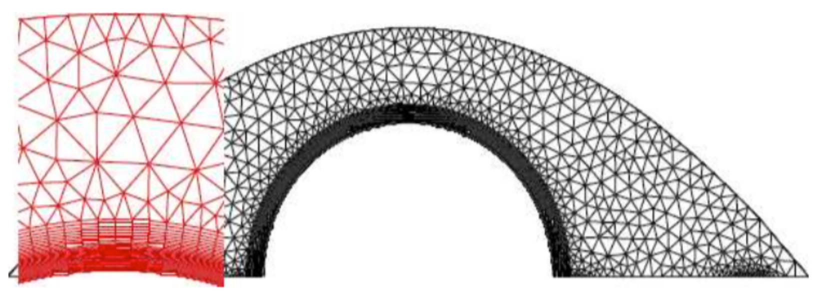
Comparison to studies using FV schemes

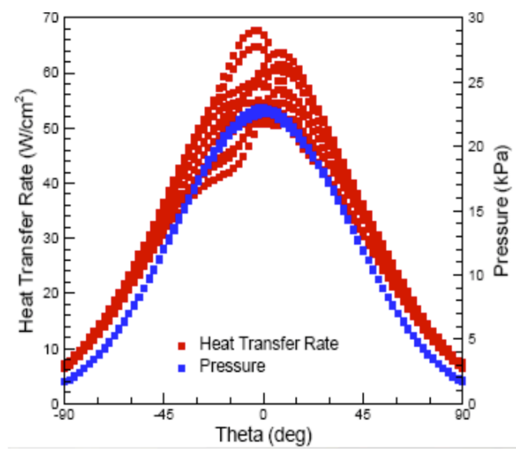
- FV schemes exhibit strong sensitivity to flux-formulation, limiter and choice of reconstruction approaches.



- FV schemes show stronger sensitivity to mesh topologies.

Randomly oriented tetrahedra



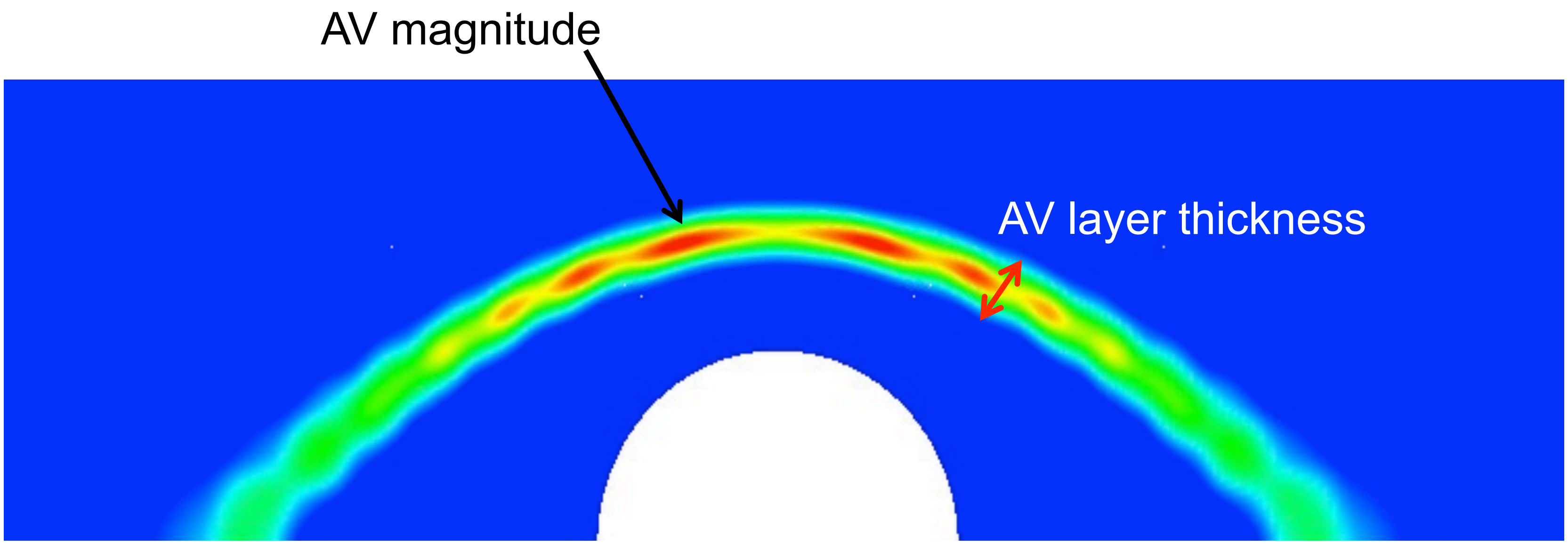


[1] Candler et al., 2009;
[2] Kitamura et al., 2010;
[3] Nompelis et al., 2004.

Design of AV formulation

- Requirements: (1) stability; (2) zero-residual solutions; (3) accuracy

- Parameterization of AV fields:



- Observations:

  Insufficient AV → violation of (1) and (2)

  Excessive AV → violation of (3)

Generation of AV field

STEP I: assign a piecewise constant AV field

$$\mu_{AV}^{0} = C\frac{h(x)}{p}f(S_e)$$

STEP II: smoothen the AV field using a differential filter

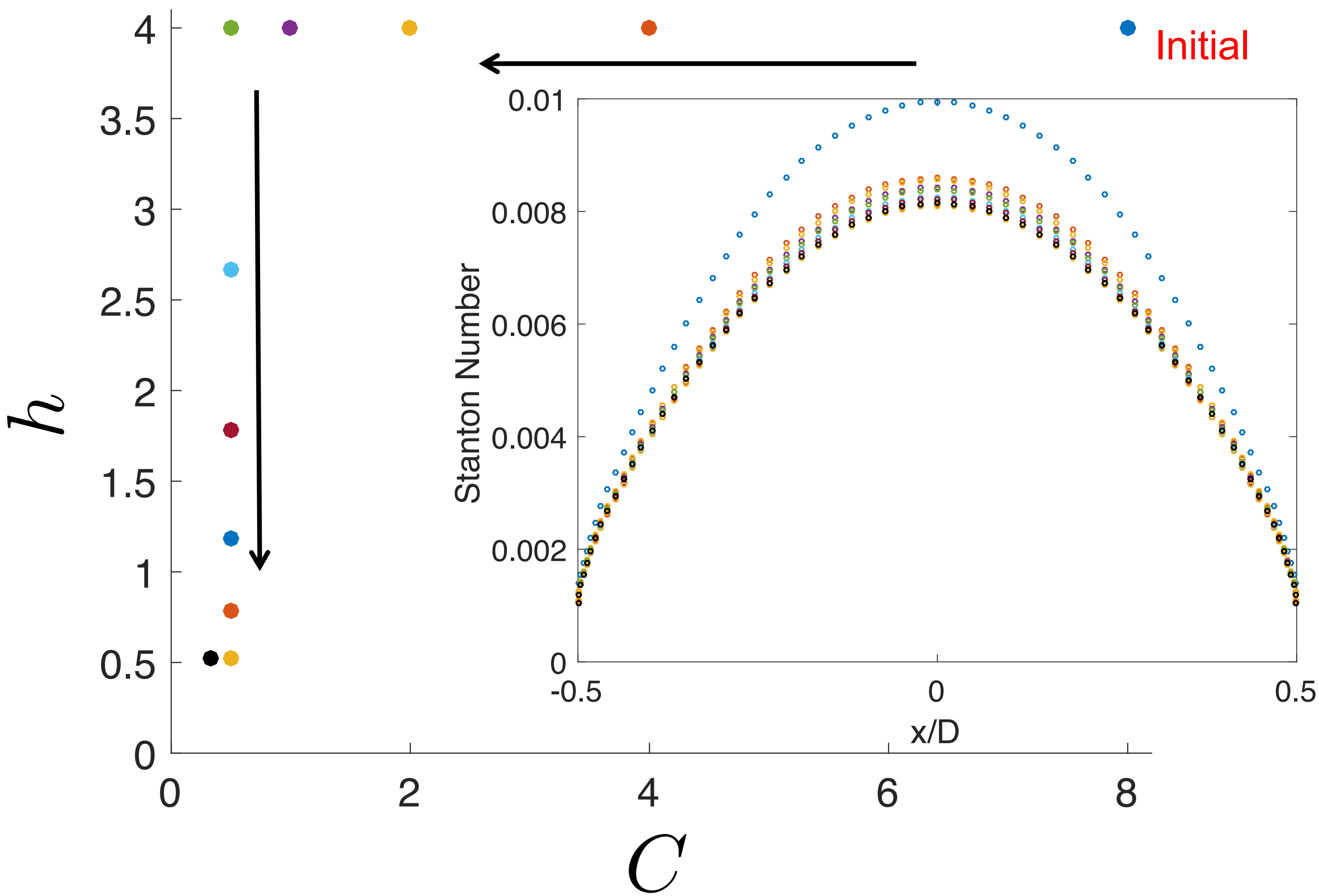
$$\mu_{AV}^{0} = \mu_{AV} - h^2\nabla^2\mu_{AV}^{0}$$

Critical parameters:

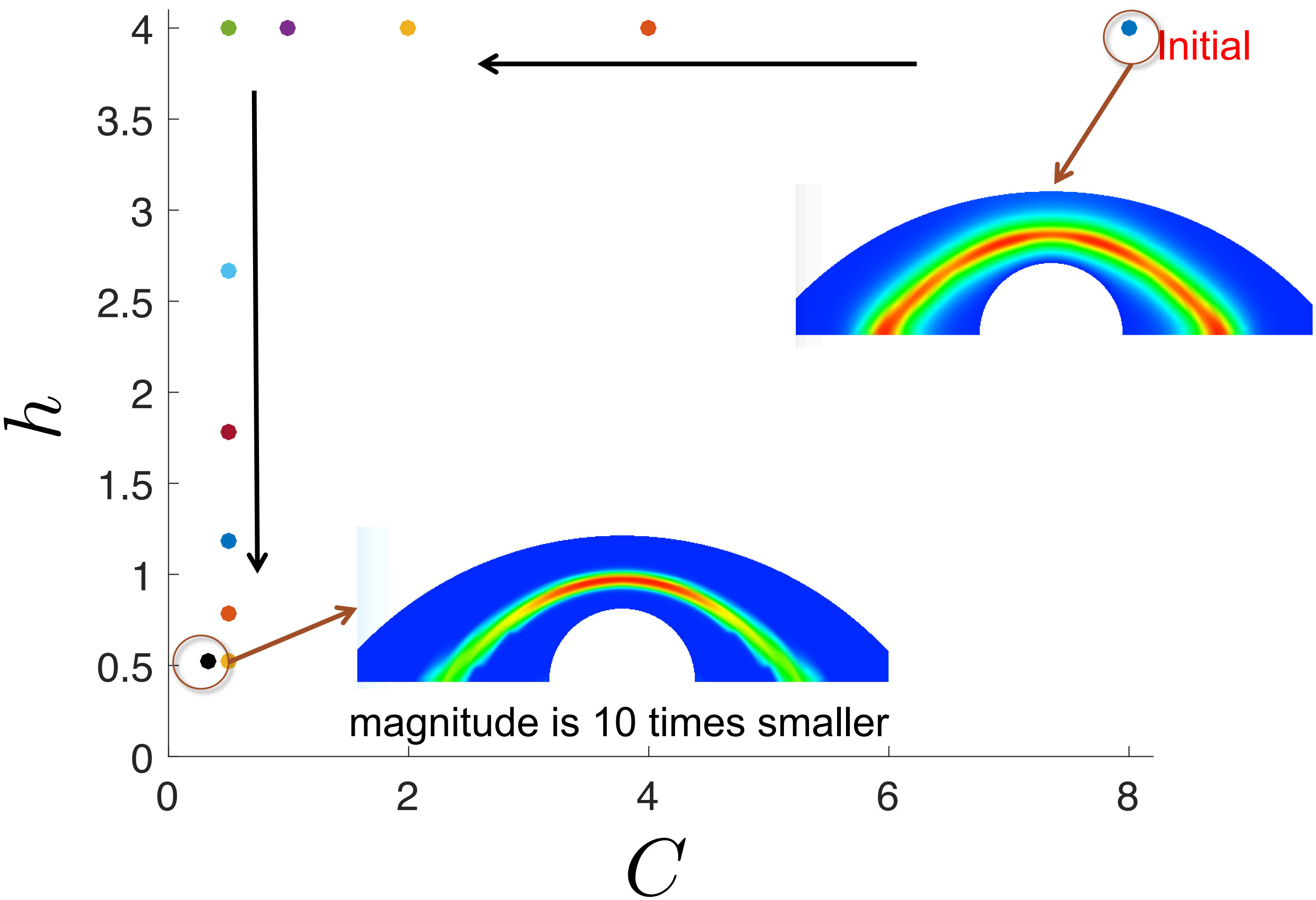
C determines AV magnitude

h determines AV-layer thickness

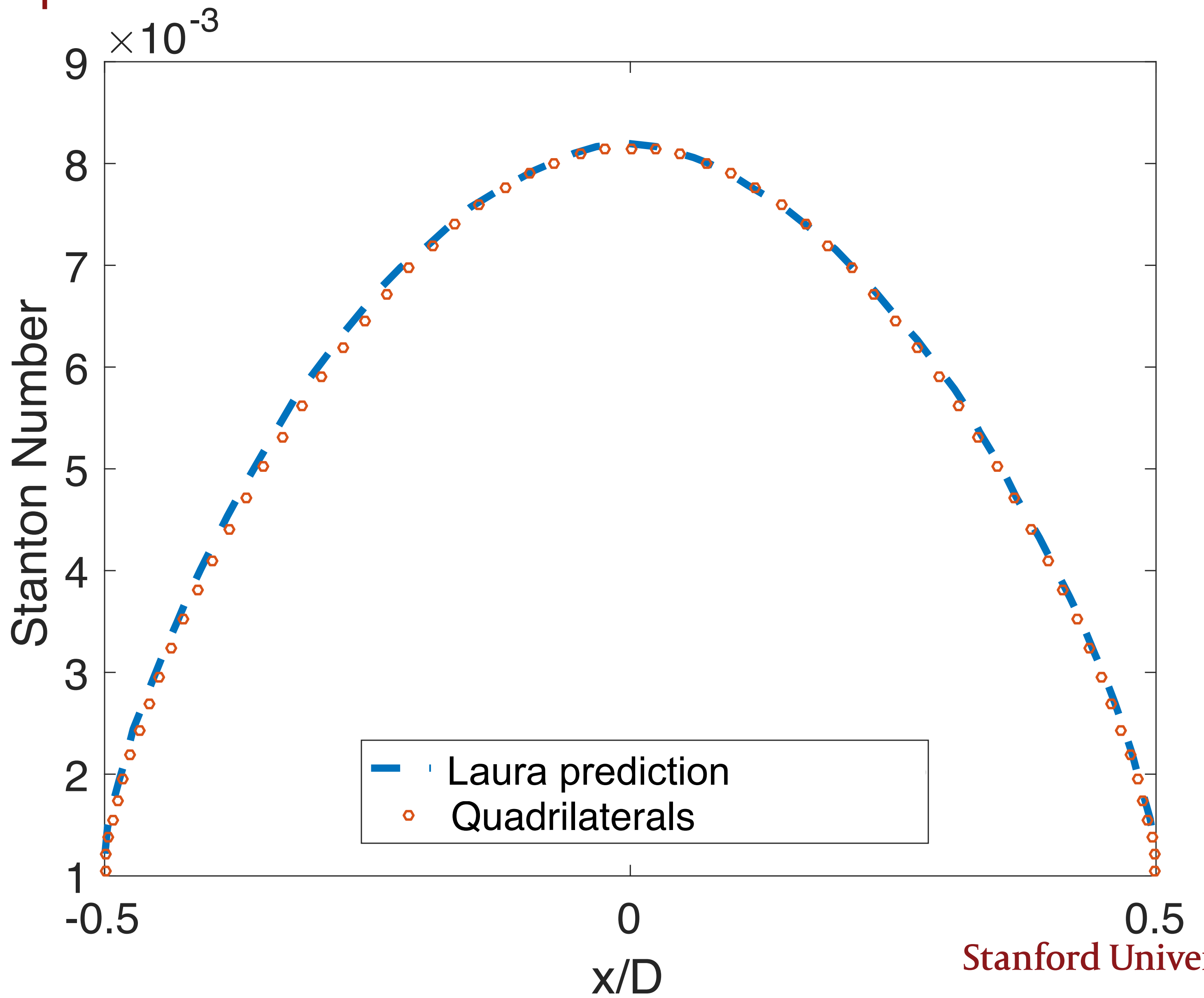
The optimal AV field



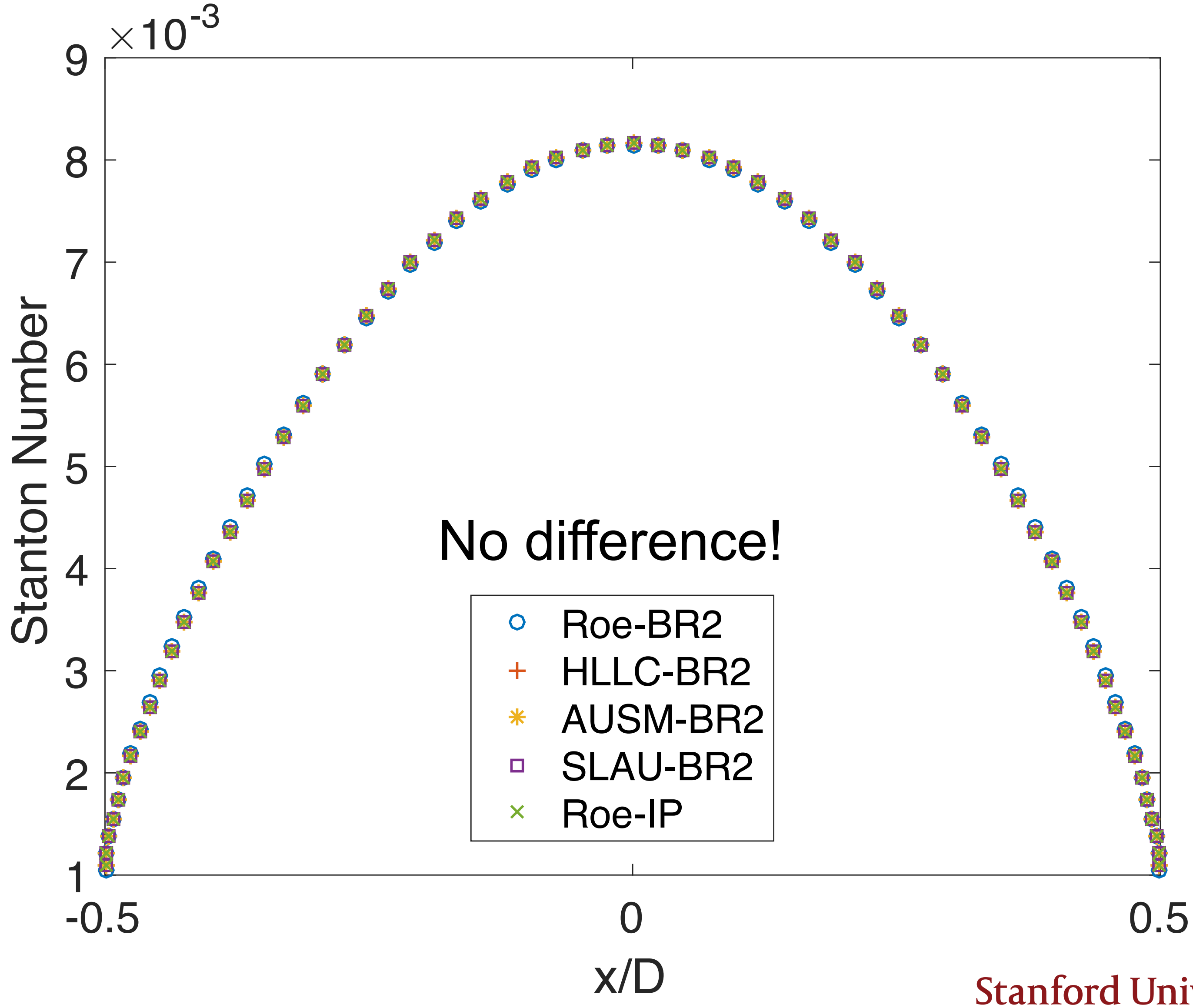
Generation of AV field using an optimization process



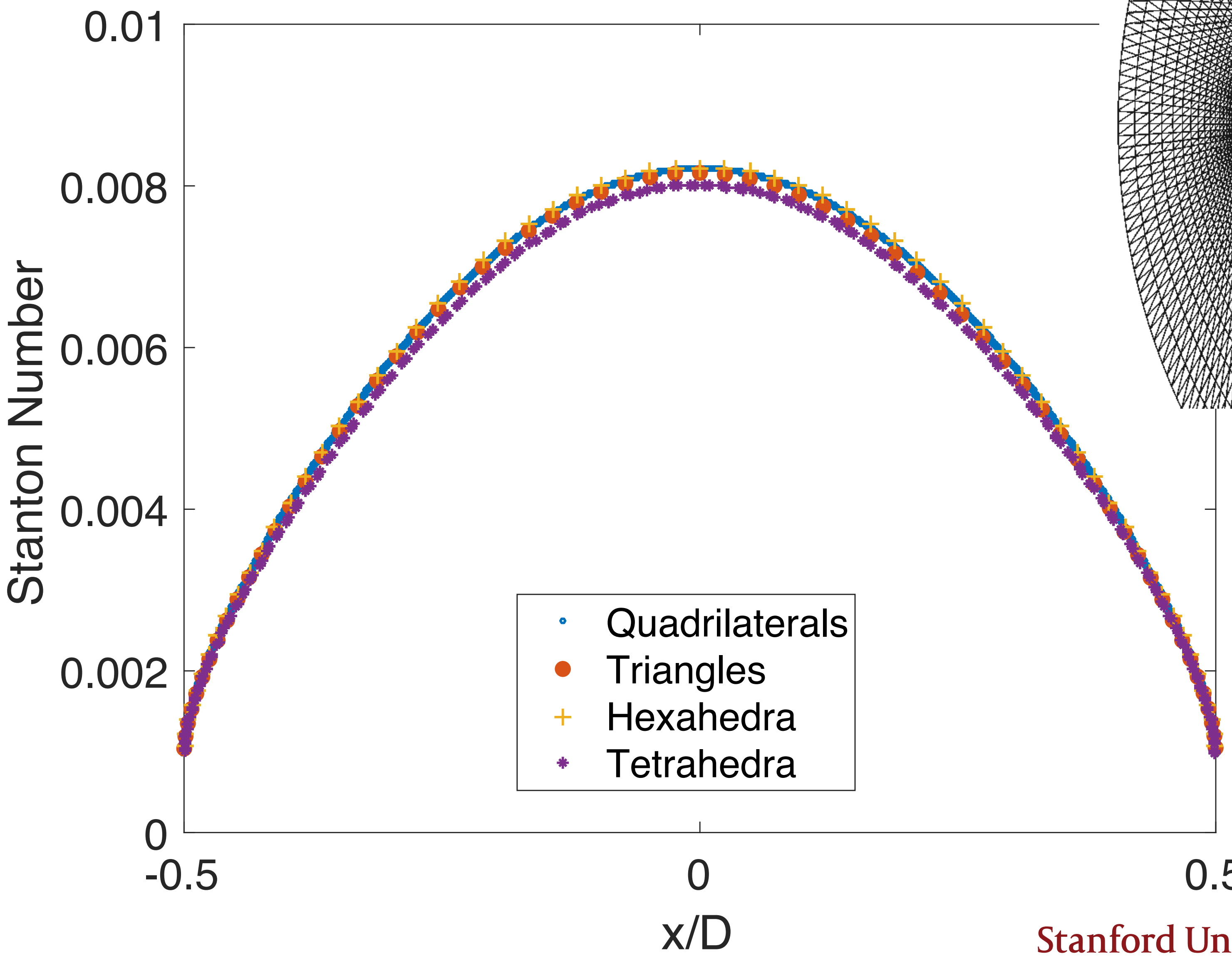
Comparison with reference data

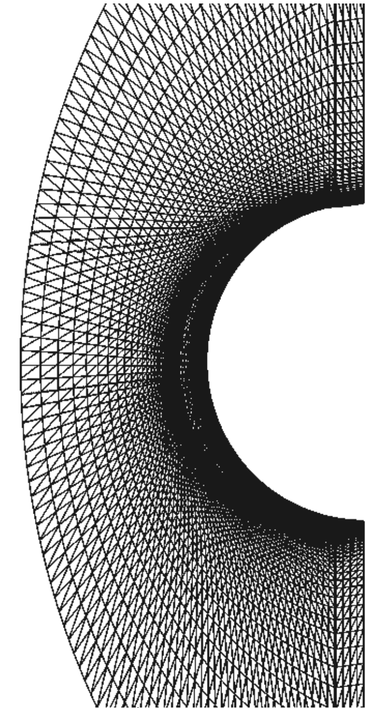


Dependence on discretization of inviscid/viscous fluxes



Dependence on mesh topologies





Conclusions and Outlook

- Entropy-bounded DG scheme is developed to support the studies of shock-containing flow problems in a variety of configurations.
- Convergence of entropy residual is analyzed in the context of DG scheme; entropy-residual shock detector is developed to exactly localize shock fronts and facilitate the application of artificial-viscosity.
- AV formulation for explicit time-integration is developed, which shows good performance in canonical test cases and applications to detonation problems.
- AV formulation for implicit steady flow problems is developed and shows good performance in the prediction of hypersonic surface heating.

In future, the developed shock-capturing capability for high-order DG scheme will be applied to flows involving more complex physics, such as hypersonic flows with radiation and ionization.

Thank you!

QUESTION?