Shock-Capturing Methods for High-Order Discontinuous Galerkin Schemes

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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

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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:
  \[ U_e(t, x) = \sum_{i=1}^{N_p} \tilde{U}_{e,i}(t) \phi_{e,i}(x), \quad x \in \Omega_e \]

- Strengths of DG scheme:
  1. High-order accuracy
  2. Compactness
  3. Energy stability
  4. Adaptation
  5. High-order geometry representation
Nonlinear instability of DG scheme
Entropy-bounded DG scheme (EBDG)
Flow models

Compressible Navier-Stokes equations:

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho u) &= 0 \\
\partial_t (\rho u) + \nabla \cdot (\rho u \otimes u + p I) &= \nabla \cdot \tau \\
\partial_t (\rho e) + \nabla \cdot (u(\rho e + p)) &= \nabla \cdot (u \cdot \tau - q)
\end{align*}
\]

\[
\partial_t U + \nabla \cdot F = \nabla \cdot Q
\]

Law of entropy:

- Entropy residual \( R = \partial_t U + \nabla \cdot F \leq 0 \) is true for any convex function \( U \) with respect to \( U \).
- Common choice of \( U \):
  \[
  U = -\rho s \quad s = \log(p \rho^{-\gamma})
  \]
- 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

Entropy stable flux (Riemann solver)

Entropy boundedness of quadrature-point solutions

\[ s(\overline{U}_e(t + \Delta t)) \geq s_0 \]

\[ U_e \rightarrow^\mathcal{L} U_e \]
\[ \mathcal{L}U_e(x_q) \geq s_0 \]

Functioning mechanism of EBDG scheme

- Solution constraining implemented using a scaling operator:
  Find
  \[ \mathcal{L} U_e = U_e + \varepsilon (\bar{U}_e - U_e) \]
  such that
  \[ s(\mathcal{L} U_e(x_q)) \geq s_0 \]
  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:
  \[ p(\mathcal{L} U_e) \geq (1 - \varepsilon)p(U_e) + \varepsilon p(\bar{U}_e) \]  
  \[ (1 - \varepsilon)\rho^\gamma(U_e) + \varepsilon \rho^\gamma(\bar{U}_e) \geq \rho^\gamma(\mathcal{L} U_e) \]

- Find \( \varepsilon \) by setting
  \[ (1) \geq (2) \times \exp(s_0) \]

# Zhang & Shu, JCP, 2010-2011.
Functioning mechanism of EBDG scheme

Entropy stable flux (Riemann solver)

Entropy boundedness of quadrature-point solutions

\[ s(\overline{U}_e(t + \Delta t)) \geq s_0 \]

Sufficient condition

\[ U_e \rightarrow^L U_e \]
\[ ^L U_e(x_q) \geq s_0 \]

Elimination of failure modes using EBDG

Demonstration of solution constraining $U_e \rightarrow L U_e$ with a Mach-20 moving shock
Elimination of failure modes using EBDG

“Vanilla” version DG

Entropy-bounded DG

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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: \( R = \partial_t U + \nabla \cdot F \)

- Interpretation: 
  1. \( R = 0 \) : smooth solution
  2. \( R < 0 \) : discontinuous solution

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

- Convergence property of entropy-residual for smooth solution*
  \[
  |R_{U}(U_e)| \leq bh^r, \quad r = \min \left\{ p - \frac{\text{dim}}{2}, 1 \right\}
  \]

- 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 $|\mathcal{R}_U(U_e)|$

- Troubled-cell detection criterion:
  $$|\mathcal{R}_U(U_e)| > \varepsilon$$

- How to set $\varepsilon$?
  For smooth solutions, no effect when $h$ is sufficiently small.

- Local and dynamic estimate for $\varepsilon$

  $$|\mathcal{R}_U| \sim \frac{1}{|\Omega_e|} \int_{\Omega_e} \frac{\partial(\rho u s)}{\partial x_1} dx ,$$
  $$\sim \frac{1}{h_e} (\bar{\rho}^* \bar{u}^* \bar{s}^* - \bar{\rho} \bar{u} \bar{s}) ,$$
  $$\sim \frac{\bar{s}}{h_e} (\bar{\rho}^* \bar{u}^* - \bar{\rho} \bar{u}) ,$$
  $$\sim \frac{\bar{s} \bar{\rho} v_s}{h_e} \left( \frac{\bar{\rho}^*}{\bar{\rho}} - 1 \right) ,$$
  $$\sim \frac{1}{h_e} \left( |\bar{u}| + \bar{c} \sqrt{\frac{\gamma - 1}{2\gamma} + \frac{\gamma + 1}{2\gamma} \bar{p}^*} \right) \frac{2}{\gamma - 1} \left( \frac{\bar{p}^*}{\bar{\rho}} - 1 \right) \bar{s} \bar{\rho} .$$

  Assume that entropy flux mostly varies along $x_1$
  
  Approximate sub-cell using neighbors' information
  
  Entropy variation is a third-order term
  
  Introduce $v_s$ as shock velocity

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Effect of threshold setting on detector performance

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

* Jiang & Shu, JCP, 1996.

Figure 9: EBDGP4 solution of shock-vortex interaction (color contours: pressure with 41 levels between 0.84 and 1.44; black regions in background represent troubled cells. troubled cells are primarily identified around the incident shock, the Mach shock and the transverse shock, which are connected through the triple point, and the elongated bow-shock. A zoom of the density profile around the triple point is also given in figures (c, f, i). It can be observed that the high-order approximation improves the resolution in predicting the Kelvin-Helmholtz instabilities along the slip-line and wall-jet. We also note that some small oscillations are not fully removed in this case, which might be due to the simplified AV specification on triangular elements. To substantiate this point, we also solve this problem on a regular mesh with rectangular elements with sizes $h = 1/100$ and $h = 1/200$. The density profiles and trouble-cell distributions are shown in Fig. 11, from which we can see that the shock detector performs equally well. As shown in Fig. 12, sharp wave fronts and fine hydrodynamic structures are nicely captured around the triple point. In addition to that, the small oscillations that are shown in figures (c, f, i) do not appear on rectangular elements. This observation indicates that for triangular elements more sophisticated AV-specification at the sub-cell might be required, and this issue is subject of further investigation.

9. Conclusions

An entropy-residual approach was proposed for shock detection with application to DG and high-order schemes. The entropy residual was introduced in a fully discretized setting and was numerically analyzed. It was shown that for smooth solutions, the detection function converges to zero. This property guarantees the deactivation of imposing shock stabilization for smooth solutions, after the required resolution is achieved such that the entropy residual stays below a given threshold. In spite of the effectiveness of the entropy residual in numerically determining under-resolved flow features, the robust application also relies on a
Numerical test – Shu-Osher problem

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

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: \( \mu_0 \) is locally added to only one cell of the domain

- Eigen-spectrum:

![Graph showing eigen-spectrum with annotations for 'Only advection' and 'With viscosity']

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

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Eigenvalue magnitude scaling

- Approximate the behavior of $\Re(\lambda)_{\text{min}}$
  $$\Re(\lambda)_{\text{min}} \approx \Re(\lambda^{AV})_{\text{min}} + \Re(\lambda^{adv})_{\text{min}}$$
Determination of AV magnitude

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

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

The range of $\beta$ 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 $\mu_0 = (\beta - 1) \frac{C_1(p)}{C_2(p)} ah$

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

Numerical test – Sod shock-tube problem

Refinement study:

EBDGP3

EBDGP4

$- h = 1/50$

$- h = 1/100$

$- h = 1/200$

8.3. Shu-Osher problem

This test aims at examining the performance of the shock-capturing scheme in the presence of high-frequency density waves. The setup was originally proposed by Shu and Osher [25]. The initial conditions are defined as:

$((ρ, u, p)^T = (3.8571, 2.6294, 10.3333)^T$ for $x \leq 0.125,$

$(1.0+0.2 \sin(50x), 0.0, 1.0)^T$ for $x > 0.125,$

$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(34)$

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Numerical test – Shu-Osher problem

Refinement study:

(a) Grid refinement study for EBDGP2

(b) Grid refinement study for EBDGP3

(c) Grid refinement study for EBDGP4

(d) AV performance (EBDGP4 and $h = 1/100$)

Figure 2: Simulation results of the Sod shock tube (Symbols in (d) indicate where artificial viscosity is applied).

8.3. Shu-Osher problem

This test aims at examining the performance of the shock-capturing scheme in the presence of high-frequency density waves. The setup was originally proposed by Shu and Osher [25]. The initial conditions are defined as:

$$(\rho, u, p)_T = \left(\frac{3}{5}, \frac{2}{5}, 10 \right)_T$$

for $x \leq 0.125$,

$$(1.0 + 0.2 \sin(50 \pi x), 0, 1.0)$$

for $x > 0.125$.

(34)

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Numerical test – double Mach reflection

Double Mach reflections: Mach 10 shock impinges on a wall with 60°

Simulation setting:
1) EBDGP4
2) $h = 1/200$
3) Entropy-residual shock indicator
4) Artificial viscosity
Numerical test – double Mach reflection

Predictions by EBDG

EBDG + entropy-residual detector + artificial viscosity
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

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*

Re-initiation through shock-wall interactions

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

![Graph showing shock angle and temperature ratio vs. shock angle with different beta values.]

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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

Inflow (Dirichlet boundary conditions)

\[ \text{Ma}_\infty = 17.6 \]
\[ \text{Re}_D = 750,000 \]

Outflow (extrapolation boundary conditions)

\[ \frac{T_{\text{wall}}}{T_\infty} = 2.5 \]

Isothermal Wall
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;
Design of AV formulation

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

- Parameterization of AV fields:

  AV magnitude

  AV layer thickness

- 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

\[ \mu^0_{AV} = C \frac{h(x)}{p} f(S_e) \]

STEP II: smoothen the AV field using a differential filter

\[ \mu^0_{AV} = \mu_{AV} - h^2 \nabla^2 \mu^0_{AV} \]

Critical parameters:

\[ C \] determines AV magnitude

\[ h \] determines AV-layer thickness
The optimal AV field

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Generation of AV field using an optimization process

The magnitude of the field is 10 times smaller.
Dependence on discretization of inviscid/viscous fluxes

No difference!

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Dependence on mesh topologies

![Graph showing Stanton Number versus x/D for different mesh topologies: Quadrilaterals, Triangles, Hexahedra, and Tetrahedra. The graph illustrates the performance of different mesh types with varying Stanton Numbers and x/D.]
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?