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Isolating Flow-field Discontinuities while Preserving Monotonicity and High-order Accuracy on Cartesian Meshes

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Introduction

- Filtering schemes offer a less dissipative alternative to the standard artificial dissipation operators when applied to high-order spatial/temporal schemes

  **Limiting Fact:** Filters impart the same amount of dissipation each time they are applied so if they are applied too frequently, they are overly dissipative

  **Limiting Fact:** Stiff systems require a preconditioned dual-time framework to be solved efficiently

  **Limiting Fact:** Filtering cannot be applied only at the physical-time level and convergence guaranteed

  **Limiting Fact:** Filtering cannot be straightforwardly applied at the pseudo-time level

**Objective:** To recast common filtering operators as equivalent artificial-dissipation schemes
Governing Equations

- **Navier-Stokes Equations:**
  \[
  \frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H
  \]
  \[
  Q = [\rho \quad \rho u_i \quad \rho e_0]^T
  \]
  \[
  F_i = [\rho u_i \quad \rho u_i u_j + p\delta_{ij} \quad u_i \rho h_0]^T \text{ where } h_0 = e_0 + \frac{p}{\rho}
  \]

- **Quasi-linear Form:**
  \[
  \frac{\partial Q}{\partial t} + A \frac{\partial Q}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H
  \]
  \[
  A = \frac{\partial F_i}{\partial Q} = \mathbf{M}A\mathbf{M}^{-1}
  \]
  \[
  \Lambda = \text{diag}\{u_i + c, u_i, u_i - c\}
  \]

- **Primitive Variables Form:**
  \[
  \Gamma_e \frac{\partial Q_p}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H \Rightarrow \Gamma_e \frac{\partial Q_p}{\partial t} + \Lambda \Gamma_e \frac{\partial Q_p}{\partial x_i} = \frac{\partial V_i}{\partial x_i} + H
  \]
  where \(\Gamma_e = \frac{\partial Q}{\partial Q_p}\) and \(Q_p = [p \quad u_i \quad T]^T\)
Governing Equations

- **Residual Form:**

\[
\begin{align*}
\frac{\partial Q}{\partial t} + R_s(Q) &= \frac{\partial Q_p}{\partial t} + \Gamma_e^{-1} R_s(Q_p) = 0 \quad \text{where} \quad R_s = \frac{\partial F_i}{\partial x_i} - \frac{\partial V_i}{\partial x_i} - H
\end{align*}
\]

- **Temporal Discretizations:**

  - **SSPRK(3, 3):**

\[
\begin{align*}
Q^{(1)} &= Q^n - \Delta t R_s(Q^n) \\
Q^{(2)} &= \frac{3}{4} Q^n + \frac{1}{4} \left( Q^{(1)} - \Delta t R_s(Q^{(1)}) \right) \\
Q^n + 1 &= \frac{1}{3} Q^n + \frac{2}{3} \left( Q^{(2)} - \Delta t R_s(Q^{(2)}) \right)
\end{align*}
\]

  - **SSPRK(4, 3):**

\[
\begin{align*}
Q^{(1)} &= Q^n - \frac{1}{2} \Delta t R_s(Q^n) \\
Q^{(2)} &= Q^{(1)} - \frac{1}{2} \Delta t R_s(Q^{(1)}) \\
Q^{(3)} &= \frac{2}{3} Q^n + \frac{1}{3} \left( Q^{(2)} - \frac{1}{2} \Delta t R_s(Q^{(2)}) \right) \\
Q^n + 1 &= Q^{(3)} - \frac{1}{2} \Delta t R_s(Q^{(3)})
\end{align*}
\]

\[Q_p^{(1)} = Q_p^n - \Delta t R_{s,p}(Q_p^n)\]

\[Q_p^{(2)} = \frac{3}{4} Q_p^n + \frac{1}{4} \left( Q_p^{(1)} - \Delta t R_{s,p}(Q_p^{(1)}) \right)\]

\[Q_p^{n+1} = \frac{1}{3} Q_p^n + \frac{2}{3} \left( Q_p^{(2)} - \Delta t R_{s,p}(Q_p^{(2)}) \right)\]

where \(R_{s,p}(Q_p^{(l)}) = \Gamma_e^{-1,(l)} R_s(Q_p^{(l)})\)
Spatial Discretizations

- Discretely-conservative High-order Upwind using Roe’s Approximate Riemann Solver:

\[
\frac{\partial F_{i,j}}{\partial x_i} = \frac{F_{i,j+1/2} - F_{i,j-1/2}}{\Delta x_i}
\]

where \( F_{i,j±1/2} = F_{LR} = f(Q_L, Q_R) \)

For instance, the standard second-order central difference can be found using:

\[
F_{+1/2} = \frac{F(Q_{+1}) + F(Q_0)}{2} \quad \text{and} \quad F_{-1/2} = \frac{F(Q_0) + F(Q_{-1})}{2}
\]

- High-order Interface States:

\[
v_{L,+1/2} = \frac{-v_{-1} + 5v_0 + 2v_1}{6}
\]

\[
v_{R,+1/2} = \frac{-v_{+2} + 5v_{+1} + 2v_0}{6}
\]

\[
v_{L,+1/2} = \frac{2v_{-2} - 13v_{-1} + 47v_0 + 27v_{+1} - 3v_{+2}}{60}
\]

\[
v_{L,+1/2} = \frac{-3v_{-3} + 25v_{-2} - 101v_{-1} + 319v_0 + 214v_{+1} - 38v_{+2} + 4v_{+3}}{420}
\]

\[
v_{L,+1/2} = \frac{4v_{-4} - 41v_{-3} + 199v_{-2} - 641v_{-1} + 1879v_0 + 1375v_{+1} - 305v_{+2} + 55v_{+3} - 5v_{+4}}{2520}
\]
Limiter: Monotonicity-preserving Method

- Limits the left and right interface quantities such that they are within an interval that is guaranteed to preserve monotonicity with an appropriate CFL number
- Uses a five-point stencil to distinguish between local extrema and discontinuities

Further details are in the paper.
Limited Quantities

• Either the conserved, the primitive, or the characteristic variables can be limited by the MP scheme

• Local characteristic limiting can be carried out as follows:

For $Q_{L,+1/2}$, the stencil consists of the set $\{Q_{-2}, Q_{-1}, Q_0, Q_{+1}, Q_{+2}\}$.

$$W_k = M_0^{-1}Q_k \quad \text{for} \quad k = -2, 2$$

$$W_{L,+1/2} = M_0^{-1}Q_{L,+1/2}$$

$$Q_{L,+1/2,\text{lim}} = M_0W_{L,+1/2,\text{lim}}$$

or

$$W_k = N_0^{-1}Q_{p,k} \quad \text{for} \quad k = -2, 2$$

$$W_{L,+1/2} = N_0^{-1}Q_{p,L,+1/2}$$

where $N_0^{-1} = M_0^{-1}\Gamma_e$. It is important to note that this necessarily implies that the same $\Gamma_e$ matrix (calculated at the midpoint of the set) resident in $N_0^{-1}$ is used for all five points in the limiting stencil.
Sod’s Shock Tube Problem

- Domain 20 m long
- 100 points
- Discontinuity initially at $x = 10$ m
- Run for 50 time steps

$$\Delta t = 0.0002s$$
$$\sigma = 0.374$$
$$t_f = 0.01s$$

$\rho_L = 1.000, \rho_R = 0.125$
$u_L = 0.0, u_R = 0.0$
$p_L = 1000000, p_R = 10000$
Lax’s Problem

- Domain 20 m long
- 100 points
- Discontinuity initially at \(x = 10\) m
- Run for 160 time steps

\[
\Delta t = 0.0002s \\
\sigma = 0.403 \\
t_f = 0.032s
\]

\[
\rho_L = 0.890, \rho_R = 1.000 \\
\rho_L = 69.8, \rho_R = 0.0 \\
\rho_L = 70560, \rho_R = 11420
\]
1D Contact Discontinuity Problem

- Domain 20 m long
- 100 points
- Discontinuities initially at $x = 5$ m and $x = 15$ m
- Run for 16,000 time steps

$$\Delta t = 6.25 \times 10^{-5} \text{s}$$
$$\sigma = 0.370$$
$$t_f = 1.00 \text{s}$$

$$\rho_L = 1000, \rho_R = 1.00$$
$$u_L = 20.0, u_R = 20.0$$
$$p_L = 1000000, p_R = 1000000$$
1D Contact Discontinuity Problem

(a) Characteristics from Conserved

Temperature vs. X for different values of $\alpha$:
- (a) $\alpha = 4$
- (b) $\alpha = 7$
- (c) $\alpha = 11$
- (d) $\alpha = 19$

(b) Characteristics from Primitive
2D Drop Problem

- Domain 1 mm square
- 100 points square
- Cold Fluid inside the drop
- Run for 25,000 time steps

\[ \Delta t = 4.0 \times 10^{-9} \text{s} \]
\[ \sigma \approx 0.4 \]
\[ t_f = 1.0 \times 10^{-4} \text{s} \]
\[ \rho_L = 15, \rho_R = 1258 \]
\[ u_L = 10.0, u_R = 10.0 \]
\[ \rho_L = 1 \times 10^7, \rho_R = 1 \times 10^7 \]

\[ Q = Q_R F + Q_L (1 - F) \]

\[ F = \frac{1}{2} \left[ 1 - \tanh \left( \frac{r - r_d}{\Delta_d} \right) \right] \]

\[ r_d = 0.2 mm \text{ and } \Delta_d = 0.015 mm \]
2D Drop Problem, Centerline T

(a) Characteristics from Conserved

(a) $\alpha = 19$

(a) Characteristics from Conserved, 2× Resolution

(b) Characteristics from Primitive

(b) $\alpha = 19$, Ninth-order

(b) Characteristics from Primitive, 2× Resolution

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2D Rotating Detonation Wave

- Unwrapped cylinder
- Follows the work of Schwer (reference in paper)
- Stoichiometric H$_2$/Air
  - $p_{\text{plenum}} = 10$ ATM
  - $T_{\text{plenum}} = 300K$
Conclusions

- Applying existing high-order monotonicity-preserving methods to the primitive variables is not straightforward.
- The MP scheme should be applied to the characteristic variables calculated from the conserved variables for the best results.
- These results will offer unique results for more-complicated equations of state (EoS) where temperature and pressure cannot be calculated from density and internal energy directly.
Future Work

• Use a detection strategy to limit the frequency with which the limiter and, with it, the conversion from conserved to primitive via the EoS is applied
  – Interpolate primitive variables
  – Detect where limiting might be needed
  – Only where needed, calculate characteristic variables from conserved variables
  – Note specifically where the MP limiter is active
  – Convert back to primitive variables only where the limiter is active
  – Use the first-order accurate value for the initial guess of temperature and pressure in the EoS routine

• In this way, efficiency and accuracy can be optimized
Questions???