High-Order Conservative Asymptotic-Preserving Schemes for Modeling Rarefied Gas Dynamical Flows with Boltzmann-BGK Equation

Min-Hung Chen[1], Manuel A. Diaz[2,3], Jaw-Yen Yang[2]

[1]Department of Mechanics
National Cheng Kung University
Tainan, Taiwan

[2]Institute of Applied Mechanics
National Taiwan University
Taipei, Taiwan

[3]National Health Research Institutes
Miaoli, Taiwan

International Conference on Flow Physics and its Simulation
In memory of Prof. Jaw-Yen Yang
Dec. 5 2016

Outline I

The Work of Prof JY Yang in Numerical Simulation of Boltzmann Equation

- Yang and Huang (JCP 1995): Discrete Ordinate Methods (**DOM**), **ENO**
- Yang, Huang and Tsuei (Proc. R. Soc. A 1995): (**DOM**), **ENO**
- Yang and Huang (AIAA 1996): DOM, **ENO**
- Yang, Chen, Tsai and Chang (JCP 1997): **Beam Scheme**, **Relativistic Gas Dynamics**
- Yang and Shi (Proc R Soc A 2006): **Beam Scheme**, **Ideal Quantum Gas**
- Yang, Hsieh and Shi (SIAM JSC 2007): **Flux Vector Splitting Scheme**, **Ideal Quantum Gas**
- Shi, Huang and Yang (JCP 2007): Beam Scheme (Generalized Coordinates), Ideal Quantum Gas
- Yang, Hsieh, Shi and Xu (JCP 2007): **High Order** Flux Vector Splitting Scheme, Ideal Quantum Gas
- Shi and Yang (JCP 2008): semiclassical Boltzmann
- Yang, Hung and Kuo (CICP 2011): Semiclassical **Lattics Boltzmann**
- Mulgadi and Yang (Proc R Soc A 2012): Semiclassical Boltzmann-BGK
- Tsai, Huang, Tsai and Yang (Phys. Rev. E 2012): Unsteady **relativistic** shock wave diffraction.
- Yang, Yan, Diaz, Huang, Li and Zhang (Proc R Soc A 2013): **Ideal Quantum Gas**, **Semiclassical Ellipsodial Statistic**
- Huang, Hsieh and Yang (JCP 2015): **Conservative** DOM, Semiclassical Boltzmann-BGK
- Diaz, Chen and Yang (CICP 2015): Boltzmann-BGK, **Flux Reconstruction (FR/CPR)**

Outline

Governing Equation

Boltzmann-BGK model equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = -\frac{f - \mathcal{M}[f]}{\tau},$$

where $f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t) \geq 0$ is a single-component density distribution in momentum space.

- The momentum space is extended by $\boldsymbol{\xi}$ to account for the δ-internal DoF,
- $\tau(\boldsymbol{x}, t)$ is the relaxation time that depends on the local macrocopic properties of the gas and the Knudsen number.[1]
- $\mathcal{M}[f](\boldsymbol{v}, \boldsymbol{\xi})$ is the local Maxwellian distribution [Xu 2001]

$$\mathcal{M}[f](\boldsymbol{v}, \boldsymbol{\xi}) = \frac{\rho}{m(2\pi\,\theta(\boldsymbol{x}))^{(D+\delta)/2}} \exp\left(-\frac{|\boldsymbol{v} - \mathbf{u}(\boldsymbol{x})|^2 + |\boldsymbol{\xi}|^2}{2\theta(\boldsymbol{x})}\right),$$

- m is the gas particle mass and ρ is the local density, $\mathbf{u}$ is the local macroscopic velocity,
- θ is a local quantity related to the local temperature T, defined as either $\theta = R_{gas}T$, where R_{gas} is the gas constant, or $\theta = k_B T/m$ where k_B is the Boltzmann constant.
- $(D + \delta) > 0$ denotes the total number of DoF.

[1] Phys.Rev.94:511-525(1954)

The local macroscopic quantities of the gas

The local macroscopic quantities such as density ρ, macroscopic velocity u, pressure tensor P, internal energy e, and heat flux Q for a $(D+\delta)$-dimensional momentum domain are defined as

$$
\begin{cases}
\rho(\boldsymbol{x}, t) = m \int d\boldsymbol{v} d\boldsymbol{\xi}\, f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t), \\
\mathbf{u}(\boldsymbol{x}, t) = \dfrac{m}{\rho(\boldsymbol{x}, t)} \int d\boldsymbol{v} d\boldsymbol{\xi}\, \boldsymbol{v}\, f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t), \\
P_{i,j}(\boldsymbol{x}, t) = m \int d\boldsymbol{v} d\boldsymbol{\xi}\, c_i c_j\, f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t), \\
e(\boldsymbol{x}, t) = \dfrac{m}{\rho(\boldsymbol{x}, t)} \int d\boldsymbol{v} d\boldsymbol{\xi} \dfrac{c^2 + \xi^2}{2} f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t) = \dfrac{D+\delta}{2} \theta(\boldsymbol{x}, t), \\
Q_i(\boldsymbol{x}, t) = m \int d\boldsymbol{v} d\boldsymbol{\xi} \dfrac{c^2 + \xi^2}{2}\, \boldsymbol{c}\, f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t),
\end{cases}
$$

where $\boldsymbol{c} = \boldsymbol{v} - \mathbf{u}$ is the peculiar velocity.

Properties of the collision operators

- The BGK relaxation term conserves mass, momentum and Energy, namely

$$-\frac{m}{\tau}\int (f-\mathcal{M}[f])\phi(\boldsymbol{v},\boldsymbol{\xi})d\boldsymbol{v}d\boldsymbol{\xi}=0, \quad \text{where } \phi(\boldsymbol{v},\boldsymbol{\xi})=\left\{1,\boldsymbol{v},\frac{v^2+\xi^2}{2}\right\}^\top,$$

- The BGK relaxation term satisfy Boltzmann H-Theorem, e.i., the production of entropy S is always positive,

$$S=-\frac{1}{\tau}\int (f-\mathcal{M}[f])\log f\, d\boldsymbol{v}d\boldsymbol{\xi}\geq 0,$$

- If f is in the continuum limit, BBGK model reduces to the closed system of Euler equations.

Outline

Literature Review

- Discretization of the velocity space
  - Discrete Velocity Methods/Discrete Ordinate Method: Chu (1965); Yang and Huang (1995)
  - Kinetic Beam Scheme: Sanders and Prendergast (1974); Yang et. al. (1997)
  - Lattice Boltzmann Methods: Mc Namara and Zanetti (1988); Higuera and Jimenez (1989)
- Discretization of the spatial space:discontinuous polynomial solution space
  - Spectral Volume Methods: Wang (2002)
  - Spectral Difference Methods: Liu et. al. (2004)
  - Discontinuous Galerkin (DG) Methods: Reed and Hill (1973); Cockburn & Shu (1989),
  - Nodal Discontinuous Galerkin (NDG) Methods: Hesthaven & Warburton (2002),
  - Correction Procedure via Reconstruction (CPR) Methods:Hyunh(2007) and Wang & Gao(2009).
- High-order DG-type method for the BGK equation
  - Ren, X., Xu, K., Shyy, W., Gu, C.. A multi-dimensional high-order discontinuous Galerkin method based on gas kinetic theory for viscous flow computations (JCP 2015)
  - Xiong, Jang, Li, and Qiu, High order asymptotic preserving nodal discontinuous Galerkin IMEX schemes for the BGK equation (JCP 2015)
  - Diaz, Chen and Yang, High-Order Conservative Asymptotic-Preserving Schemes for Modeling Rarefied Gas Dynamical Flows with Boltzmann-BGK Equation (CICP 2015)

Boltzmann-BGK model equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = -\frac{f - \mathcal{M}[f]}{\tau},$$

where $f(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{\xi}, t) \geq 0$ is a single-component density distribution in momentum space.

To remove functional dependency on the velocity space in the Boltzmann-BGK equation, the discrete ordinate method is usually introduced (Yang and Huang 1995).

Discrete Ordinate Method (DOM)

$$\frac{\partial f_\sigma}{\partial t} + \frac{\partial}{\partial x} \upsilon_\sigma f_\sigma = -\frac{f_\sigma - \mathcal{M}_\sigma[f_\sigma]}{\tau_\sigma}, \quad \text{and } \sigma = 1, \cdots, N_\upsilon \tag{1}$$

where $f_\sigma = f(x, \upsilon_\sigma, \boldsymbol{\xi}_\sigma, t)$, by setting σ as global index for the discrete velocities in our system, and N_υ is the total number of discrete velocities.
The vector of conserved properties is approximated by a suitable quadrature method as

$$[\rho, \rho\, u, \rho\, e]^\intercal = \int d\upsilon d\boldsymbol{\xi}\, \phi(\upsilon, \boldsymbol{\xi}) f(x, \upsilon, \boldsymbol{\xi}, t), \approx \sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\upsilon_\sigma, \boldsymbol{\xi}_\sigma) f_\sigma .$$

where $\phi(\boldsymbol{v}, \boldsymbol{\xi}) = \left[1, \boldsymbol{v}, \frac{\upsilon^2 + \xi^2}{2}\right]^\top$

Discrete Ordinate Method (DOM)

$$[\rho, \rho\, u, \rho\, e]^\intercal = \int d\upsilon d\boldsymbol{\xi}\, \phi(\upsilon, \boldsymbol{\xi}) f(x, \upsilon, \boldsymbol{\xi}, t), \approx \sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\upsilon_\sigma, \boldsymbol{\xi}_\sigma) f_\sigma .$$

where $\phi(\boldsymbol{\upsilon}, \boldsymbol{\xi}) = \left[1, \boldsymbol{\upsilon}, \frac{\upsilon^2+\xi^2}{2}\right]^\top$

Notice that the moment equation above requires $(D+\delta)$ fold integrals over the momentum space. For instance, let us consider a one-dimensional $(D=1)$ mono-atomic gas $(D+\delta=3)$, so that the quadrature approximation takes the form

$$\sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\upsilon_\sigma, \boldsymbol{\xi}_\sigma) f_\sigma = \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} \sum_{\gamma=1}^{n} W_\alpha W_\beta W_\gamma \phi(\{\upsilon_\alpha, \xi_\beta, \xi_\gamma\}) f_{\alpha,\beta,\gamma}, \tag{2}$$

where subindices α, β and γ refer to discrete velocities in Cartesian directions. In this notation $W_\sigma = W_\alpha W_\beta W_\gamma$ and discrete velocities $(\upsilon_\sigma, \boldsymbol{\xi}_\sigma) = (\upsilon_\alpha, \xi_\beta, \xi_\gamma)$, are designed with index σ using the relation $\sigma = \alpha + n\,(\beta-1) + n^2\,(\gamma-1)$.

Note: We can consider Gauss-Hermite quadrature rules or any quadrature rules on a bounded domain $\Omega_\upsilon = [-\upsilon_c, \upsilon_c] \times [-\xi_c, \xi_c]^2$

Modification: Impose Conservation of the BGK collision term (CDOM)

However, Mieussens in (JCP 2000) pointed out,

$$\int \phi(\boldsymbol{\upsilon},\boldsymbol{\xi})(\mathcal{M}[f](\boldsymbol{\upsilon},\boldsymbol{\xi}) - f)d\boldsymbol{\upsilon}d\boldsymbol{\xi} \approx \sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\boldsymbol{\upsilon}_\sigma,\boldsymbol{\xi}_\sigma)(\mathcal{M}[f_\sigma] - f_\sigma) \neq 0,$$

We then need to enforce the conservation property numerically in our scheme as

$$\sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\boldsymbol{\upsilon}_\sigma,\boldsymbol{\xi}_\sigma)(\mathcal{M}[f_\sigma] - f_\sigma) = 0,$$

so that the Maxwellian and solution of $f^{(j)}$ in every stage of the AP formulation have the same macroscopic moments. As in Huang (2011), by performing such correction on the local Maxwellian, the numerical quadrature will be termed conservative DOM or simply CDOM.

Conservative Discrete Ordinate Method(CDOM)

We follow the method in Mieussens (2000) and introduce an alternative formulation for the Maxwellian distributions as

$$\mathcal{M}[f](\boldsymbol{\upsilon},\boldsymbol{\xi}) = \mathcal{M}(\alpha,\phi(\boldsymbol{\upsilon},\boldsymbol{\xi})) = \exp\left(\alpha\cdot\phi(\boldsymbol{\upsilon},\boldsymbol{\xi})\right)$$

where α is a vector that depends on the local macroscopic properties $\rho(x,t)$, $u_i(x,t)$ and $\theta(x,t)$, considering 1-D mono-atomic gas, it is defined by

$$\alpha = (\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5)^T = (\log\left(\frac{\rho}{(2\pi\theta)^{(1+2)/2}}\right) - \frac{u_1^2+\xi_2^2+\xi_3^2}{2\theta}, \frac{u_1}{\theta}, \frac{u_2}{\theta}, \frac{u_3}{\theta}, -\frac{1}{\theta})^T.$$

The discrete version of the conservation can be written as

$$\sum_{\sigma=1}^{N_\upsilon} W_\sigma \phi(\boldsymbol{\upsilon}_\sigma)(\mathcal{M}_\sigma(\alpha,\phi(\boldsymbol{\upsilon},\boldsymbol{\xi})) - f_\sigma) = 0. \quad (3)$$

This is a discrete system of three equations that has to be solved for the α_i values that fulfill the equality. This approximate system can be expressed in the following form,

$$F(\alpha) = 0,$$

and can be solved by a Newton nonlinear solver.

IMEX-RK scheme

Let us exemplify a 1st-order scheme by considering a single σ-equation,

$$\partial_t f + \partial_x F = -\frac{f - \mathcal{M}[f]}{\tau}, \quad t \geq 0 \text{ and } x \in \mathbb{R}, \upsilon \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^{\delta},$$

where F represents the product $\upsilon \cdot f$. In this work, we explore a 3rd and 4th-order Additive Runge-Kutta (ARK) schemes following the work of Kennedy & Carpenter (Appl.Num.Math. 44(12):139-181,2003). So that an IMEX-RK / ARK formulation reads

IMEX-RK scheme

For every stages $i = 1, \ldots, \nu$

$$f^{(i)} = f^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \partial_x F^{(j)} + \Delta t \sum_{j=1}^{i} a_{ij} \frac{1}{\tau^{(j)}} (\mathcal{M}[f^{(j)}] - f^{(j)}),$$

and the final stages is given by

$$f^{n+1} = f^n - \Delta t \sum_{j=1}^{\nu} \tilde{b}_i \partial_x F^{(j)} + \Delta t \sum_{j=1}^{\nu} b_i \frac{1}{\tau^{(j)}} (\mathcal{M}[f^{(j)}] - f^{(j)}),$$

Asymptotic-Preserving (AP) discretization

Following the work of Jin (1999) and Pieraccini and Puppo (2007), we consider

$$\frac{f^{(n+1)} - f^{(n)}}{\Delta t} = -\partial_x F^{(n)} + \frac{1}{\tau^{(n+1)}} \left(\mathcal{M}[f^{(n+1)}] - f^{(n+1)} \right).$$

or

$$f^{(n+1)} = (f^{(n)} - \Delta t\, \partial_x F^{(n)}) + \frac{\Delta t}{\tau^{(n+1)}} \left(\mathcal{M}[f^{(n+1)}] - f^{(n+1)} \right)$$

However note that $\tau \to 0$, $f \to \mathcal{M}[f]$.,

$$\begin{aligned} \int_{\infty}^{\infty} \phi(\upsilon) f^{(n+1)} d\upsilon &= \int_{\infty}^{\infty} \phi(\upsilon)(f^{(n)} - \Delta t\, \partial_x F(U^{(n)}))d\upsilon \\ &+ \frac{\Delta t}{\tau^{(n+1)}} \int_{\infty}^{\infty} \phi(\upsilon)(\mathcal{M}[f^{(n+1)}](\upsilon) - f^{(n+1)})d\upsilon \end{aligned} \tag{4}$$

yields

$$\begin{bmatrix} \rho^{(n+1)} \\ (\rho\, u)^{(n+1)} \\ (\rho\, e)^{(n+1)} \end{bmatrix} = \int_{\infty}^{\infty} \phi(\upsilon)(f^{(n)} - \Delta t\, \partial_x F(f^{(n)}))d\upsilon,$$

so that we can find

$$\mathcal{M}[U^{(n+1)}](\upsilon)$$

Discontinuous Galerkin Methods

Here again we start by considering a single equation of our system, namely

$$\partial_t u + \partial_x f(u) = s(u), \quad x \in \Omega \in [a, b], \tag{5}$$

We expect that discontinuities may appear in the solution of this equation, therefore, we choose to modify our equation to use a dissipative model following Persson & Peraire(AIAA,2006),

$$\partial_t u + \partial_x f(u) = s(u) + \partial_x(\epsilon\, \partial_x u), \quad x \in \Omega \in [a, b], \tag{6}$$

where ϵ is a parameter that controls the amount of viscosity and will be introduced later. Therefore we consider a first order system,

$$\begin{cases} \partial_t u + \partial_x f - s = \epsilon\, \partial_x q, \\ q = \partial_x u. \end{cases} \tag{7}$$

and apply the discontinuous Galerkin methods,

- Discontinuous Galerkin (DG): Cockburn & Shu (1989),
- Nodal Discontinuous Galerkin (NDG): Hesthaven & Warburton (2002),
- Correction Procedure via Reconstruction (CPR):Hyunh(2007) and Wang & Gao(2009).

Approximate solutions and the Standard Element

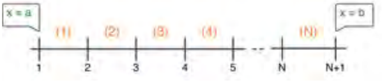


Figure: Domain Discretization

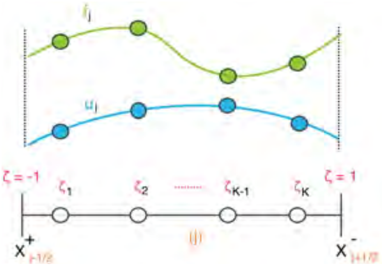


Figure: DG & CPR elements

let u_h, f_h and q_h be linear approximations that belong to a polynomial space defined as $V^h = \oplus_{i=1}^{K} \{\psi_j^i\}_{j=1}^{N}$, where ψ_j^i represents a polynomial basis function spanned in Ω. The global solutions are approximated as piecewise p-th order polynomial approximation of the form

$$u_h^i(\xi, t) = \sum_{l=1}^{p} u_l^i(t)\, \psi_l(\xi) \qquad (8)$$

Where $\xi \in [-1, 1]$ is a local variable set on very elements interval. With the knowledge of the element's size and center, a mapping between our local and global variables is given by

$$x_{i,j} = x_i + \frac{\Delta x_i}{2}\xi_j. \qquad (9)$$

Here we consider three approximations for our local solution polynomials for $\xi \in I$,

$$u^i(\xi,t) \approx u_h^i(\xi,t) = \underbrace{\sum_{l=0}^{p} u_l^{M,i}(t) P_l(\xi)}_{\text{modal expansion}} = \underbrace{\sum_{l=0}^{p} \tilde{u}_l^i(t)\mathcal{P}_l(\xi),}_{\text{normalized modal expansion}} = \underbrace{\sum_{j=1}^{N_p} u^i(\xi_j,t)\mathcal{L}_j(\xi)}_{\text{nodal expansion}} \tag{10}$$

where $P_l(\xi)$ are the Legendre Polynomials defined by,

$$P_0(\xi) = 1, \qquad P_n(\xi) = \frac{1}{2^n n!}\frac{d^n(\xi^2-1)^n}{d\xi^n}, \qquad n = 1,\dots,p, \tag{11}$$

$\mathcal{P}_l(\xi)$ the normalized Legendre polynomials and $\mathcal{L}_l(\xi)$ are Lagrange polynomials, also termed shapes function (as finite element methods), defined by

$$\mathcal{L}_n(\xi) = \prod_{j=1,\ j\neq n}^{p} \frac{\xi-\xi_j}{\xi_n-\xi_j}, \quad n = 1,\dots,N_p. \tag{12}$$

Discontinuous Galerkin Methods

Consider the first order system

$$\begin{cases} \partial_t u + \partial_x f - s = \epsilon \, \partial_x q, \\ q = \partial_x u. \end{cases}$$

Multiplying the system by test functions ϕ_h^i, $\psi_h^i$and derive the weak form,

$$\int_{-1}^{1} \partial_t u_h^i \phi_h^i - f_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i - s_h^i \phi_h^i + \epsilon^i \, q_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i \, d\xi = - \frac{2}{\Delta x_i} \left(f^* \phi_h^i + \epsilon^i \, q^* \phi_h^i \right)_{-1}^{1}$$

$$\int_{-1}^{1} q_h^i \psi_h^i - u_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i \, d\xi = - \frac{2}{\Delta x_i} \left(u^* \psi_h^i \right)_{-1}^{1}$$

Replacing f^*, q^*, u^* by numerical fluxes $\hat{f}$, $\hat{q}$, $\hat{u}$ and we get

$$\int_{-1}^{1} \partial_t u_h^i \phi_h^i - f_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i - s_h^i \phi_h^i + \epsilon^i \, q_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i \, d\xi = - \frac{2}{\Delta x_i} \left(\hat{f} \phi_h^i + \epsilon^i \, \hat{q} \phi_h^i \right)_{-1}^{1}$$
$$\int_{-1}^{1} q_h^i \psi_h^i - u_h^i \frac{2}{\Delta x_i} \partial_\xi \psi_h^i \, d\xi = - \frac{2}{\Delta x_i} \left(\hat{u} \psi_h^i \right)_{-1}^{1} \tag{13}$$

The numerical fluxes $\hat{f}$, $\hat{q}$, $\hat{u}$ are chosen so that the scheme is stable.

DG formulation:

$$\int_{-1}^{1} \partial_t u_h^i \phi_h^i - f_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i - s_h^i \phi_h^i + \epsilon^i \, q_h^i \frac{2}{\Delta x_i} \partial_\xi \phi_h^i \, d\xi = -\frac{2}{\Delta x_i} \left(\hat{f} \phi_h^i + \epsilon^i \, \hat{q} \phi_h^i \right)_{-1}^{1}$$

$$\int_{-1}^{1} q_h^i \psi_h^i - u_h^i \frac{2}{\Delta x_i} \partial_\xi \psi_h^i \, d\xi = -\frac{2}{\Delta x_i} \left(\hat{u} \psi_h^i \right)_{-1}^{1}$$

Substitute the u_h^i, f_h^i, s_h^i and q_h^i by their modal expansions and get,

$$\begin{aligned} M_{l,m} \frac{d}{dt} u^i - \frac{2}{\Delta x_i} S_{l,m} (f^i + \epsilon^i q^i) - M_{l,m} s^i &= -\frac{2}{\Delta x_i} \left(f_{LF}^i P_m + \epsilon^i \, q_C^i P_m \right)_{-1}^{1} \\ M_{l,m} q_l^i - \frac{2}{\Delta x_i} S_{l,m} u^i &= -\frac{2}{\Delta x_i} \left(u_C^i P_m \right)_{-1}^{1} \end{aligned} \tag{14}$$

where M and S are the mass and stiffness matrices for the standard element

$$M_{l,m} = \int_{-1}^{1} P_l(\xi) P_m(\xi) d\xi, \quad S_{l,m} = \int_{-1}^{1} P_l(\xi) \frac{dP_m(\xi)}{d\xi} d\xi.$$

We then solve the differential system (14) with ARK time-integration and Asymptotic-Preserving (AP) schemes.

Nodal DG

Integrate (13) and we get the strong formulation of our problem

$$\int_{-1}^{1}\left(\partial_t u_h^i + \frac{2}{\Delta x_i}\partial_\xi f_h^i - s_h^i - \frac{2}{\Delta x_i}\epsilon^i\,\partial_\xi q_h^i\right)\phi_h^i\,d\xi = \frac{2}{\Delta x_i}\left([f_h^i - f^*]\phi_h^i + \epsilon^i\,[q_h^i - q^*]\phi_h^i\right)_{-1}^{1},$$
$$\int_{-1}^{1}\left(q_h^i - \frac{2}{\Delta x_i}\partial_\xi u_h^i\right)\phi_h^i\,d\xi = \frac{2}{\Delta x_i}\left([u_h^i - u^*]\phi_h^i\right)_{-1}^{1}$$

and substitute u_h^i, f_h^i and q_h^i by the nodal expansion suggested in (10), then our local nodal DG formulation can be written as

$$M_{j,n}\frac{d}{dt}u_j^i + \frac{2}{\Delta x_i}S_{l,m}\left(f_j^i - \epsilon^i\,q_j^i\right) - M_{l,m}s_j^i = \frac{2}{\Delta x_i}\left([f_j^i - f_{LF}^i]\mathcal{L}_j + \epsilon\,[q_j^i - q_C^i]\mathcal{L}_j\right)_{-1}^{1},$$
$$M_{l,m}q_j^i - \frac{2}{\Delta x_i}S_{l,m}u_j^i = \frac{2}{\Delta x_i}\left([u_j^i - u_C^i]\mathcal{L}_j\right)_{-1}^{1} \tag{15}$$

where $M_{l,m}$ and $S_{l,m}$ are the mass and stiffness matrices of standard element respectively and computed as

$$M_{l,m} = (\tilde{\mathcal{V}}\tilde{\mathcal{V}}^T)^{-1} \quad \text{and} \quad S_{l,m} = MD_\xi, \tag{16}$$

where D_ξ is defined by

$$D_{\xi,(l,m)} = \left.\frac{dP_l(\xi)}{d\xi}\right|_{\xi_j}. \tag{17}$$

Similarly, let us define a flux function

$$\frac{dF_j^i}{d\xi} = [S]f_j^i + [f_{LF}^i(1) - f^i(1)]\mathcal{L}_j(1) - [f_{LF}^i(-1) - f^i(-1)]\mathcal{L}_j(-1) + \epsilon^i \left([S]q_j^i + [q_C^i(1) - q^i(1)]\mathcal{L}_j(1) - [q_C^i(-1) - q^i(-1)]\mathcal{L}_j(-1)\right), \tag{18}$$

where the q_j^i nodal information is computed before hand by

$$q_j^i = \frac{2}{\Delta x_i}\left([Dr]u_j^i + [u_C^i(1) - u^i(1)]\mathcal{L}_j(1) - [u_C^i(-1) - u^i(-1)]\mathcal{L}_j(-1)\right). \tag{19}$$

Therefore the discrete formulation of the NDG flux term is

$$\partial_x^{NDG} f_j^i = -\frac{2}{\Delta x_i}[M]^{-1}\frac{dF_j^i}{d\xi} \tag{20}$$

FR/CPR scheme

Let us consider the strong formulation of our system and rearrange the terms as,

$$\int_{-1}^{1}\partial_t u_j^i\phi\,d\xi+\frac{2}{\Delta x_i}\left([f_j^i(1)-f_{LF}^i(1)]\phi(1)-[f_j^i(-1)-f_{LF}^i(-1)]\phi(-1)+\int_{-1}^{1}\partial_\xi f_j^i\phi\,d\xi\right)+$$
$$\epsilon^i\frac{2}{\Delta x_i}\left([q_j^i(1)-q_C^i(1)]\phi(1)-[q_j^i(-1)-q_C^i(-1)]\phi(-1)+\int_{-1}^{1}\partial_\xi q_j^i\phi\,d\xi\right)=\int_{-1}^{1}s_j^i\phi\,d\xi, \tag{21a}$$

$$\int_{-1}^{1}q_j^i\phi\,d\xi=\frac{2}{\Delta x_i}\left([u_j^i(1)-u_C^i(1)]\phi(1)-[u_j^i(-1)-u_C^i(-1)]\phi(-1)+\int_{-1}^{1}\partial_\xi u_j^i\phi\,d\xi\right). \tag{21b}$$

This system can be further simplified if

$$\phi(1)=\int_{-1}^{1}g'_{RB}\phi\,d\xi \qquad \text{and} \qquad -\phi(-1)=\int_{-1}^{1}g'_{LB}\phi\,d\xi \tag{22}$$

$$\int_{-1}^{1}\partial_t u_j^i\phi\,d\xi+\frac{2}{\Delta x_i}\left(\int_{-1}^{1}([f_j^i(1)-f_{LF}^i(1)]g'_{RB}-[f_j^i(-1)-f_{LF}^i(-1)]g'_{LB}+\partial_\xi f_j^i)\phi\,d\xi\right)+$$
$$\epsilon^i\frac{2}{\Delta x_i}\left(\int_{-1}^{1}([q_j^i(1)-q_C^i(1)]g'_{RB}-[q_j^i(-1)-q_C^i(-1)]g'_{LB}+\partial_\xi q_j^i)\phi\,d\xi\right)=\int_{-1}^{1}s_j^i\phi\,d\xi,$$
$$\int_{-1}^{1}q_j^i\phi\,d\xi=\frac{2}{\Delta x_i}\left(\int_{-1}^{1}([u_j^i(1)-u_C^i(1)]g'_{RB}-[u_j^i(-1)-u_C^i(-1)]g'_{LB}+\partial_\xi u_j^i)\phi\,d\xi\right).$$

$$\phi(1) = \int_{-1}^{1} g'_{RB}\phi \, d\xi \qquad \text{and} \qquad -\phi(-1) = \int_{-1}^{1} g'_{LB}\phi \, d\xi$$

By using integration by parts on the RHS terms of the equations above we find,

$$\phi(1) = g_{RB}(1)\phi(1) - g_{RB}(-1)\phi(-1) - \int_{-1}^{1} g_{RB}\phi' \, d\xi, \tag{24}$$

$$-\phi(-1) = g_{LB}(1)\phi(1) - g_{LB}(-1)\phi(-1) - \int_{-1}^{1} g_{LB}\phi' \, d\xi, \tag{25}$$

these relations indicate that g_{RB} and g_{LB} are some functions that take the following values at the element boundaries

$$g_{RB}(1) = 1 \quad \text{and} \quad g_{RB}(-1) = 0; \qquad g_{LB}(1) = 0 \quad \text{and} \quad g_{LB}(-1) = 1;$$

and by noting the contribution of the integral term,

$$\int_{-1}^{1} g_{RB}\phi' \, d\xi = 0; \qquad \int_{-1}^{1} g_{LB}\phi' \, d\xi = 0$$

g_{RB} and g_{LB} should be orthogonal to the space span by all the test function ϕ', i.e. the left and right Radau polynomials!

By substituting (22) back into (21), we can get rid of all test functions inside our integrals. The remaining expression indicates,

$$\begin{aligned}\frac{dF^i(\xi)}{d\xi} = [f_j^i(1) - f_C^i(1)]g'_{RB}(\xi) + [f_j^i(-1) - f_C^i(-1)]g'_{LB}(\xi) + \frac{d}{d\xi}f^i(\xi) + \\ \epsilon^i\left\{[q_j^i(1) - q_C^i(1)]g'_{RB}(\xi) + [q_j^i(-1) - q_C^i(-1)]g'_{LB}(\xi) + \frac{d}{d\xi}q^i(\xi)\right\}\end{aligned} \tag{26}$$

where the function $q_i(\xi)$ is initially computed by

$$q^i(\xi) = \frac{2}{\Delta x_i}\left([u_j^i(1) - u_C^i(1)]g'_{RB}(\xi) + [u_j^i(-1) - u_C^i(-1)]g'_{LB}(\xi) + \frac{d}{d\xi}u^i(\xi)\right). \tag{27}$$

Finally, the semi-discrete formulation of the CPR system is simply,

$$\partial_x^{CPR} f_j^i = -\frac{2}{\Delta x_i}\frac{dF_j^i}{d\xi} \tag{28}$$

Discontinuity Sensor

As originally introduced in the work of Persson & Peraire (AIAA,2006), consider the solution of order p within each element as a modal basis expansion and the truncated expansion

$$u = \sum_{i=1}^{p+1} u_i \psi_i, \qquad \hat{u} = \sum_{i=1}^{p} u_i \psi_i. \tag{29}$$

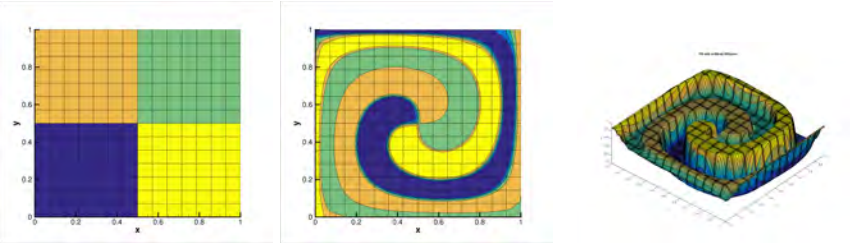
Within each element E_i the following smoothness indicator is defined,

$$s_i = \log_{10}\left(\frac{(u-\hat{u})_i \cdot (u-\hat{u})_i}{(u \cdot u)_i}\right) \tag{30}$$

Once the shock has been sensed, the amount of viscosity is taken to be constant over each element and determined by following smooth function,

$$\epsilon^i = \begin{cases} 0 & \text{if } s_i < s_0 - k \\ \frac{\epsilon_0}{2}\left(1 + \sin\frac{\pi(s_i - s_0)}{2k}\right) & \text{if } s_0 - k \le s_i \le s_0 + k \\ \epsilon_0 & \text{if } s_i > s_0 + k \end{cases} \tag{31}$$

In this work we choose $\epsilon_0 = \mathcal{S}\frac{\Delta x}{P}|\upsilon_\sigma|$, $s_0 = -4.0$, $k = 1.5$
where $\mathcal{S}$ is $1/20$ for 1-D and $1/10$ for 2-D.



(a) $t = 2.5$ (b) $t = 2.5$ (c) $t = 2.5$

Figure: Solution of $\partial_t u - \sin(\pi x)\cos(\pi y)\partial_x u + \cos(\pi x)\sin(\pi y)\partial_y u = 0$ in $(x, y) \in [0, 1]^2$ using a FR/CPR scheme with RK4(5)-SSP with 14×14 elements of degree P8 with artificial diffusion ($\mathcal{S} = 1/20$) for a initial discontinuous data in (a), up to a time $t = 2.5$ (b). A time step $dt = 0.0014$. A sharp and well behaved profile is obtained in 196 cells without resorting to limiting strategies (c).

Outline

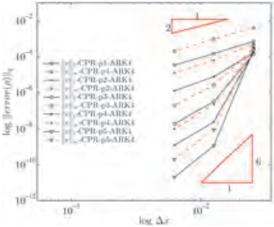
Test 1: Convergence Test for IMEX implementations (Pieraccini & Puppo2007)

- 1-D smooth test
- gas with three DoF ($D + \delta = 3$) is considered.
- The ratio of heat capacity: $\gamma = \frac{D+\delta+2}{D+\delta} = 5/3$.
- AP-BBGK solver: FR/CPR with ARK4
- $\tau = $ 1E-5
- Domain: (x, υ) , where $x \in [-1, 1]$ and $\upsilon \in [-10, 10]$,
- initial data:

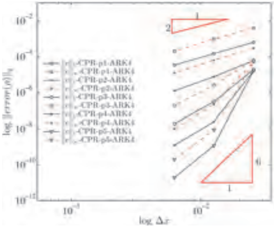
$$\{\rho_0, u_0, \theta_0\} = \left\{1, \frac{1}{\sigma}\left(\exp(-(\sigma x - 1)^2) - \exp(-(\sigma x + 1)^2)\right), 1\right\}, \qquad (32)$$

- Reference Solution: WENO7 with $N_x \times N_v = 1280 \times 1280$
- $N_x = N_v = 20, 40, 80$

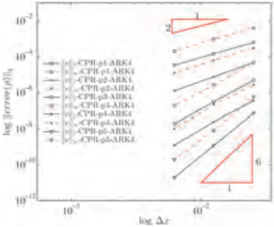
Test 1: Convergence Test for IMEX implementations



(a) ARK4-DOM(N_υ)



(b) ARK4-CDOM(N_υ)



(c) ARK4-DOM($N_\upsilon + 10$)

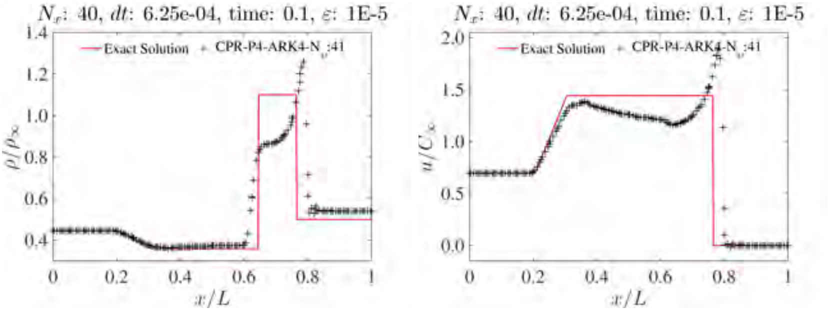
Test 2: Shock Tube Test Problems

- Lax shock tube problem
- gas with three DoF ($D + \delta = 3$)
- The ratio of heat capacity of the gas:$\gamma = \frac{D+\delta+2}{D+\delta} = 5/3$.
- $\tau = 1 \times 10^{-5}$
- initial data

$$\begin{cases} (\rho_L, u_L, \theta_L) = (0.445, 0.698, 7.928) & \text{if} \;\; 0 \leqslant x \leqslant 0.5, \\ (\rho_R, u_R, \theta_R) = (0.5, 0.0, 1.142) & \text{if} \;\; 0.5 < x \leqslant 1, \end{cases} \tag{33}$$

- $x \in ([0, 1]$ and $\upsilon \in [-14, 14])$.
- $N_x = 40$
- FR/CPR with P^4 elements
- ARK4

Test 2: Shock Tube Test Problems

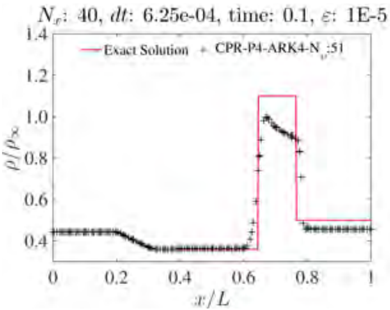


(a) CDOM: Density (b) CDOM: Velocity

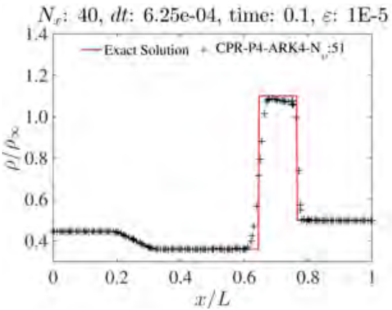
Figure: Test 2. Density and Velocity profiles for Lax shock tube problem at $t = 0.1$ with $CFL = 0.20$. $N_v = 41$

Note: The DOM solution blows up.

Test 2: Shock Tube Test Problems



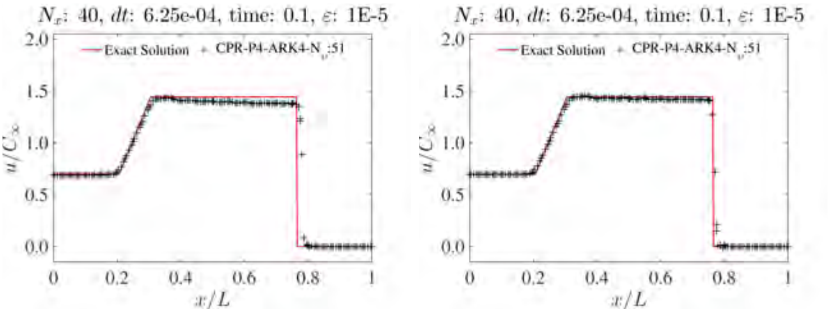
(a) DOM: Density



(b) CDOM: Density

Figure: Test 2. Density profiles of DOM and CDOM methods for Lax shock tube problem at $t = 0.1$ with $CFL = 0.20$. $N_v = 51$

Test 2: Shock Tube Test Problems

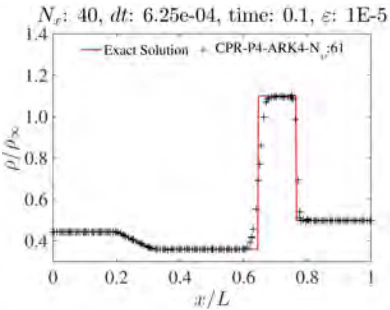


(a) DOM: Velocity

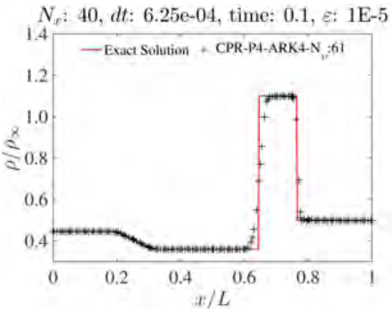
(b) CDOM: Velocity

Figure: Test 2. Velocity profiles of DOM and CDOM methods for Lax shock tube problem at $t = 0.1$ with $CFL = 0.20$. $N_v = 51$

Test 2: Shock Tube Test Problems



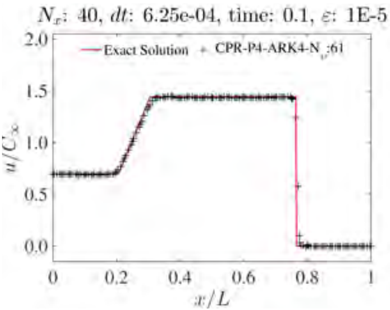
(a) DOM: Density



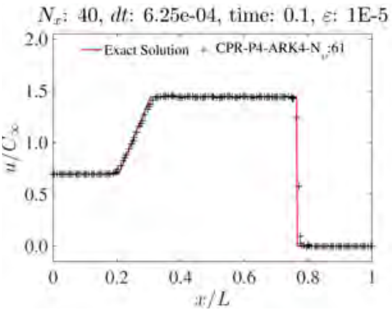
(b) CDOM: Density

Figure: Test 2. Density profiles of DOM and CDOM methods for Lax shock tube problem at $t = 0.1$ with $CFL = 0.20$. $N_v = 61$

Test 2: Shock Tube Test Problems



(a) DOM: Velocity



(b) CDOM: Velocity

Figure: Test 2. Velocity profiles of DOM and CDOM methods for Lax shock tube problem at $t = 0.1$ with $CFL = 0.20$. $N_v = 61$

Test 3: Viscous Shock-Tube Problems

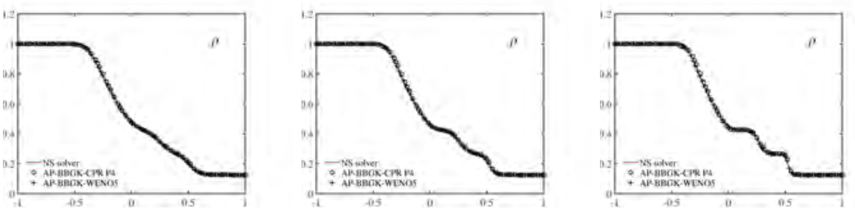
- Viscous Shock-Tube Problems
- gas with five DoF ($D + \delta = 5$)
- The ratio of heat capacity: $\gamma = \frac{D+\delta+2}{D+\delta} = 7/5$.
- Sod's shock tube initial condition

$$\begin{cases} (\rho_L, u_L, \theta_L) = (1, 0, 1) & \text{if } \ 0 \leqslant x \leqslant 0.5, \\ (\rho_R, u_R, \theta_R) = (0.1, 0, 0.125) & \text{if } \ 0.5 < x \leqslant 1. \end{cases} \tag{34}$$

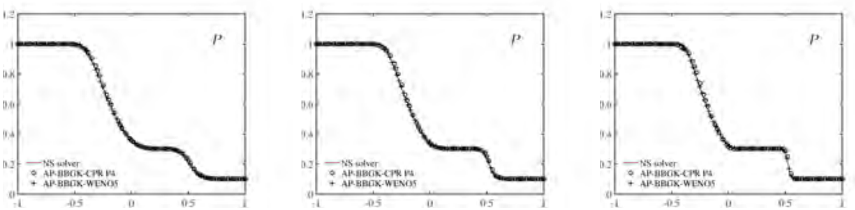
- ARK4 with WENO5 ($N_x = 100$) and FR/CPR-P^4 $N_x = 20$
- DOM with Gauss-Hermite quadrature with $N_\upsilon = 80$
- Final time: $t = 0.10$
- $\Delta t = 0.0024$ for WENO5 and $\Delta t = 0.0013$ for FR/CPR.
- Reference Solutin: compressible Navier-Stokes (CNS) equation solver

Test 3: Viscous Shock-Tube Problems

Density profiles



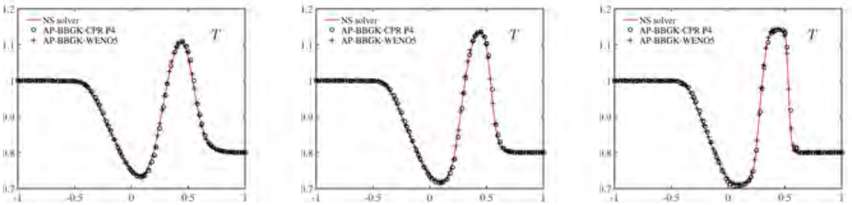
Pressure profiles



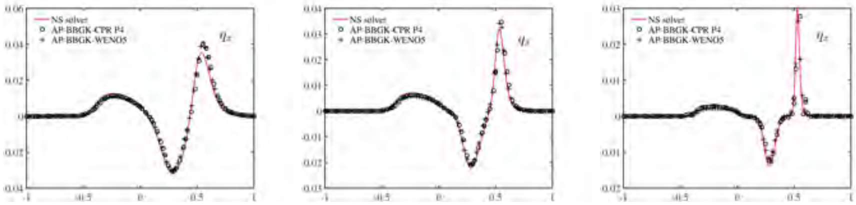
(a) $R_e = 200$ (b) $R_e = 400$ (c) $R_e = 1000$

Test 3: Viscous Shock-Tube Problems

Temperature profiles



Heat flux profiles



(a) $R_e = 200$ (b) $R_e = 400$ (c) $R_e = 1000$

Test 4: 2-D Riemann Problem, Configuration 5

Configuration 5: $J_{32}^{-} \begin{matrix} J_{21}^{-} \\ J_{34}^{-} \end{matrix} J_{41}^{-}$

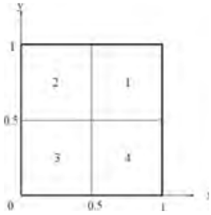
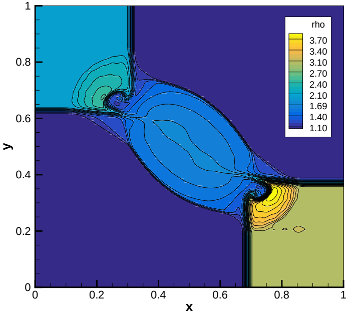


Figure: Domain configuration of 2-D Riemann problems.

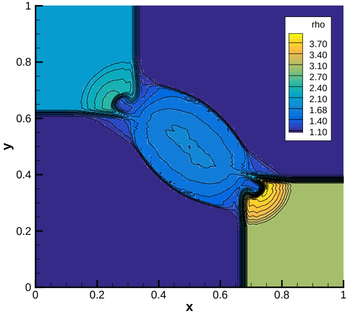
$p_2 = 1, \quad \rho_2 = 2,$ $u_{x,2} = -0.75, \quad u_{y,2} = 0.5,$	$p_1 = 1, \quad \rho_1 = 1,$ $u_{x,1} = -0.75, \quad u_{y,1} = -0.5,$
$p_3 = 1, \quad \rho_3 = 1,$ $u_{x,3} = 0.75, \quad u_{y,3} = 0.5,$	$p_4 = 1, \quad \rho_4 = 3,$ $u_{x,4} = 0.75, \quad u_{y,4} = -0.5.$

- Gas with five DoF ($D + \delta = 5$).
- The ratio of specific heat capacity $\gamma = \frac{D+\delta+2}{D+\delta} = 7/5$.
- $\tau = 10^{-6}$ (Euler hydrodynamic limit).
- FR/CPR with $Q4$ elements
- Gauss-Hermite with 20×20 quadrature points
- Positivep-preserving limiter (Zhang and Shu, JCP 2010)

Test 4: Configure 5



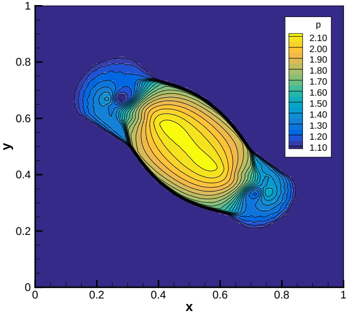
(a) WENO5 $\Delta x = \Delta y = 1/200$



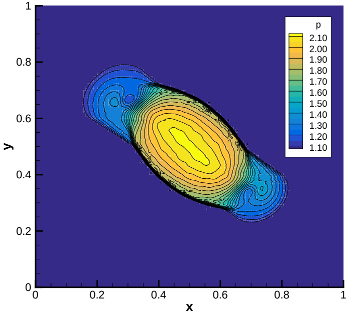
(b) FR/CPR $\Delta x = \Delta y = 1/32$

Figure: Density contour plots of 2-D Riemann problems for a time $t = 0.23$ with $\Delta t = 0.0009$.

Test 4: Configure 5



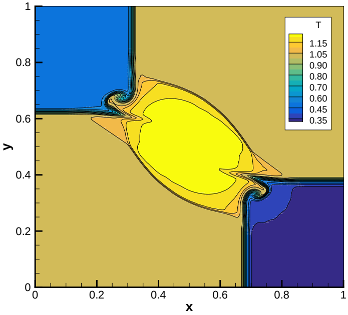
(a) WENO5 $\Delta x = \Delta y = 1/200$



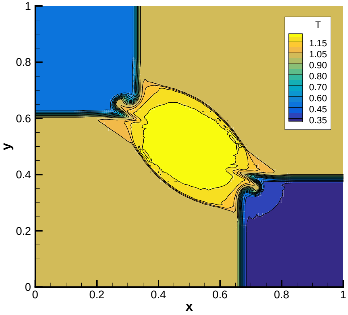
(b) FR/CPR $\Delta x = \Delta y = 1/32$

Figure: Pressure contour plots of 2-D Riemann problems for a time $t = 0.23$ with $\Delta t = 0.0009$

Test 4: Configure 5



(a) WENO5 $\Delta x = \Delta y = 1/200$



(b) FR/CPR $\Delta x = \Delta y = 1/32$

Figure: Temperature contour plots of 2-D Riemann problems for a time $t = 0.23$ with $\Delta t = 0.0009$

Outline

Discussion

1. About **High-order AP scheme:**
   Here we demostrated that high-order schemes for non-linear Boltzmann Equation can be achieved by taking advantage of ARK and FR/CPR schemes.
2. About **AP Scheme:**
   Taking advantage of an Asymptotic-Preserving scheme can provide improved stability and overcome the numerical stiffness imposed by the collision term. However, it alone cannot garantee correct convergence and it's accuracy.
3. About **Conservative DOM:**
   Based on our observations, imposing numerical conservation is important to ensure the correct convergence of our schemes. Here, we remark that this is important mainly for lower-order schemes.
4. About **High-order Advections schemes with Artificial Viscosity:**
   CPR scheme performs very well for smooth IC problems and can achieve results comparable to WENO methods with about the same number of degrees of freedom.

Thank you for your attention