A conservative semi-Lagrangian scheme for the Boltzmann equation

Seung Yeon Cho

Department of Mathematics
Gyeongsang National University
Jinju, Republic of Korea

France-Korea IRN webinar in PDE
6th Nov 2023

joint work with S. Boscarino and G. Russo

Motivation

Semi-Lagrangian (SL) schemes are very effective for the treatment of convection (and drift) terms in kinetic equations.

- Obtained by integrating the equations along characteristics.
- Large time steps are possible, therefore improving efficiency
- SL scheme may not be conservative.

Conservation is very relevant for

- Boltzmann or BGK-type equations
  (essential for example for capturing shocks)
- long time behaviour of Vlasov-like equations

Purpose of the talk: - Introduction to a finite-difference high order conservative semi-Lagrangian method for the Boltzmann equation.

The Boltzmann equation

The Boltzmann equation describes collisions among particles.

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f).$$

- $f = f(x, v, t)$ stands for the velocity distribution function of molecules with position $x \in \mathbb{R}^3$ and velocity $v \in \mathbb{R}^3$ at time $t > 0$.
- convection term $v \cdot \nabla_x f$ describes the free streaming of molecules
- collision operator $Q(f, f)$ describes the binary collisions of molecules.
- the parameter $\varepsilon > 0$ is called *Knudsen number*, and defined by

$$\varepsilon = \frac{\text{mean free path between collisions}}{\text{macroscopic length scale}}.$$

The Boltzmann equation

The collision operator $Q(f,f)$ describes the binary collisions of the particles:

$$Q(f,f)(x,v,t) = \int_{\mathbb{R}^3}\int_{S^2} B(|v-v_*|,\omega)[f(v')f(v'_*) - f(v)f(v_*)]\,d\omega\,dv_*.$$

- (v, v_*) and (v', v'_*) are pre- and post-collision velocities that satisfy microscopic momentum and energy conservation

$$v' + v'_* = v + v_*, \quad |v'|^2 + |v'_*|^2 = |v|^2 + |v_*|^2.$$

- ω is a vector of the unit sphere S^2.
- $B(|v-v_*|,\omega)$ is called collision kernel.
- $f(v') = f(x,v',t),\ f(v'_*) = f(x,v'_*,t),\ f(v) = f(x,v,t),\ f(v_*) = f(x,v_*,t)$

Properties of the Boltzmann equation:

Macroscopic variables such as density, mean velocity, energy and temperature of gas are defined by

$$\rho = \int_{\mathbb{R}^3} f \, dv, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^3} vf \, dv, \quad E = \int_{\mathbb{R}^3} \frac{|v|^2}{2} f \, dv$$

$$T = \frac{1}{3R\rho} \int_{\mathbb{R}^3} |v - u|^2 f \, dv$$

where R is the gas constant

Properties of the Boltzmann equation:

- Conservation laws of mass/momentum/energy:

$$\int_{\mathbb{R}^3} Q(f,f) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} dv = 0.$$

- H-theorem:

$$\int_{\mathbb{R}^3} Q(f,f) \ln(f(v)) dv \leq 0.$$

- The density, mean velocity and temperature of gas are defined by

$$\rho = \int_{\mathbb{R}^3} f\, dv, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^3} vf\, dv, \quad T = \frac{1}{3R\rho} \int_{\mathbb{R}^3} |v-u|^2 f\, dv$$

where R is the gas constant

- Local equilibrium (Maxwellian):

$$\int_{\mathbb{R}^3} Q(f,f) \ln(f(v)) dv = 0 \leftrightarrow f = M(f)(x,v,t) := \frac{\rho(x,t)}{\sqrt{(2\pi RT(x,t))^3}} e^{-\frac{|v-u(x,t)|^2}{2RT(x,t)}}$$

Computational challenges

The Boltzmann equation presents several computational difficulties:

1. the high dimensionality of the problem: $(x, v, t) \in \mathbb{R}^7$
2. collision operator $Q(f, f)$ is a five-dimensional integral on $\mathbb{R}^3 \times S^2 \Rightarrow$ very expensive to compute
3. difficult to preserve conservative quantities numerically (conservation laws)
4. stability issues from convection term and small Knudsen number.
5. positivity of the solution has to be maintained at a discrete level.

High order methods

- Eulerian based methods are obtained by discretizing

$$\partial_t f + v \cdot \nabla_x f = \frac{Q(f,f)}{\varepsilon}.$$

  - Strang splitting based method (Filbet and Russo, 2003): 2nd order accuracy.
  - Implicit-explicit penalization technique (Filbet and Jin, 2010): 2nd order accuracy.
  - Exponential time integrator (Li and Pareschi, 2014): arbitrary high order accuracy.
  - Implicit-explicit penalization technique + unstructured mesh (Boscheri and Dimarco, 2021): arbitrary high order accuracy.

->CFL condition: $\max_j |v_j| \frac{\Delta t}{\Delta x} < 1$

High order methods

Semi-Lagrangian methods are obtained by discretizing :

$$\frac{df}{dt}(x(t), v, t) = \frac{Q(f,f)}{\varepsilon}(x(t), v, t), \quad \frac{dx}{dt} = v.$$

1. Strang splitting based method (Dimarco, Hauck, Loubère): second order accuracy.
2. Non-splitting based method (in this work): arbitrary high order accuracy

->Time step is not restricted by CFL condition

Semi-Lagrangian scheme

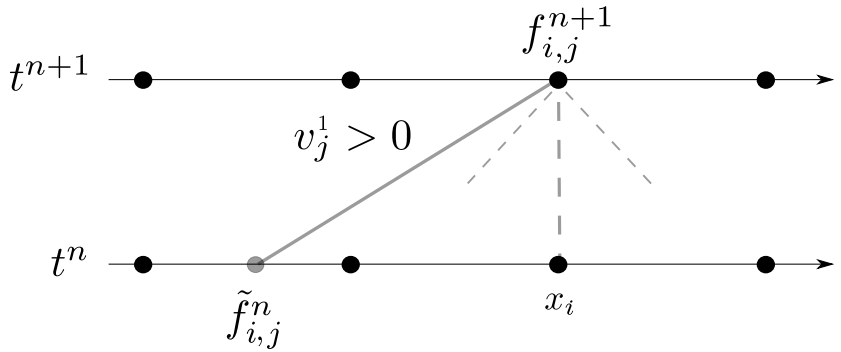
To derive the first order SL method, we begin by writing the BTE in characteristic form:

$$\begin{aligned} &\frac{df}{dt} = \frac{1}{\varepsilon} Q(f,f) := K \qquad \frac{dx}{dt} = v^1 \\ &x(0) = \tilde{x}, \quad f(0,x,v) = f_0(x,v), \quad t \geq 0, \quad x, v \in \mathbb{R} \times \mathbb{R}^2. \end{aligned} \tag{2.1}$$

- Applying the explicit Euler method to (2.1), we obtain

$$f^{n+1}(x,v) = f^n(x - v^1 \Delta t, v) + \Delta t K^n(x - v^1 \Delta t, v),$$

where $f^n(x,v) = f(x,v,t_n)$ and $K^n(x,v) = \frac{1}{\varepsilon} Q(f^n, f^n)(x,v,t_n)$.



$\tilde{f}_{i,j}^n$ and $\tilde{K}_{i,j}^n$ are computed on the same characteristic foot $x_i - v_j^1 \Delta t$ at time t_n.

- Discretization in space and velocity further gives

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}^n + \Delta t \tilde{K}_{i,j}^n. \tag{2.2}$$

where $\tilde{f}_{i,j}^n \approx f(x_i - v_j^1 \Delta t, v_j, t_n)$, $\quad \tilde{K}_{i,j}^n \approx K\left(x_i - v_j^1 \Delta t, v_j, t_n\right)$.

Semi-Lagrangian scheme

First order explicit SL scheme:

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}^{n} + \Delta t \tilde{K}_{i,j}^{n}$$

where $\tilde{f}_{i,j}^{n} \approx f(x_i - v_j^1 \Delta t, v_j, t^n)$, $\tilde{K}_{i,j}^{n} \approx K(x_i - v_j^1 \Delta t, v_j, t^n)$.

- Since $\tilde{f}_{i,j}^{n}$ and $\tilde{K}_{i,j}^{n}$ need to be computed on off-grid points, one should consider a 'suitable' reconstruction.
- Moreover, one has to consider very 'efficient' method for computing collision part $K_{i,j}^{n} = \frac{1}{\varepsilon} Q_{i,j}^{n}$.
- At the end, we want our scheme satisfies 'discrete conservation' in time:

$$\sum_{i,j} f_{i,j}^{n+1} \phi(v_j) \Delta x (\Delta v)^2 = \sum_{i,j} f_{i,j}^{n} \phi(v_j) \Delta x (\Delta v)^2$$

High order semi-Lagrangian method

Our strategy is to use:

- a high order non-oscillatory conservative reconstruction (Boscarino, Cho, Russo, Yun, 2021):
  -> high accuracy in space, non-oscillatory solution near discontinuity, and preservation of mass/momentum/energy
- fast spectral method (Mouhot and Pareschi, 2006) for the collision operator:
  -> spectral accuracy and fast computation of the collision operator $O(M^{d_v-1}N^{d_v}\log(N^{d_v}))$, $M << N$.
- Weighted L^2-minimization technique:
  -> the corrected values of collision operator satisfy

$$\sum_j Q^n_{i,j}\phi(v_j) = 0, \quad \phi(v) = 1, v, |v|^2.$$

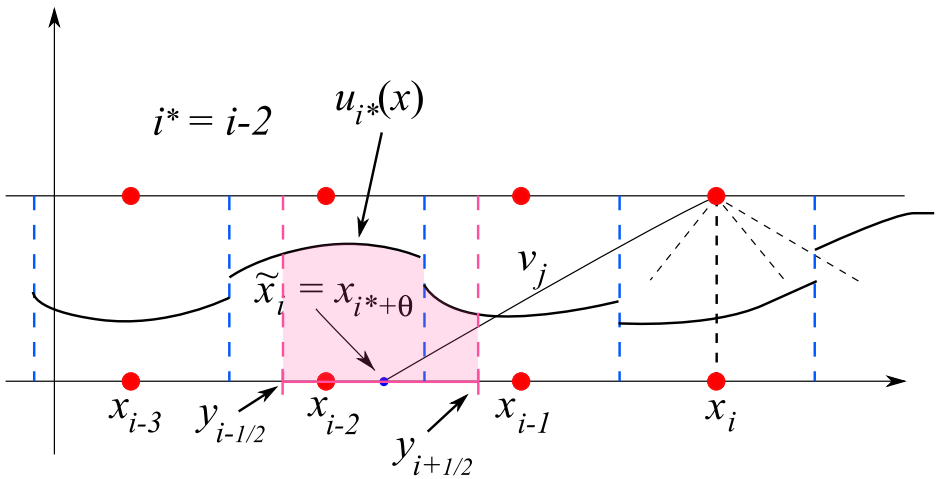
Conservative SL reconstruction

S. Y. Cho, S.Boscarino, G. Russo, S.-B. Yun, J. Comp. Phys., 2021

Example Given $\bar{u}_i$, we construct a conservative polynomial $u_i(x)$ in interval I_i obtained by non-linear reconstruction (e.g.CWENO23):

$$u_i(x) = u_i + u_i'(x - x_i) + \frac{1}{2}u_i''(x - x_i)^2, \quad \bar{u}_i = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_i(x)dx$$

with u_i, u_i', u_i'' suitable approximation of the point-wise value of u and its derivatives. In order to interpolate $\bar{u}(x_i + \theta\Delta x)$, $\theta \in [0, 1)$, we use



$$Q_{i+\theta} = \frac{1}{\Delta x}\int_{y_{i-\frac{1}{2}}}^{y_{i+\frac{1}{2}}} u_i(x)dx$$

$$\rightarrow \sum_i Q_{i+\theta}\Delta x = \sum_i \bar{u}_i\Delta x$$

- Thus, the use of a conservative reconstruction technique implies

$$\sum_i \tilde{f}_{i,j}^n \phi(v_j)\Delta x = \sum_i f_{i,j}^n \phi(v_j)\Delta x, \quad \sum_i \tilde{K}_{i,j}^n \phi(v_j)\Delta x = \sum_i K_{i,j}^n \phi(v_j)\Delta x$$

  for each j.

- Then, the scheme satisfies

$$\begin{aligned}\sum_{i,j} f_{i,j}^{n+1} \phi(v_j)\Delta x(\Delta v)^2 &= \sum_{j,i} \left(\tilde{f}_{i,j}^n + \Delta t \tilde{K}_{i,j}^n\right) \phi(v_j)\Delta x(\Delta v)^2 \\ &= \sum_{j,i} f_{i,j}^n \phi(v_j)\Delta x(\Delta v)^2 + \underbrace{\sum_i \sum_j K_{i,j}^n \phi(v_j)\Delta x(\Delta v)^2}_{=0?}\end{aligned}$$

Fast Spectral method

Mouhot and Pareschi, Math. Comp., 2000

The spectral method (also called Fourier-Galerkin method) is based on the Fourier series expansion of the velocity distribution function and the collision operator:

$$f_N(v) = \sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{f}_k e^{i\frac{\pi}{L}k\cdot v}, \quad i = \sqrt{-1}$$

- $[-L, L]^2$ is the velocity domain
- $k = (k_1, k_2)$ is the multi-index for frequencies such that $-\frac{N}{2} \leq k_1, k_2 \leq \frac{N}{2} - 1$.
- the summation with respect to k means

$$\sum_{k=-\frac{N}{2}}^{\frac{N}{2}-1} = \sum_{k_1,k_2=-\frac{N}{2}}^{\frac{N}{2}-1}$$

- $\hat{f}_k$ is the the Fourier mode that corresponds to the frequency index k

In classical spectral method of [Pareschi and Russo], the explicit form of Fourier mode of collision operator is provided as follows:

$$\hat{Q}_k = \sum_{m=-\frac{N}{2}}^{\frac{N}{2}-1} \hat{\beta}(k-m,m)\hat{f}_{k-m}\hat{f}_m, \quad -\frac{N}{2} \le k \le \frac{N}{2}-1$$

- $m = (m_1, m_2)$.
- $\hat{\beta}(k-m,m) = \beta(k-m,m) - \beta(m,m)$ is the so-called *kernel mode*. The explicit form of $\beta(k-m,m)$ for the Maxwellian and hard sphere molecules are computed.
- computational cost: $O(N^{2d_v})$

In FSM, the authors use the Carleman representation and approximate the coefficients $\beta(k-m,m)$ with $\beta^f(k-m,m)$:

$$\beta(k-m,m) \approx \beta^f(k-m,m) = \frac{\pi}{M}\sum_{p=1}^{M}\alpha_p(k-m)\alpha'_p(m),$$

- $\alpha_p(k-m) := \phi_R^2((k-m)\cdot e_{\theta_p}), \quad \alpha'_p(m) = \phi_R^2(m\cdot e_{\theta_p+\frac{\pi}{2}})$
- $e_\theta = (\cos(\theta),\sin(\theta)) \in S^1$
- $\phi_R^2(s) = 2R\frac{\sin s}{s}$, $\theta_p = \pi p/M$

This finally gives us a convolution structure:

$$\hat{Q}_k^f = \frac{\pi}{M}\sum_{p=1}^{M}\sum_{m=-\frac{N}{2}}^{\frac{N}{2}-1}\left(\alpha_p(k-m)\hat{f}_{k-m}\alpha'_p(m)\hat{f}_m - \hat{f}_{k-m}\alpha_p(m)\alpha'_p(m)\hat{f}_m\right).$$

- computational cost: $O(M^{d_v-1}N^{d_v}\log(N^{d_v}))$.

Consequently, we can obtain the values of collision operator:

$$\text{Inverse Fast Fourier Transform} : \{\hat{Q}_k^f\}_k \Longrightarrow Q_{\mathcal{J}}$$

In FSM, the authors use the Carleman representation and approximate the coefficients $\beta(k-m,m)$ with $\beta^f(k-m,m)$:

$$\beta(k-m,m) \approx \beta^f(k-m,m) = \frac{\pi}{M}\sum_{p=1}^{M}\alpha_p(k-m)\alpha'_p(m),$$

- $\alpha_p(k-m) := \phi_R^2((k-m)\cdot e_{\theta_p}), \quad \alpha'_p(m) = \phi_R^2(m\cdot e_{\theta_p+\frac{\pi}{2}})$
- $e_\theta = (\cos(\theta),\sin(\theta)) \in S^1$
- $\phi_R^2(s) = 2R\frac{\sin s}{s}$, $\theta_p = \pi p/M$

This finally gives us a convolution structure:

$$\hat{Q}_k^f = \frac{\pi}{M}\sum_{p=1}^{M}\sum_{m=-\frac{N}{2}}^{\frac{N}{2}-1}\left(\alpha_p(k-m)\hat{f}_{k-m}\alpha'_p(m)\hat{f}_m - \hat{f}_{k-m}\alpha_p(m)\alpha'_p(m)\hat{f}_m\right).$$

- computational cost: $O(M^{d_v-1}N^{d_v}\log(N^{d_v}))$.

Consequently, we can obtain the values of collision operator:

$$\text{Inverse Fast Fourier Transform} : \{\hat{Q}_k^f\}_k \Longrightarrow Q_{\mathcal{J}}$$

However,

$$\sum_j Q_j\phi(v_j) \neq 0, \quad \phi(v_j) = 1, v_j, |v_j|^2.$$

Weighted L^2-minimization

S.Boscarino, S. Y. Cho, G. Russo, J. Comp. Phys., 2022

Given $\mathcal{U} := (\rho, \rho U, E)^\top$ and an initial guess $f \in \mathbb{R}^{(N_v)^2}$, we consider a weight function $1/h$ and look for a solution g of the following weighted L^2-minimization problem:

$$\min_g \left\| f \circ \frac{1}{h} - g \right\|_2^2 \quad \text{s.t} \quad Cg = \mathcal{U}$$

where $\circ$ denotes the componentwise multiplication and

$$f,\ g,\ h \in \mathbb{R}^{(N_v)^2}, \quad C := \begin{pmatrix} h_j(\Delta v)^2 \\ h_j v_j (\Delta v)^2 \\ h_j \frac{|v_j|^2}{2} (\Delta v)^2 \end{pmatrix} \in \mathbb{R}^{(1+2+1)\times(N_v)^2}.$$

Here g is constructed as close as possible to the ratio of f with respect to h which corresponds to the macroscopic quantities $\mathcal{U}$, while $g \circ h$ gives the approximation of f reproducing exactly the same discrete moments $\mathcal{U}$. The explicit form of $g \circ h$ is obtained by the method of Lagrange multiplier:

$$g \circ h = f + C^\top (CC^\top)^{-1} \left(\mathcal{U} - C\left(f \circ \frac{1}{h} \right) \right) \circ h.$$

Here the matrix $CC^\top$ is invertible because it is symmetric and positive definite.

- Letting $\mathcal{U} := (\rho, \rho U, E)^\top = (0,0,0,0)$, and applying the L^2 projection method, we can modify the values of collision operator to satisfy

$$\sum_j Q^n_{i,j}\phi(v_j) = 0, \quad \phi(v_j) = 1, v_j, |v_j|^2$$

- Consequently, the scheme satisfies

$$\begin{aligned}\sum_{i,j} f^{n+1}_{i,j}\phi(v_j)\Delta x(\Delta v)^2 &= \sum_{j,i}\left(\tilde{f}^n_{i,j} + \Delta t \tilde{K}^n_{i,j}\right)\phi(v_j)\Delta x(\Delta v)^2 \\ &= \sum_{j,i} f^n_{i,j}\phi(v_j)\Delta x(\Delta v)^2 + \underbrace{\sum_i \sum_j K^n_{i,j}\phi(v_j)\Delta x(\Delta v)^2}_{=0} \\ &= \sum_{i,j} f^n_{i,j}\phi(v_j)\Delta x(\Delta v)^2\end{aligned}$$

Semi-Lagrangian scheme

First order explicit SL scheme:

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}^{n} + \Delta t \tilde{K}_{i,j}^{n}$$

where $\tilde{f}_{i,j}^{n} \approx f(x_i - v_j^1 \Delta t, v_j, t^n)$, $\tilde{K}_{i,j}^{n} \approx K(x_i - v_j^1 \Delta t, v_j, t^n)$.

- For each i, j, we interpolate $\tilde{f}_{i,j}^{n}$ from $f_{\mathcal{I},j}^{n}$.
- For each i, from $f_{i,\mathcal{J}}^{n}$, we compute $Q_{i,\mathcal{J}}^{n}$ using the fast spectral method (Mouhot and Pareschi).
- For each i, to prevent loss of conservation we adopt L^2-minimization to impose

$$\sum_j Q_{i,j}^{n} \phi_j (\Delta v)^2 = 0, \quad \phi_j = 1, v_j, v_j^2/2$$

- For each i, j, we set $K_{i,j}^{n} = \frac{Q_{i,j}^{n}}{\varepsilon_i^n}$ and interpolate $\tilde{K}_{i,j}^{n}$ from $K_{\mathcal{I},j}^{n}$.
- update $f_{i,j}^{n+1}$

High order semi-Lagrangian method

For high order extension in time, we consider the following things:

- For relatively large $\varepsilon \geq 0.01$, there is no stiffness in the collision term. Therefore, for high order extension in time variable, it is enough to consider high order explicit Runge-Kutta or Adam's Bashforth methods
  -> stable and high order accuracy in time
- To have better efficiency, we chose RK methods which include many zeros in it's Butcher's table and dupulicated values of c values. In case of RK3, we set $\alpha = \frac{1}{3}$:

$$\text{RK3} = \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \alpha & \alpha & 0 & 0 \\ 1 & 1+\frac{1-\alpha}{\alpha(3\alpha-2)} & -\frac{1-\alpha}{\alpha(3\alpha-2)} & 0 \\ \hline & \frac{1}{2}-\frac{1}{6\alpha} & \frac{1}{6\alpha(1-\alpha)} & \frac{2-3\alpha}{6(1-\alpha)} \end{array}, \quad \text{RK4} = \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}$$

High order time discretization

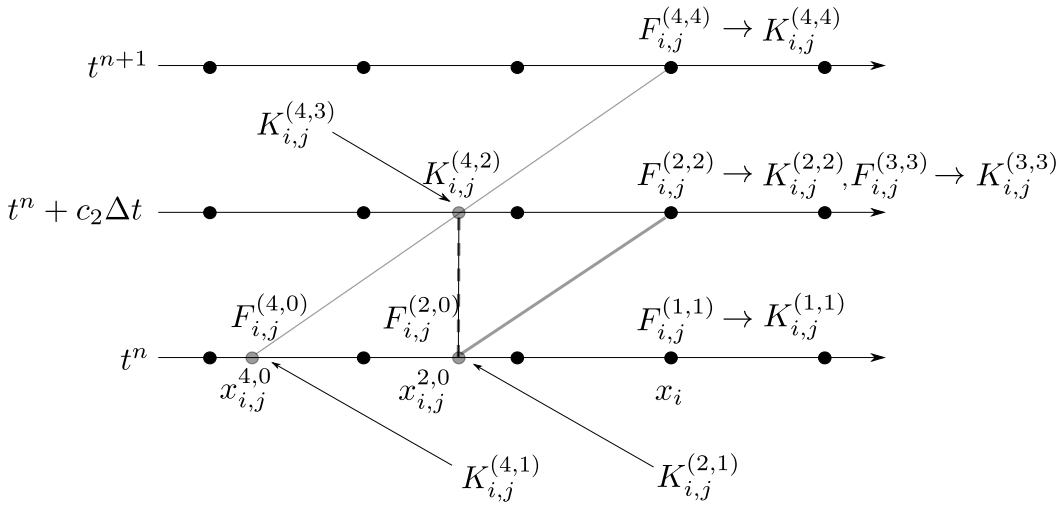


Illustration of RK4. The quantities on grey points need interpolation.

1st-stage value: $F_{i,j}^{(1,1)} = f_{i,j}^n \implies Q_{i,j}^{(1,1)}$

2nd-stage value: $F_{i,j}^{(2,2)} = F_{i,j}^{(2,0)} + \frac{\Delta t}{2} K_{i,j}^{(2,1)} \implies Q_{i,j}^{(2,2)}$

3rd-stage value: $F_{i,j}^{(3,3)} = F_{i,j}^{(2,0)} + \frac{\Delta t}{2} K_{i,j}^{(2,2)} \implies Q_{i,j}^{(3,3)}$

4th-stage value: $F_{i,j}^{(4,4)} = F_{i,j}^{(4,0)} + \Delta t K_{i,j}^{(4,3)} \implies Q_{i,j}^{(4,4)}$

numerical solution: $f_{i,j}^{n+1} = F_{i,j}^{(4,0)} + \frac{\Delta t}{6} K_{i,j}^{(4,1)} + \frac{\Delta t}{3} K_{i,j}^{(4,2)} + \frac{\Delta t}{3} K_{i,j}^{(4,3)} + \frac{\Delta t}{6} K_{i,j}^{(4,4)}.$

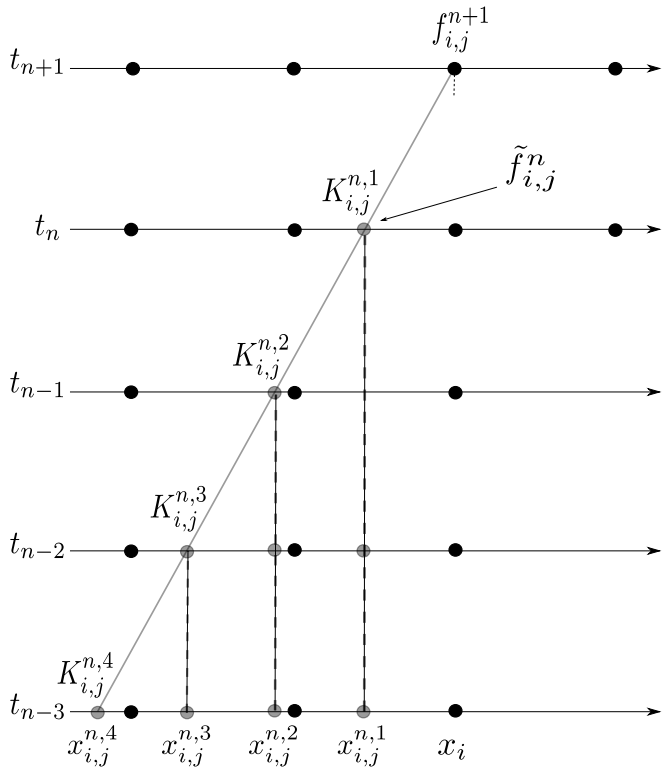


Illustration of AB4 method. The quantities on grey points need interpolation.

$$f_{i,j}^{n+1} = \tilde{f}_{i,j}^{n} + \Delta t \left(\frac{55}{24} K_{i,j}^{n,1} - \frac{59}{24} K_{i,j}^{n,2} + \frac{37}{24} K_{i,j}^{n,3} + \frac{9}{24} K_{i,j}^{n,4} \right) \quad \Longrightarrow Q_{i,j}^{(1,1)}$$

Remark: Yoshida's fourth order splitting method requires
4 interpolations + 3×4 computations of collision operator.

X1D-V2D Accuracy test with smooth data. $\varepsilon \approx 1$

Smooth initial data on the periodic domain $x \in [-0.5, 0.5]$ with

$$\rho_0(x) = \frac{2 + \sin 2\pi x}{2}, \quad u_0(x) = (0.75,\ -0.75), \quad T_0(x) = \frac{5 + 2\cos 2\pi x}{20}.$$

- Equilibrium initial data

$$f_0^{eq}(x, v) = \frac{\rho_0(x)}{2\pi T_0(x)} \exp\left(-\frac{|v - u_0|^2}{2T_0(x)}\right).$$

- Non-equilibrium initial data

$$f_0^{neq}(x, v) = \frac{1}{2}\frac{\rho_0(x)}{2\pi T_0(x)}\left(\exp\left(-\frac{(v - u_0(x))^2}{2T_0(x)}\right) + \exp\left(-\frac{(v + u_0(x))^2}{2T_0(x)}\right)\right)$$

- Maxwell molecules: $B(|v - v_*|, \omega) = C$

X1D-V2D Accuracy test with smooth data. $\varepsilon \approx 1$

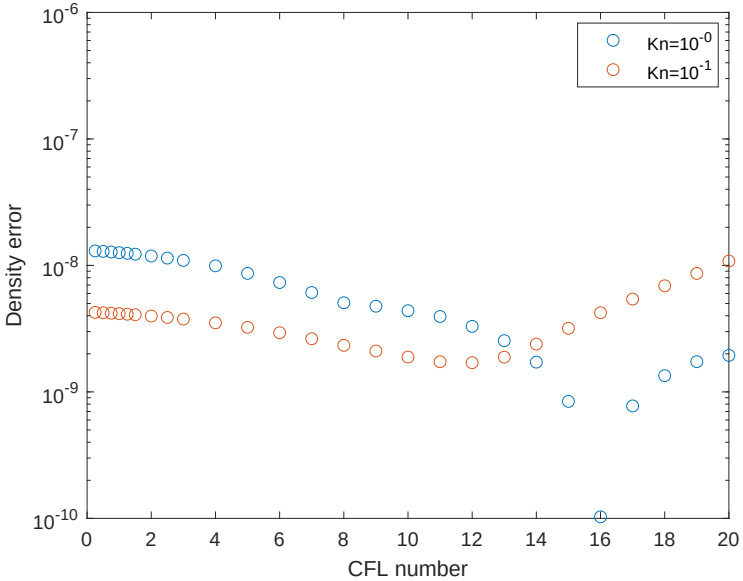
Relative L^1 error and convergence rate of density ρ								
	Non-equilibiurm				Equilibiurm			
	CFL= 4		CFL= 10		CFL= 4		CFL= 10	
$(N_x, 2N_x)$	error	rate	error	rate	error	rate	error	rate
(40, 80)	2.572e-07	4.89	1.684e-07	4.26	3.534e-06	4.96	1.670e-06	4.81
(80, 160)	8.663e-09	4.96	8.802e-09	4.18	1.139e-07	4.99	5.943e-08	4.87
(160, 320)	2.787e-10		4.844e-10		3.591e-09		2.036e-09	

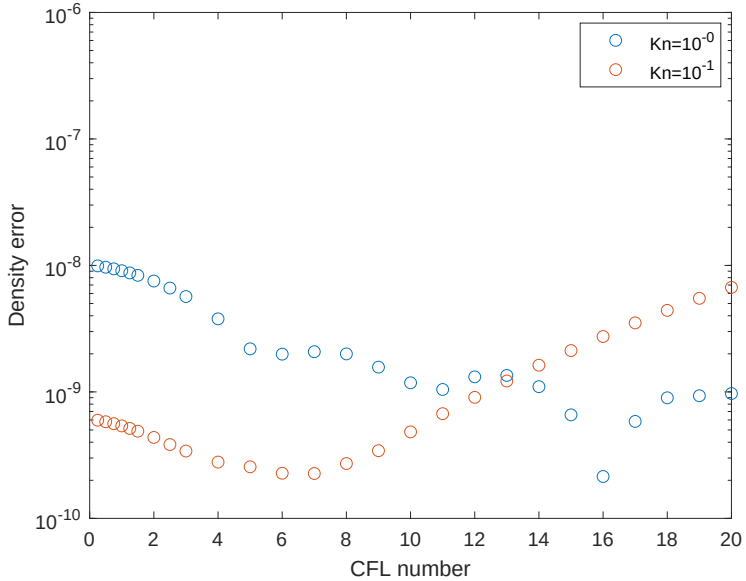
Table: RK4+QCWENO35+SL

Relative L^1 error and convergence rate of density ρ								
	Non-equilibiurm				Equilibiurm			
	CFL= 4		CFL= 10		CFL= 4		CFL= 10	
$(N_x, 2N_x)$	error	rate	error	rate	error	rate	error	rate
(40, 80)	1.021e-06	4.19	4.272e-05	4.18	3.739e-06	4.85	5.525e-05	5.00
(80, 160)	5.597e-08	4.14	2.358e-06	4.14	1.294e-07	4.87	1.726e-06	4.29
(160, 320)	3.182e-09		1.342e-07		4.432e-09		8.799e-08	

Table: AB4+QCWENO35+SL

Optimal CFL number





(Left:equilibrium initial data, Right:non-equilibrium initial data)

X1D-V2D Sod problem $\varepsilon \approx 0.01$

Discontinuous initial data on the periodic domain $x \in [-2, 2]$ with

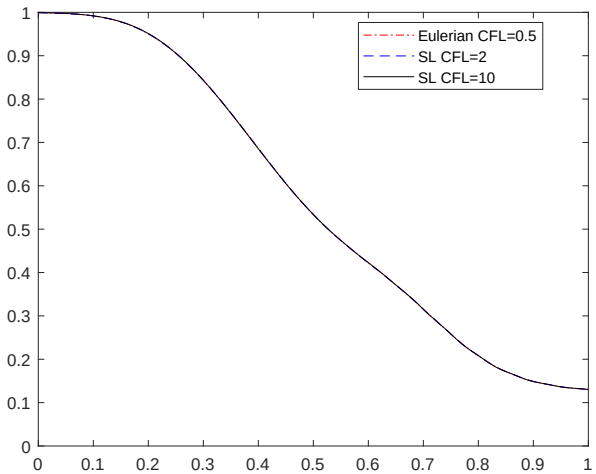
$$(\rho_0,\ u_{10},\ u_{20},\ T_0) = \begin{cases} (1, 0, 0, 1), & \text{if} \quad -1 \leq x \leq 0.5 \\ \left(\frac{1}{8}, 0, 0, \frac{1}{4}\right), & \text{otherwise} \end{cases} .$$

- Equilibrium initial data

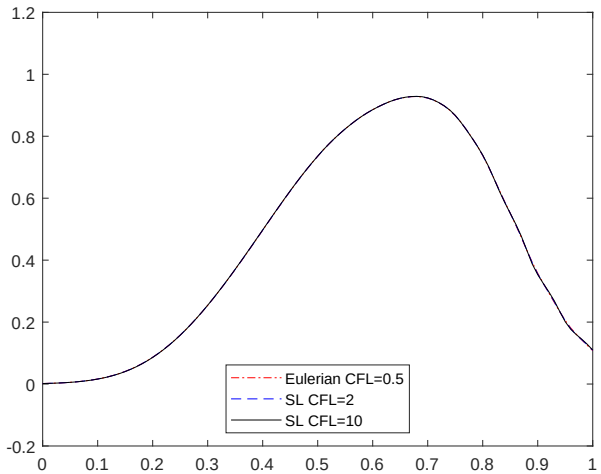
$$f_0^{eq}(x, v) = \frac{\rho_0(x)}{2\pi T_0(x)} \exp\left(-\frac{|v - u_0|^2}{2T_0(x)}\right).$$

- Maxwell molecules: $B(|v - v_*|, \omega) = C$

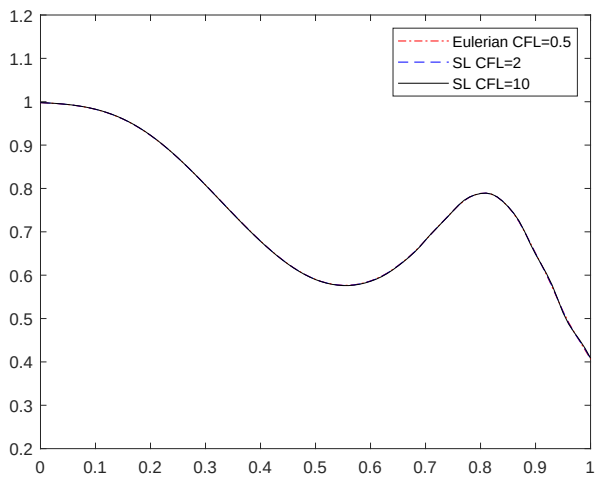
X1D-V2D Sod problem $\varepsilon \approx 0.01$



ρ



u



T

Conservation test

		without L^2-minimization		L^2-minimization	
	N_v	$L = 8$	$L = 10$	$L = 8$	$L = 10$
Mass	32	9.493e-08	7.269e-06	-6.096e-15	-9.144e-15
	64	-1.358e-09	-5.628e-09	-7.803e-15	-1.024e-14
Momentum	32	9.483e-08	2.755e-07	-2.314e-17	6.028e-17
	64	5.533e-08	8.564e-10	2.263e-17	-3.488e-17
Energy	32	-9.281e-06	-1.013e-04	-7.132e-15	-9.090e-15
	64	-5.407e-06	-2.339e-07	-7.132e-15	-1.035e-14

Table: Conservation error for RK4+QWENO35+SL

X1D-V2D Convergence towards global equilibrium

$\varepsilon \approx 1$, $CFL = 6$

- Non-equilibrium initial data on the periodic space domain $x \in [-1, 1]$ with

$$f_0(x, v) = \frac{1 + A_0 \sin(\pi x)}{2\pi T_0} \left[\exp\left(-\frac{|v - u_0|^2}{2T_0} \right) + \exp\left(-\frac{|v + u_0|^2}{2T_0} \right) \right]$$

$$A_0 = \frac{1}{2}, \quad T_0 = 0.125, \quad u_0 = \left(\frac{1}{2}, \frac{1}{2} \right)$$

The corresponding global equilibrium is given by

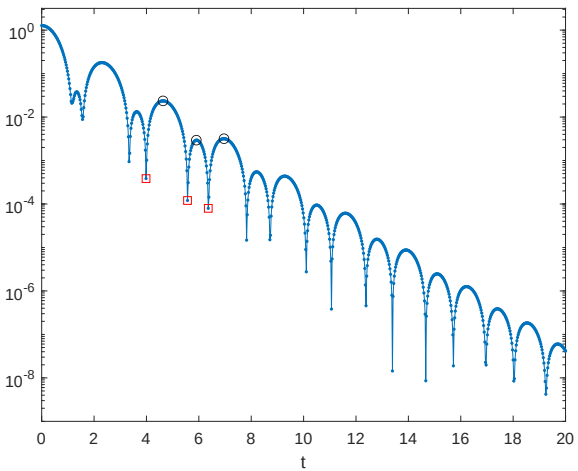
$$\mathcal{M}_g = \frac{\rho_g}{2\pi T_g} \exp\left(-\frac{|v|^2}{2T_g} \right)$$

where

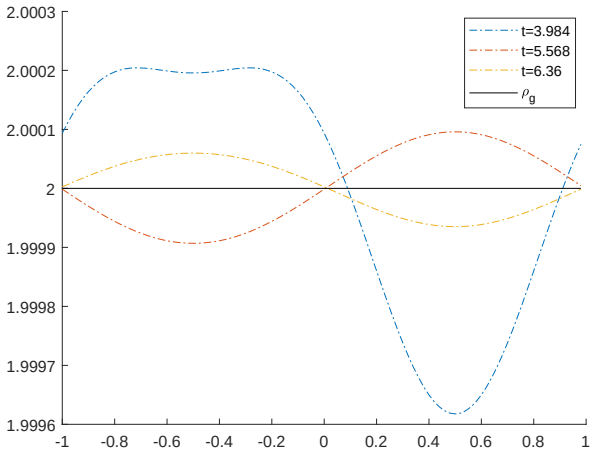
$$\rho_g = \int_{-1}^{1} \int_{\mathbb{R}^2} f_0(x, v) dv\, dx, \quad T_g = \frac{1}{2\rho_g} \int_{-1}^{1} \int_{\mathbb{R}^2} f_0(x, v) |v|^2 dv\, dx$$

X1D-V2D Convergence towards global equilibrium

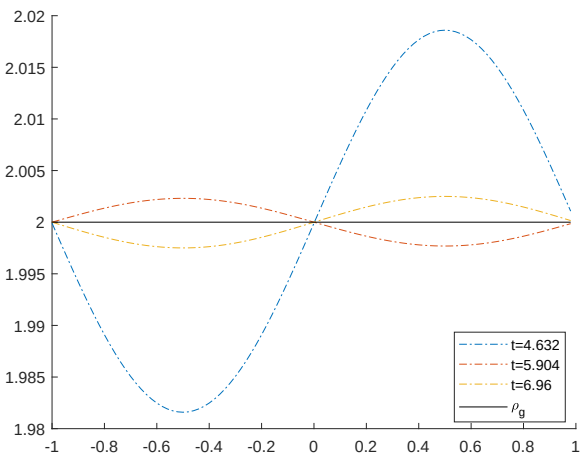
$\varepsilon \approx 1$, $CFL = 6$



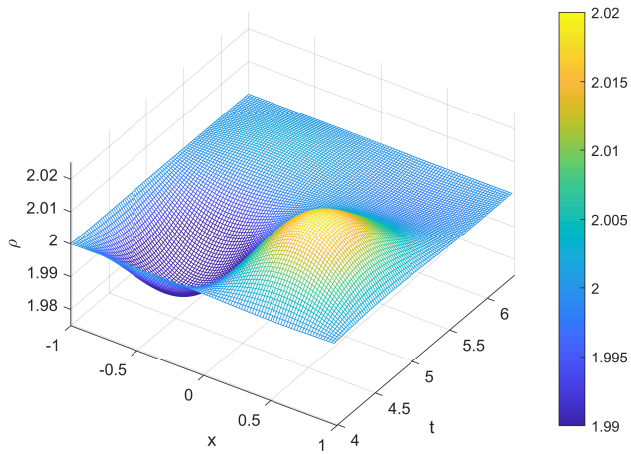
Time evolution of $\|\rho - \rho_g\|_1$



red squares



black circles



zoom at time $t \in [4, 6.5]$

X1D-V3D Sod problem $\varepsilon \approx 0.01$

Discontinuous initial data on the periodic domain $x \in [-2, 2]$ with

$$(\rho_0,\ u_{10},\ u_{20},\ u_{30},\ T_0) = \begin{cases} (1,0,0,0,1), & \text{if} \quad -1 \leq x \leq 0.5 \\ \left(\frac{1}{8},0,0,0,\frac{1}{4}\right), & \text{otherwise} \end{cases} .$$

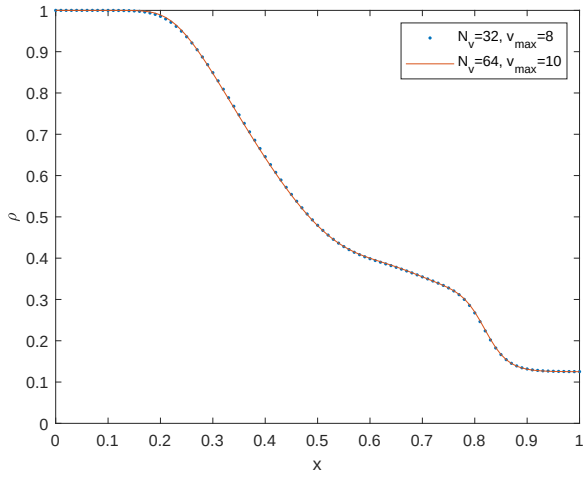
- Equilibrium initial data

$$f_0^{eq}(x,v) = \frac{\rho_0(x)}{(2\pi T_0(x))^{\frac{3}{2}}} \exp\left(-\frac{|v-u_0|^2}{2T_0(x)}\right).$$

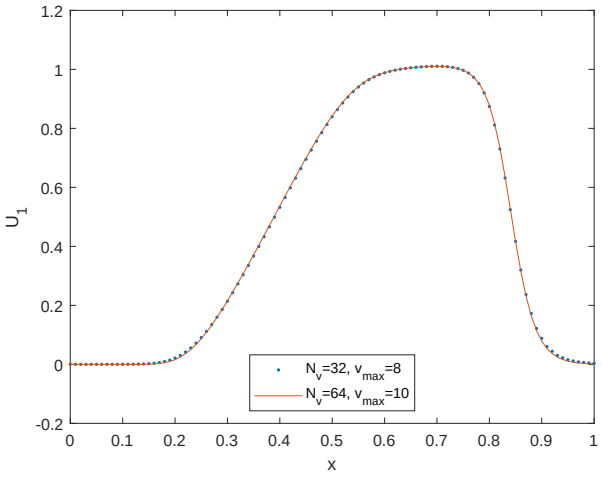
- Hard-sphere molecules: $B(|v-v_*|,\omega) = C|v-v_*|$

X1D-V3D Sod problem with hard-sphere molecules

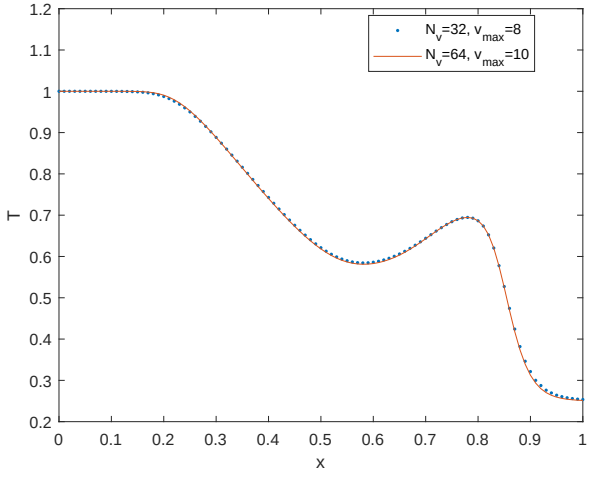
$\varepsilon \approx 0.01$, $CFL = 4$



ρ



u



T

X2D-V2D Vortex problem $\varepsilon \approx 0.1$

Smooth initial data on the periodic domain $(x, y) \in [0, 10]^2$ with

$$u(x, y, 0) = (1, 1) + (\delta u_1, \delta u_2), \quad T(x, y, 0) = 1 + \delta T$$

where

$$\delta u_1 = -(y - 5)\frac{5}{2\pi} \exp\left(\frac{1 - r^2}{2}\right),$$

$$\delta u_2 = (x - 5)\frac{5}{2\pi} \exp\left(\frac{1 - r^2}{2}\right),$$

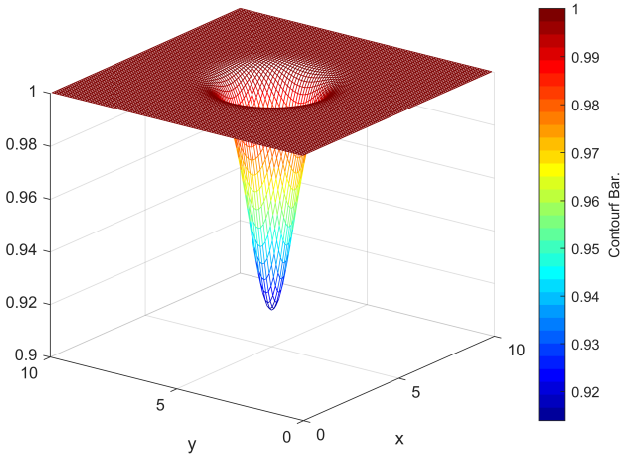
$$\delta T = -\frac{5}{16\pi^2} \exp\left(1 - r^2\right)$$

with $r^2 = (x - 5)^2 + (y - 5)^2$. For density, we use

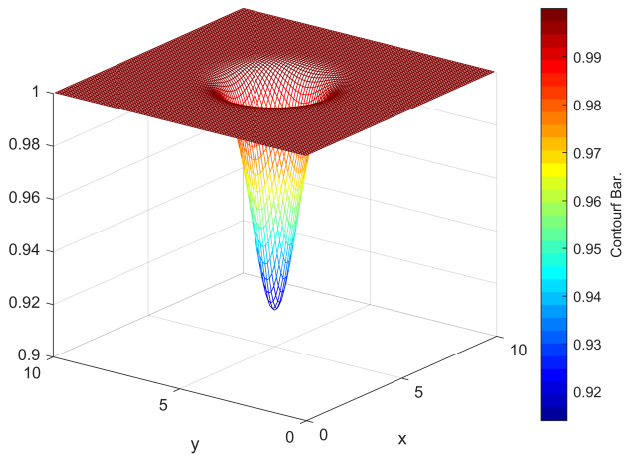
$$\rho(x, y, 0) = T(x, y, 0)$$

- Maxwell molecules.

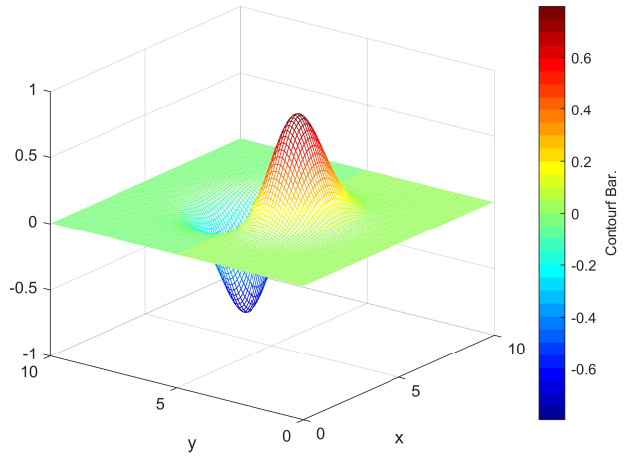
X2D-V2D Vortex problem $\varepsilon \approx 0.1$ at $t = 0$



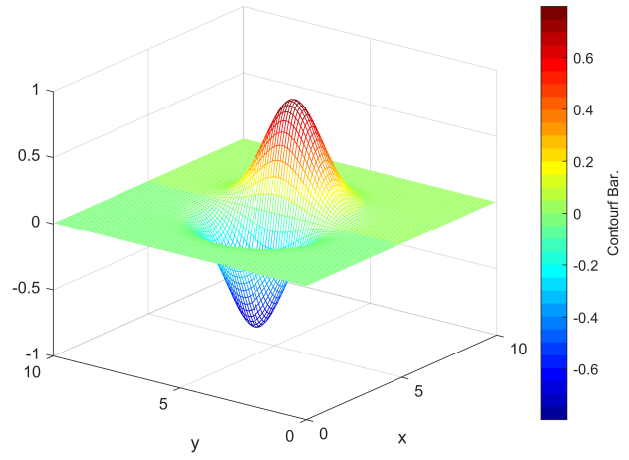
$\rho(x, y, 0)$



$T(x, y, 0)$

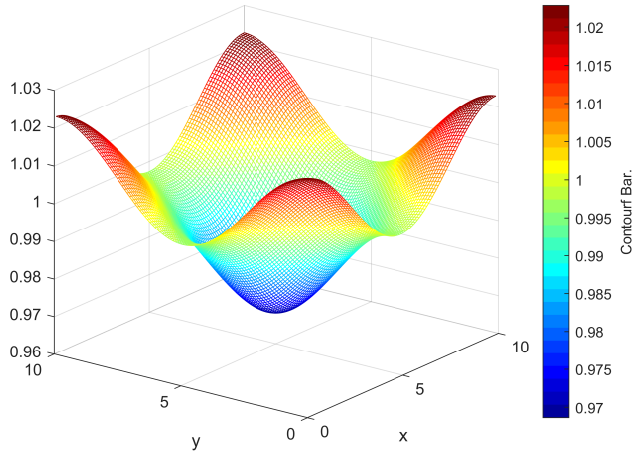


$u_1(x, y, 0) - 1$

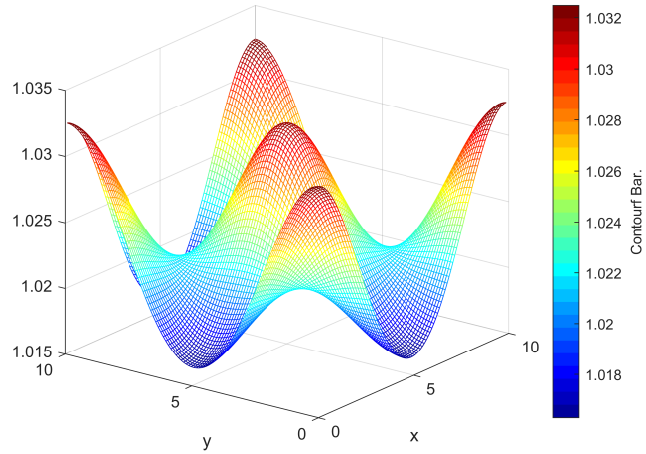


$u_2(x, y, 0) - 1$

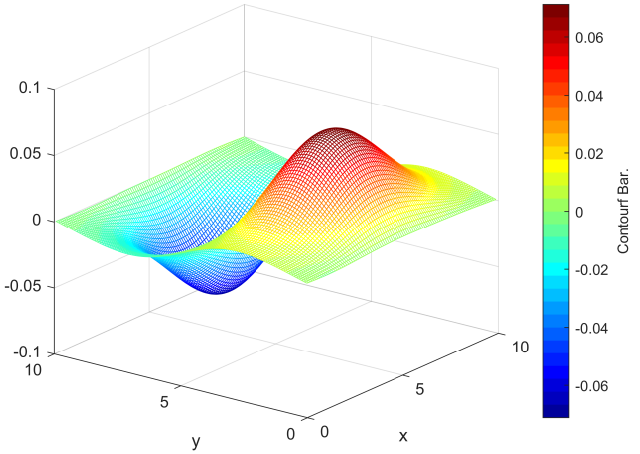
X2D-V2D Vortex problem $\varepsilon \approx 0.1$ at $t = 10$



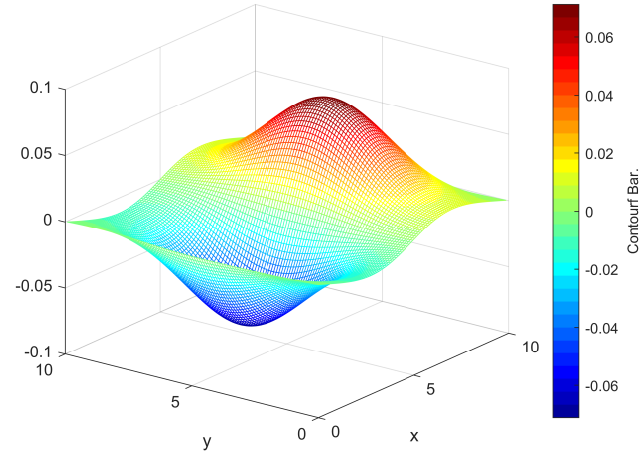
$\rho(x, y, 10)$



$T(x, y, 10)$



$u_1(x, y, 10) - 1$



$u_2(x, y, 10) - 1$

Conclusion

1. The proposed method attains high accuracy and conservation is maintained.
2. The scheme could be very effective for solving rarefied gas flow $\varepsilon \geq 0.01$.
3. Compared to RK methods, multi-step AB methods are very efficient and requires less memory (more efficient than splitting methods)
4. When we consider small Knudsen number $Kn << 1$, stiffness becomes important, SL approach can be combined with IMEX penalization technique.

Thank you for your attention!