Apply for Postdoctoral Position

Modeling and Simulation of Multiscale Transport Problems

Construction and Application of Unified Gas-Kinetic Scheme

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Webinar with Prof. Martin Frank and Steinbuch Centre for Computing, KIT
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Outline

- Personal Information
- Intro of Research during Ph.D. Study
- Conclusion and Outlook

Personal information

Name: Tianbai Xiao (肖天白)

Birth: Mar. 1992

Nationality: China

Education:

- **Ph. D.** Peking University, Beijing, China, Jun. 2019 (expected)
  (Thesis topic: Numerical Methods for Multiscale Transport Problems, Advisor: Qingdong Cai)
- **B.S.** Wuhan University, Wuhan, China, Jun. 2014

Experience

- Research Assistant, Department of Mathematics, Hong Kong University of Science and Technology, Apr. - Oct., 2016, Sep. 2017 - Mar., 2018, Sep. 2018 - Jan. 2019. (Advisor: Kun Xu)
- Teaching Assistant for Advanced Mathematics, Peking University, Sep. 2015 - Jan. 2016.

Theoretical mechanics:
continuous in mind,
discrete in equations

Distinct governing equations on different scales

- Euler
- Navier-Stokes
- Moment

...

- Boltzmann

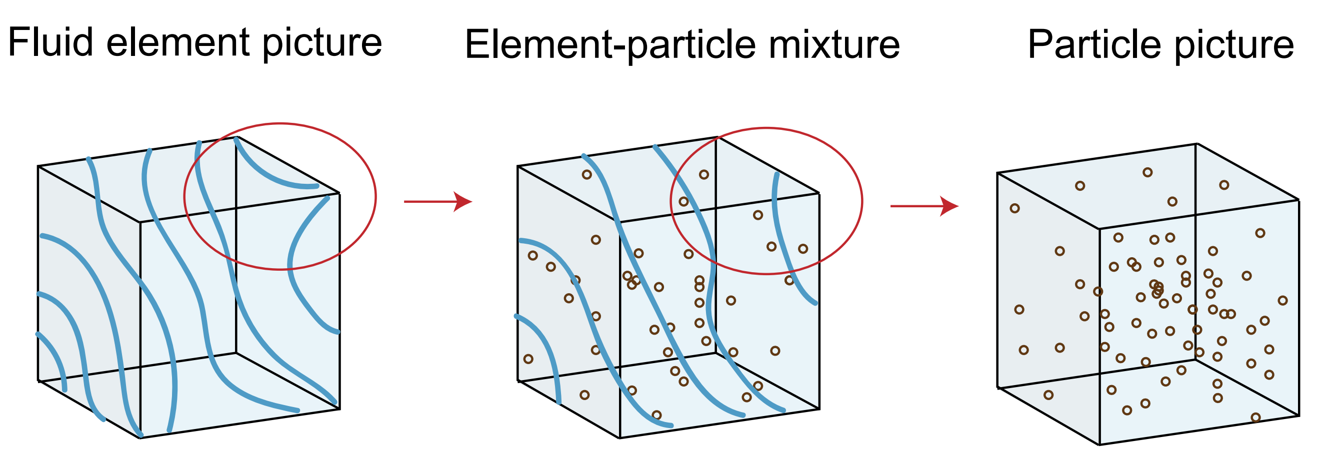
Computational mechanics:
discrete in numbers,
continuous in reality

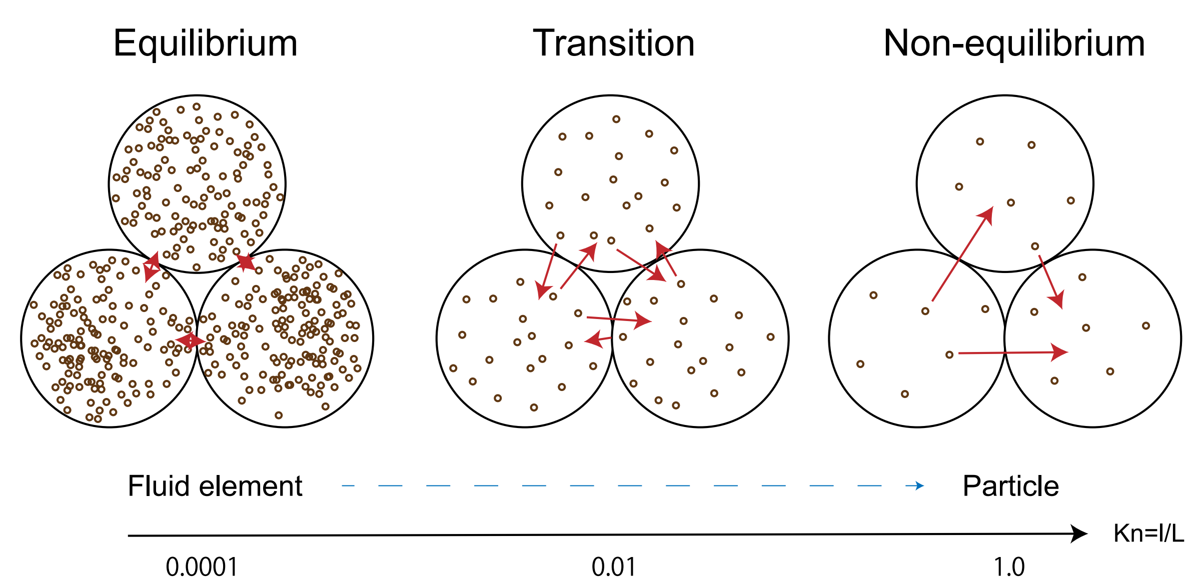
Distinct computational methods for numerical PDEs

- Equation based
- Particle based

...

Aim: connect individual equations seamlessly





Attempts of multiscale modeling and simulation

Hybrid method[1] —> Asymptotic-preserving (AP) scheme[2]:

- preserves the discrete analogy of the **asymptotic expansion** when Kn —> 0 (Hilbert, Chapman-Enskog, Hermite, etc.)

- overcomes the **stiffness** by kinetic relaxation scales (space & time)

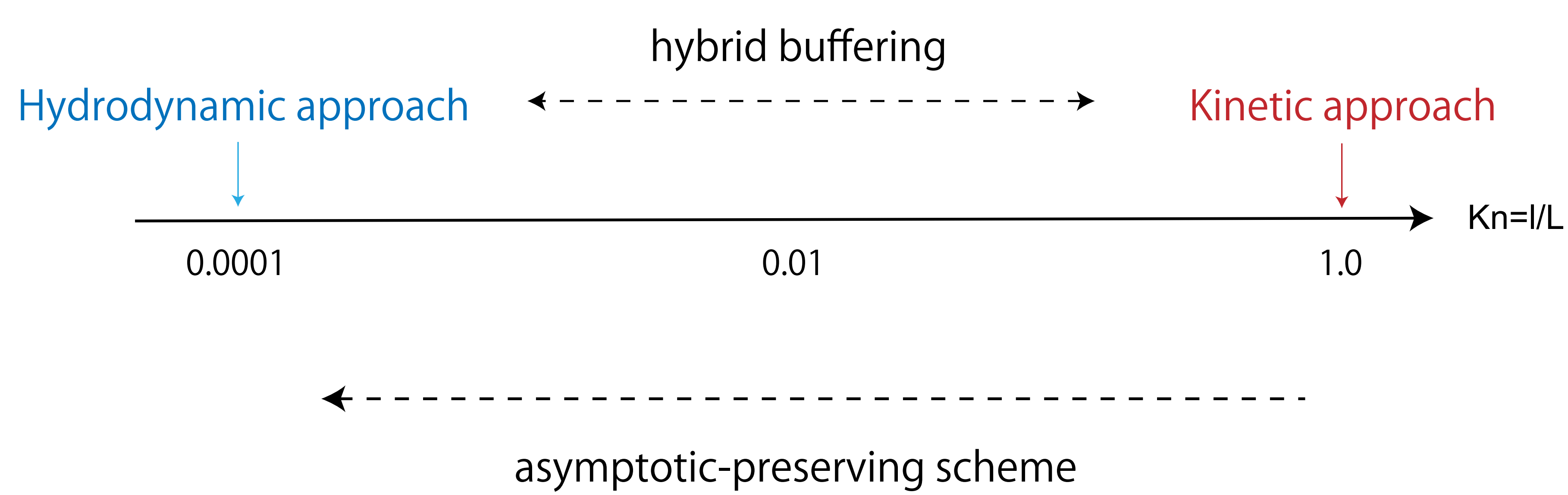


Figure: Two choices of developing multiscale algorithm

[1] Schwartzentruber, T. E., and Boyd, I. D. (2006). A hybrid particle-continuum method applied to shock waves. Journal of Computational Physics, 215(2), 402-416.
[2] Filbet, F., and Jin, S. (2010). A class of asymptotic-preserving schemes for kinetic equations and related problems with stiff sources. Journal of Computational Physics, 229(20), 7625-7648.

Framework of unified gas-kinetic scheme (UGKS)

Direct modeling for **macroscopic** and **microscopic variables** on the cell size and time step scales[1]

gas: distribution function —> mass, momentum, energy density
radiative transfer: radiative intensity —> energy, flux, pressure
and **neutron**, **phonon**, **plasma** transport problems

$$\mathbf{W}^{n+1} = \mathbf{W}^n + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_r^W dt + \int_{t^n}^{t^{n+1}} \mathbf{G}_i dt$$

$$f^{n+1} = f^n + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_r^f dt + \int_{t^n}^{t^{n+1}} Q(f) dt + \int_{t^n}^{t^{n+1}} G(f) dt$$

- Interface modeling: multiscale flux function
- In-cell modeling: correct collision effects
- Hydro physics *drives* kinetic dynamics, kinetic quantities *inform* hydro dynamics (like a combination of moment and kinetic formulation but no closure problem)

[1] Xu, K., and Huang, J. C. (2010). A unified gas-kinetic scheme for continuum and rarefied flows. Journal of Computational Physics, 229(20), 7747-7764.

Three Typical Scenarios

1. Gas dynamics under external force field
2. Supersonic and Hypersonic flows
3. Multicomponent gas and plasma physics

1. Force-Related Gas Dynamics

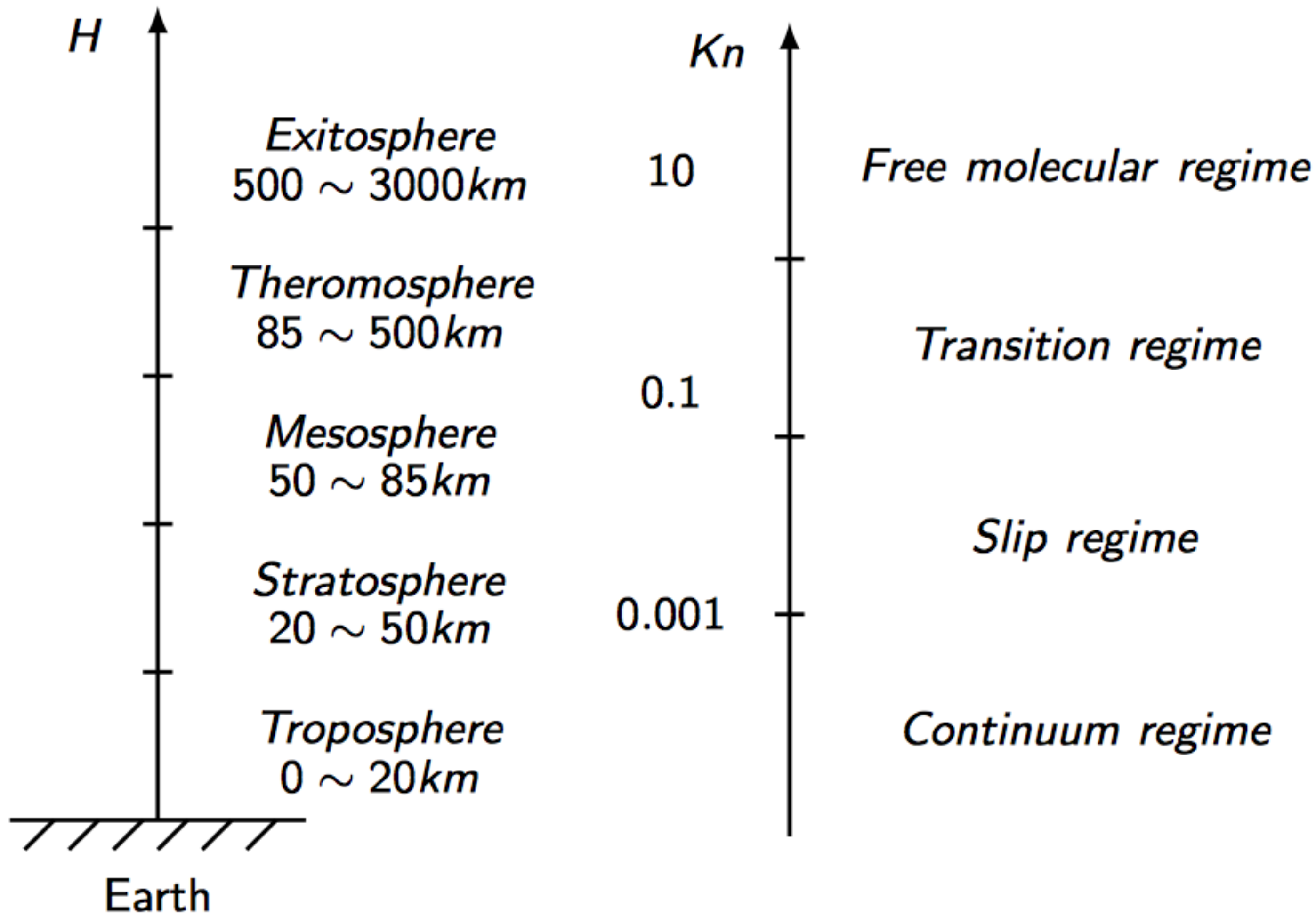


Figure: Schematic of atmosphere multilayer structure

Interface modeling

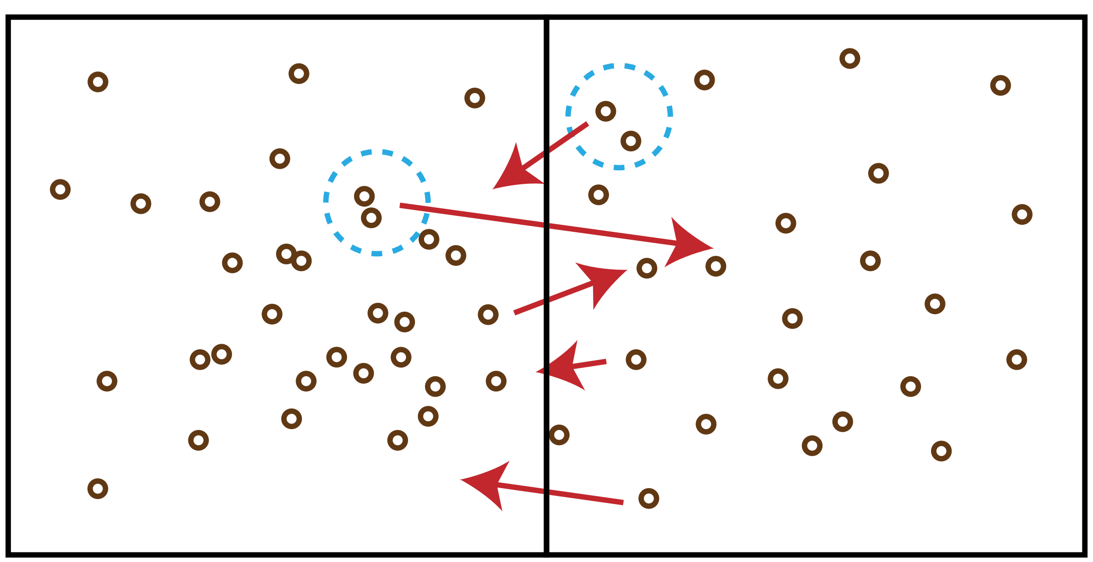
- Godunov's interface modeling: involve Euler physics into numerical scheme

- UGKS: involve kinetic asymptotic-preserving physics instead

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{u}} f = \frac{f^+ - f}{\tau}$$

$$f(\mathbf{x}, t, \mathbf{u}) = \frac{1}{\tau} \int_{t^n}^{t} f^+(\mathbf{x}', t', \mathbf{u}) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_0(\mathbf{x}^n, t^n, \mathbf{u})$$

Interface



Fluxes:

$$F_f = \int_{t^n}^{t^{n+1}} \mathbf{u} \cdot \mathbf{n} f(\mathbf{x}, t, \mathbf{u}) dt$$

$$\mathbf{F_W} = \int_{t^n}^{t^{n+1}} \int \psi \mathbf{u} \cdot \mathbf{n} f(\mathbf{x}, t, \mathbf{u}) d\mathbf{u} dt$$

Numerical implementation of interface fluxes

Construct interface distribution function ($x_{i+1/2}$=0, t^n=0)

$$f\left(0,t,\mathbf{u}_k\right)=\frac{1}{\tau}\int_0^t f^+\left(\mathbf{x}',t',\mathbf{u}_k'\right)e^{-\left(t-t'\right)/\tau}dt'+e^{-t/\tau}f_0\left(\mathbf{x}^0,0,\mathbf{u}_k^0\right)$$

particle trajectories under acceleration **a** (no forcing —> forcing)

$$\mathbf{x}'=\mathbf{x}-\mathbf{u}\left(t-t'\right)\longrightarrow\mathbf{x}'=\mathbf{x}-\mathbf{u}'\left(t-t'\right)-\frac{1}{2}\mathbf{a}\left(t-t'\right)^2,\quad\mathbf{u}'=\mathbf{u}-\mathbf{a}\left(t-t'\right)$$

initial distribution f_0:

$$f_0\left(x,0,u_k\right)=\begin{cases}f^L_{i+1/2,k}+\sigma_{i,k}x, & x\le 0\\ f^R_{i+1/2,k}+\sigma_{i+1,k}x, & x>0\end{cases}$$

$$\sigma_{i,k}=\left(\mathrm{sign}\left(s_1\right)+\mathrm{sign}\left(s_2\right)\right)\frac{|s_1||s_2|}{|s_1|+|s_2|}$$

$$s_1=\left(f_{i,k}-f_{i-1,k}\right)/\left(x_i-x_{i-1}\right)$$

$$s_2=\left(f_{i+1,k}-f_{i,k}\right)/\left(x_{i+1}-x_i\right)$$

equilibrium distribution f^+:

$$f^+=f_0^+\left(1+\theta x+\eta t\right)$$

$$\frac{\partial\mathbf{W}}{\partial x}=\int\theta f_0^+\psi du$$

$$\frac{\partial\mathbf{W}}{\partial t}=\int\eta f_0^+\psi du$$

Numerical implementation of interface fluxes

Interface distribution function

$$
\begin{aligned}
f(0,t,u_k) = &\left(1 - e^{-t/\tau}\right) f_0^+ \\
&+ \left[\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right] \theta u_k f_0^+ \\
&- \left[\tau\left(\tau(-1 + e^{-t/\tau}) + te^{-t/\tau}\right) + \frac{1}{2}t^2 e^{-t/\tau}\right] \theta a f_0^+ \\
&+ \tau\left(t/\tau - 1 + e^{-t/\tau}\right) \eta f_0^+
\end{aligned}
$$

equilibrium part
(collision contribution)

$$
\begin{aligned}
&+ e^{-t/\tau}\left[\left(f^L_{i+1/2,k^0} - \left(u_k - \frac{1}{2}at^2\right)\sigma_{i,k^0}\right) H[u_k - \frac{1}{2}at] \right. \\
&\left. + \left(f^R_{i+1/2,k^0} - \left(u_k t - \frac{1}{2}at^2\right)\sigma_{i+1,k^0}\right)(1 - H[u_k - \frac{1}{2}at])\right]
\end{aligned}
$$

initial part
(particle transport contribution)

Fluxes

$$
F_{f_k} = \int_{t^n+1}^{t^{n+1}} u_k f(0,t,u_k) dt
$$

$$
\mathbf{F_W} = \int_{t^n}^{t^{n+1}} \sum_k \psi u_k f(0,t,u_k) dt
$$

In-cell modeling

Boltzmann collision operator

$$Q(f) = \int_{-\infty}^{\infty} \int_{0}^{4\pi} (f^* f_1^* - f f_1) g_r \sigma d\mathbf{\Omega} d\mathbf{u}_1$$

FFT-based fast spectral method with computational cost O(MN³ logN)

$\hat{f} = \text{ FFTSHIFT } \{\text{IFFT}[\text{FFTSHIFT } (f)]\}$ 1

$Q^+ = 0$

For $\theta_p = (1, 2, \cdots, M-1)\pi/M$

For $\varphi_q = (1, 2, \cdots, M)\pi/M$ 2

End

End

$\text{Q}^+ = \left(4\pi^2/\text{Kn}' M^2\right) \text{FFTSHIFT} \left[\Re\left(Q^+\right)\right]$

$\nu = \left(4\pi^2/\text{Kn}' M^2\right) \text{ FFTSHIFT } \left\{\Re\left[\text{ FFT } \left[\text{ FFTSHIFT } \left(\hat{f} \cdot \phi_{\text{ loss}}\right)\right]\right]\right\}$ 3

$Q^- = \nu f$

$Q = Q^+ - Q^-$ 4

[1] Mouhot, C., and Pareschi, L. (2006)
[2] Wu, L., White, C., Scanlon, T. J., Reese, J. M., and Zhang, Y. (2013)
[3] Gamba, I. M., Haack, J. R., Hauck, C. D., & Hu, J. (2017)
[4] Jaiswal, S., Alexeenko, A. A., and Hu, J. (2019)

FFTSHIFT: shift the zero-frequency component to the center of spectrum, IFFT: inverse FFT, R: real part

Numerical implementation of collision term

Shakhov relaxation model O(N³) ~ 20x faster

$$Q(f) = \frac{f^+ - f}{\tau}$$

$$f^+ = \rho\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{m}{2kT}(\mathbf{u}-\mathbf{U})^2}\left[1+(1-Pr)\mathbf{c}\cdot\mathbf{q}\left(\mathbf{c}^2\frac{m}{kT}-5\right)\frac{m}{5pkT}\right]$$

Boltzmann operator coupled with BGK term in a penalty way

$$\int_{t^n}^{t^{n+1}} Q\left(f_{i,k}\right) dt = \Delta t\left[\exp\left(-\Delta t/\tau_i^{n+1}\right) Q\left(f_{i,k}^n, f_{i,k}^n\right) + \left(1-\exp\left(-\Delta t/\tau_i^{n+1}\right)\right)\frac{f_{i,k}^{(n+1)+} - f_{i,k}^{n+1}}{\tau_i^{n+1}}\right]$$

[1] Filbet, F., and Jin, S. (2010).

Numerical implementation of solution algorithm

Update conservative variables

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x_i}(F^W_{i-1/2} - F^W_{i+1/2}) + \frac{1}{\Delta x_i}\int_{t^n}^{t^{n+1}} \mathbf{G}_i dt$$

Update particle distribution function

$$f_{i,k}^{n+1} = f_{i,k}^n + \frac{1}{\Delta x_i}\left(F^f_{i-1/2,k} - F^f_{i+1/2,k}\right) + \frac{\Delta t}{2}\left[\frac{f_{i,k}^{+(n+1)} - f_{i,k}^{n+1}}{\tau^{n+1}} + Q(f_{i,k}^n)\right] - a\frac{\Delta t}{2}\left(\frac{\partial}{\partial u}f_{i,k}^{n+1} + \frac{\partial}{\partial u}f_{i,k}^n\right)$$

full Boltzmann integration / BGK-type relaxation term

upwind difference over velocity space

NO staggered grid or iterative techniques are needed to achieve asymptotic-preserving property

Well-balanced discrete velocity method

well-balanced property is precisely preserved

$$\rho_0 = p_0 = e^{-x}$$

$$p = p_0 + 0.01e^{-100(x-0.5)^2}$$

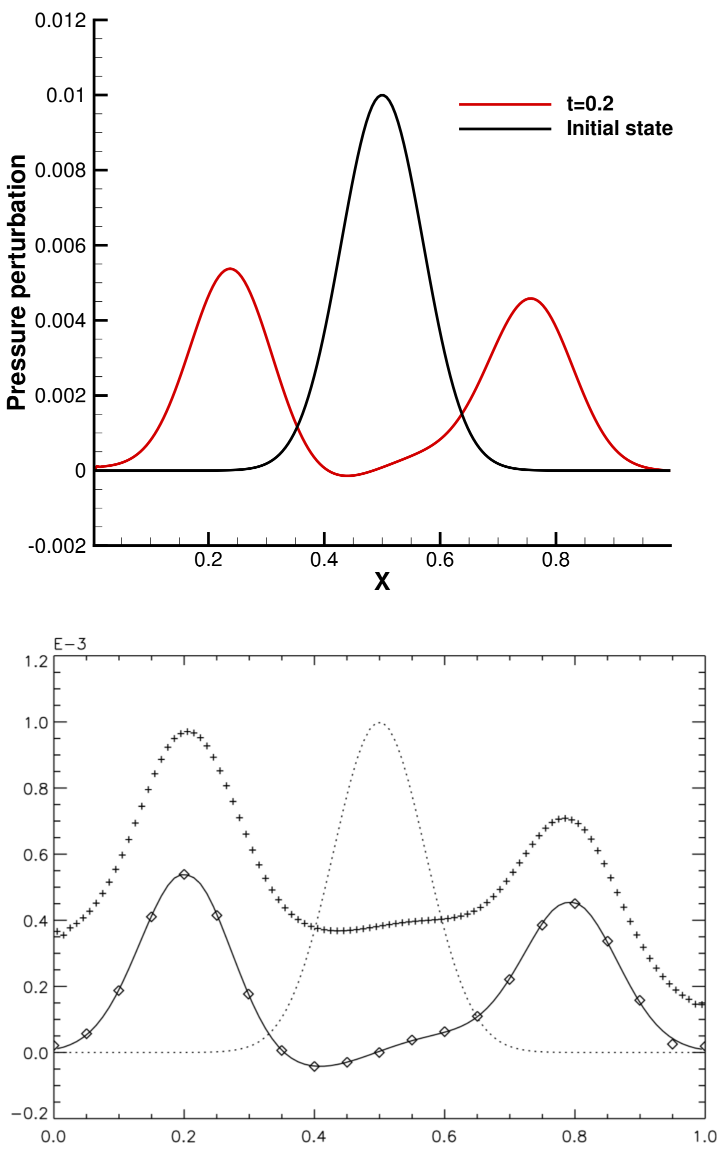


Figure: hydrostatic solution + perturbation

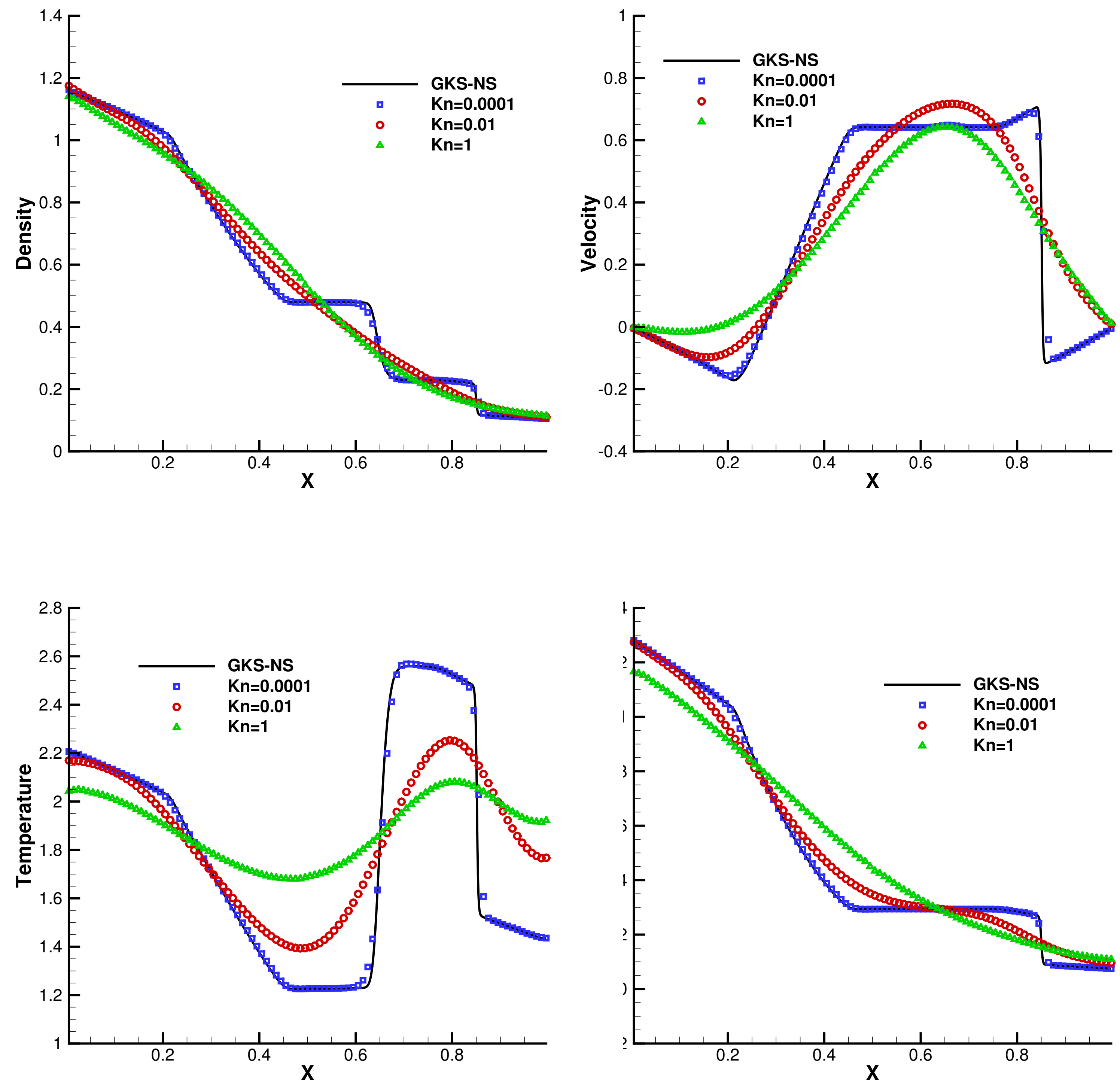
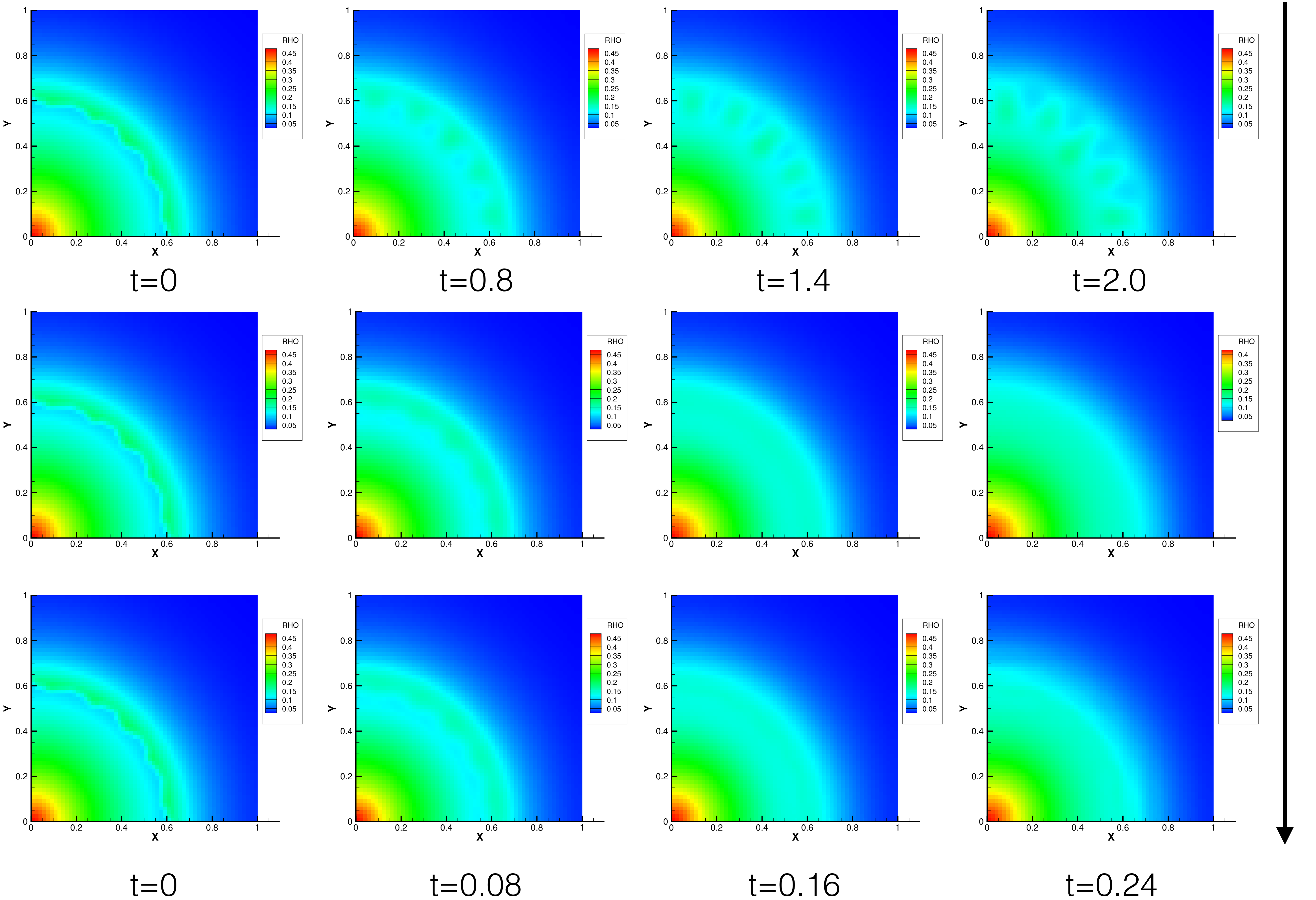


Figure: Sod shock tube under external force field

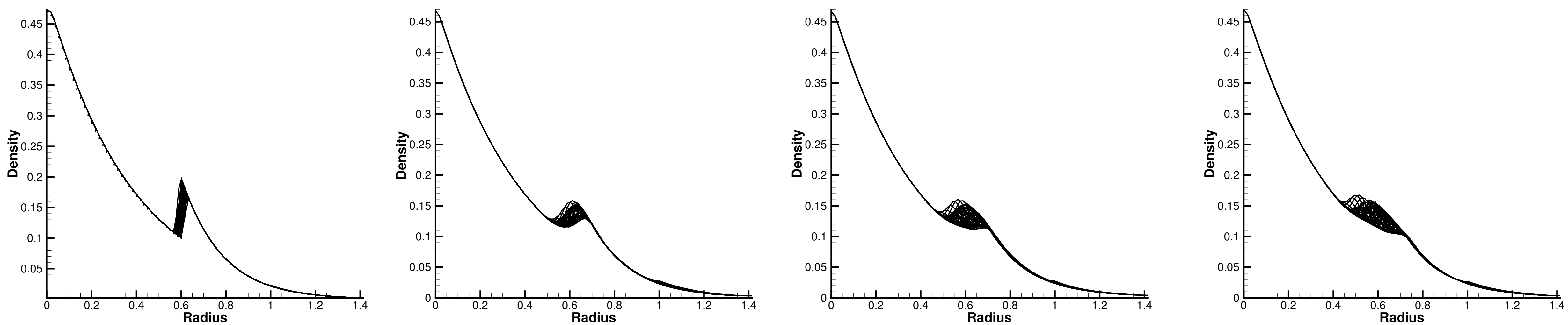
Rayleigh-Taylor Instability

Kn



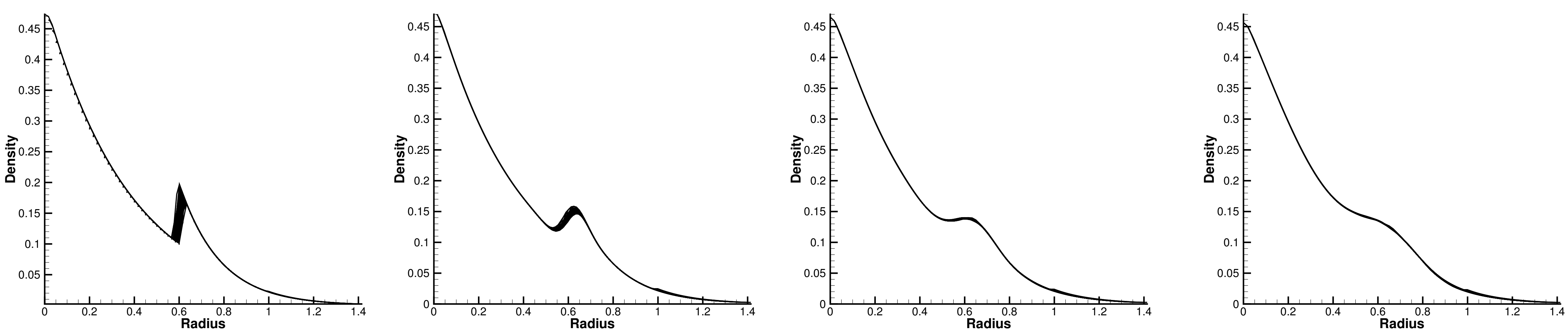
Rayleigh-Taylor Instability

Kn=0.0001



t=0 t=0.8 t=1.4 t=2.0

Kn=0.01



t=0 t=0.08 t=0.16 t=0.24

Figure: Density evolution along radial direction

Non-equilibrium heat transfer: theoretical analysis

Integral solution of BGK equation

$$f\left(0,t,u\right)=\frac{1}{\tau}\int_0^t f^+\left(x',t',u'\right)e^{-\left(t-t'\right)/\tau}dt'+e^{-t/\tau}f_0\left(-ut+\frac{1}{2}at^2,0,u-at\right)$$

Taylor expansion

$$\tilde{f}_0=e^{-t/\tau}\left[f_0(0,0,u)-\frac{\partial f_0}{\partial x}ut-\frac{\partial f_0}{\partial u}at\right]+O\left(t^2\right)$$

Assume homogeneous field and Maxwellian in initial distribution f_0

$$\Delta q=\frac{e^{-t/\tau}}{2}\int(u-U)^3\left(-taf_u^+\right)du$$

Linear theory

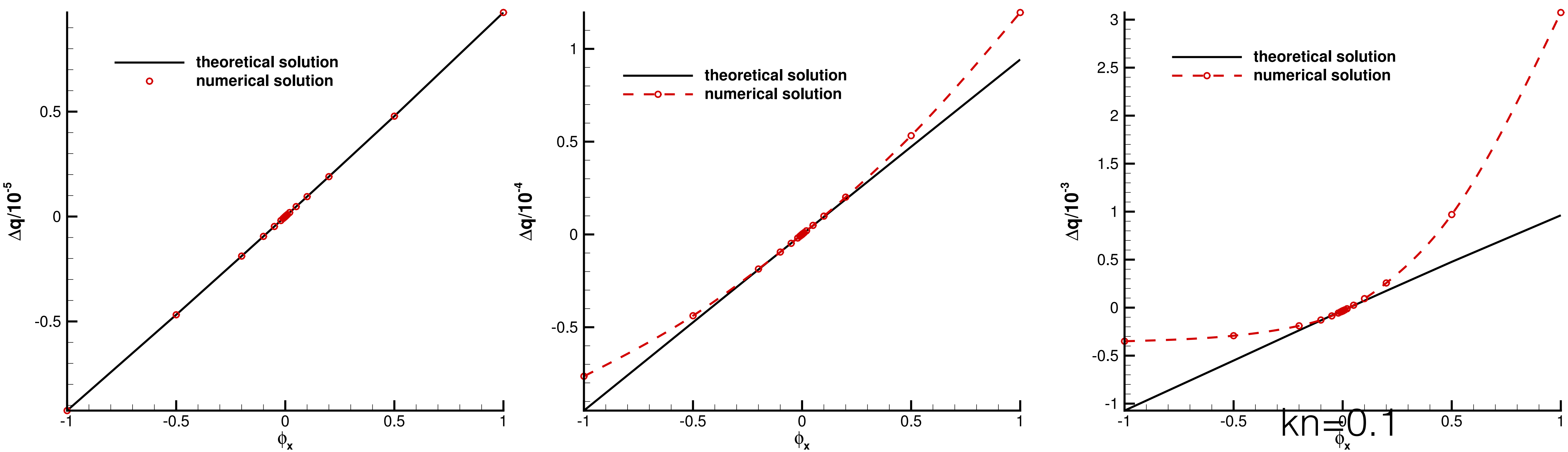
$$\mathbf{q}_{force}=\frac{5\rho kT}{2m}\sigma e^{-\sigma/\tau}\mathbf{a}$$

[1] Xiao, T., Xu, K., Cai, Q., and Qian, T. (2018). An investigation of non-equilibrium heat transport in a gas system under external force field. *International Journal of Heat and Mass Transfer*, *126*, 362-379.

Non-equilibrium heat transfer: numerical experiments

Fourier flow between two infinite plates
Kn=0.001, 0.01, 0.1 and **a** varies from -1 to 1

$$\Delta q = q_{kinetic} - q_{fourier}$$



kn=0.1

kn=0.001

kn=0.01

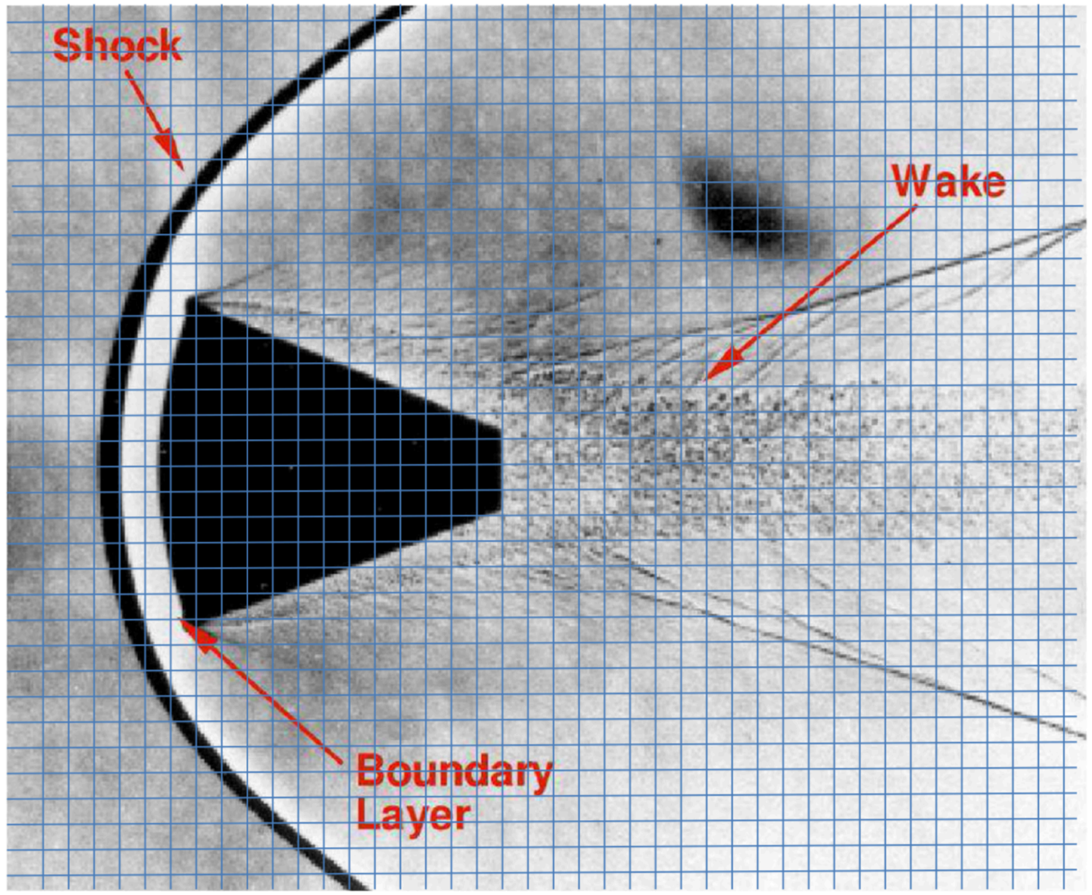
Figure: force-induced heat flux in Fourier flow (line: theoretical solutions, points: numerical results)

[1] Xiao, T., Xu, K., Cai, Q., and Qian, T. (2018). An investigation of non-equilibrium heat transport in a gas system under external force field. *International Journal of Heat and Mass Transfer*, *126*, 362-379.

2. High Speed Flows

- Computational deficiency and memory burden of AP scheme (**discretized velocity space**)

- No necessary for near-equilibrium region



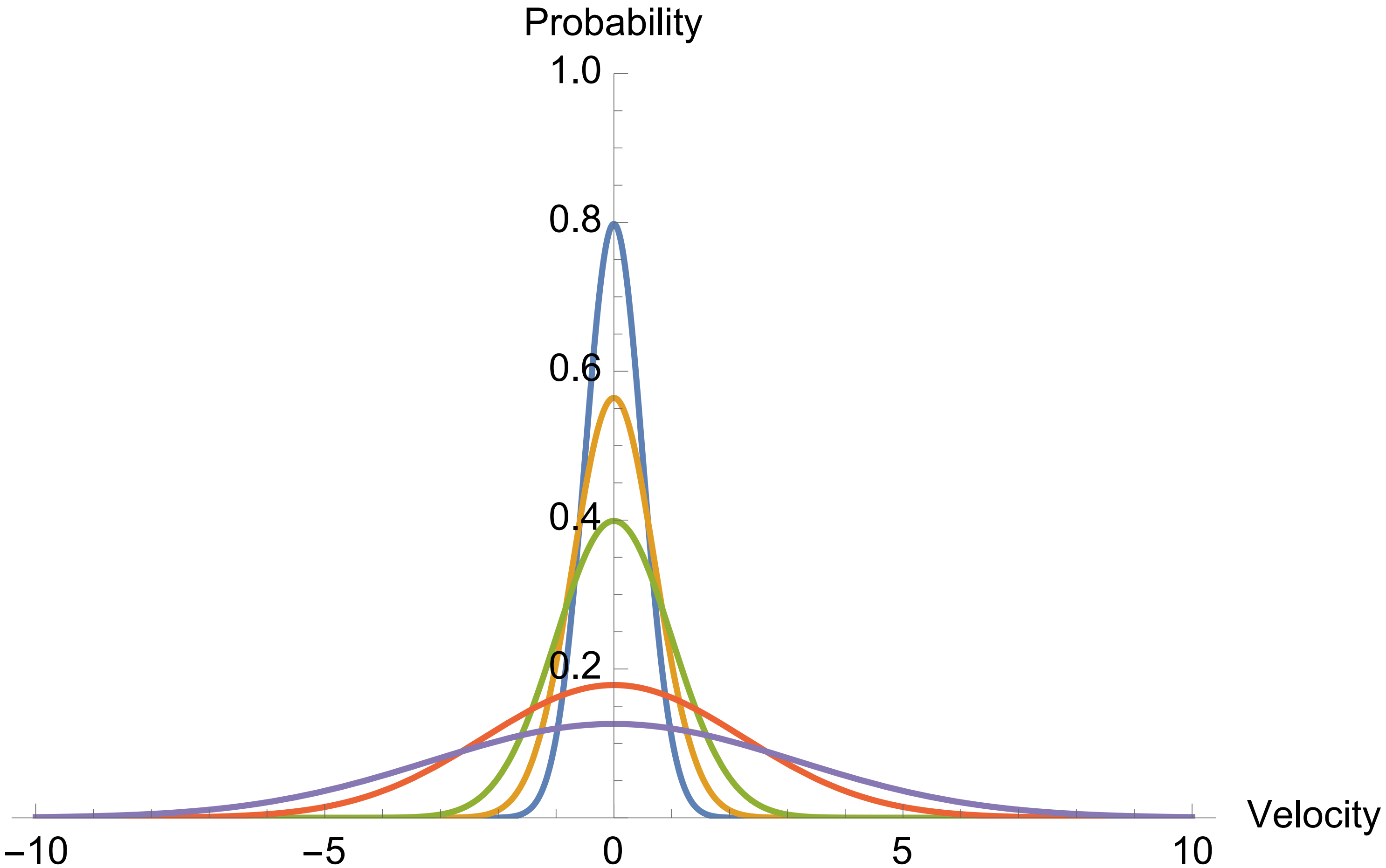


Figure: Supersonic flow around vehicle and particle distribution function versus temperature

Near-equilibrium gas kinetic scheme

Near-equilibrium: no need to update distribution function

$$\mathbf{W}^{n+1} = \mathbf{W}^n + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_r^W dt$$

$$\cancel{f^{n+1} = f^n + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_r^f dt + \int_{t^n}^{t^{n+1}} Q(f) dt}$$

Formulation of distribution function continuously:
Chapman-Enskog ansatz / moment methods / data driven

$$f = f^+[1 - \tau(\mathbf{a} \cdot \mathbf{u} + A)] \qquad f = f^+ \left(1 + \frac{p_{ij}}{2pRT} c_i c_j - \frac{S_i c_i}{2pRT} \left(1 - \frac{c^2}{5RT}\right)\right)$$

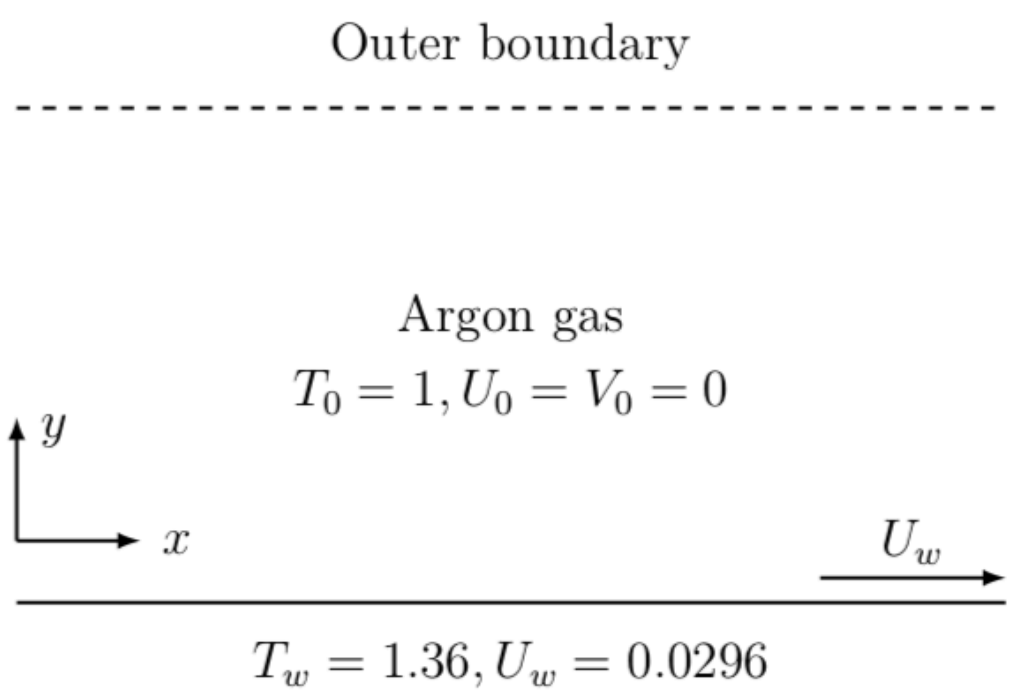
$$F = \mathcal{M}(\boldsymbol{\alpha}) \equiv \exp\left(\mathbf{a}^T \mathbf{m}(v)\right) \qquad \mathcal{B}(\boldsymbol{\alpha}) := \eta'_* \left(\boldsymbol{\alpha}^T \mathbf{m}\right) = \frac{2h\nu^3}{c^2} \frac{1}{\exp\left(-\frac{h\nu c}{k} \boldsymbol{\alpha}^T \mathbf{m}\right) - 1}$$

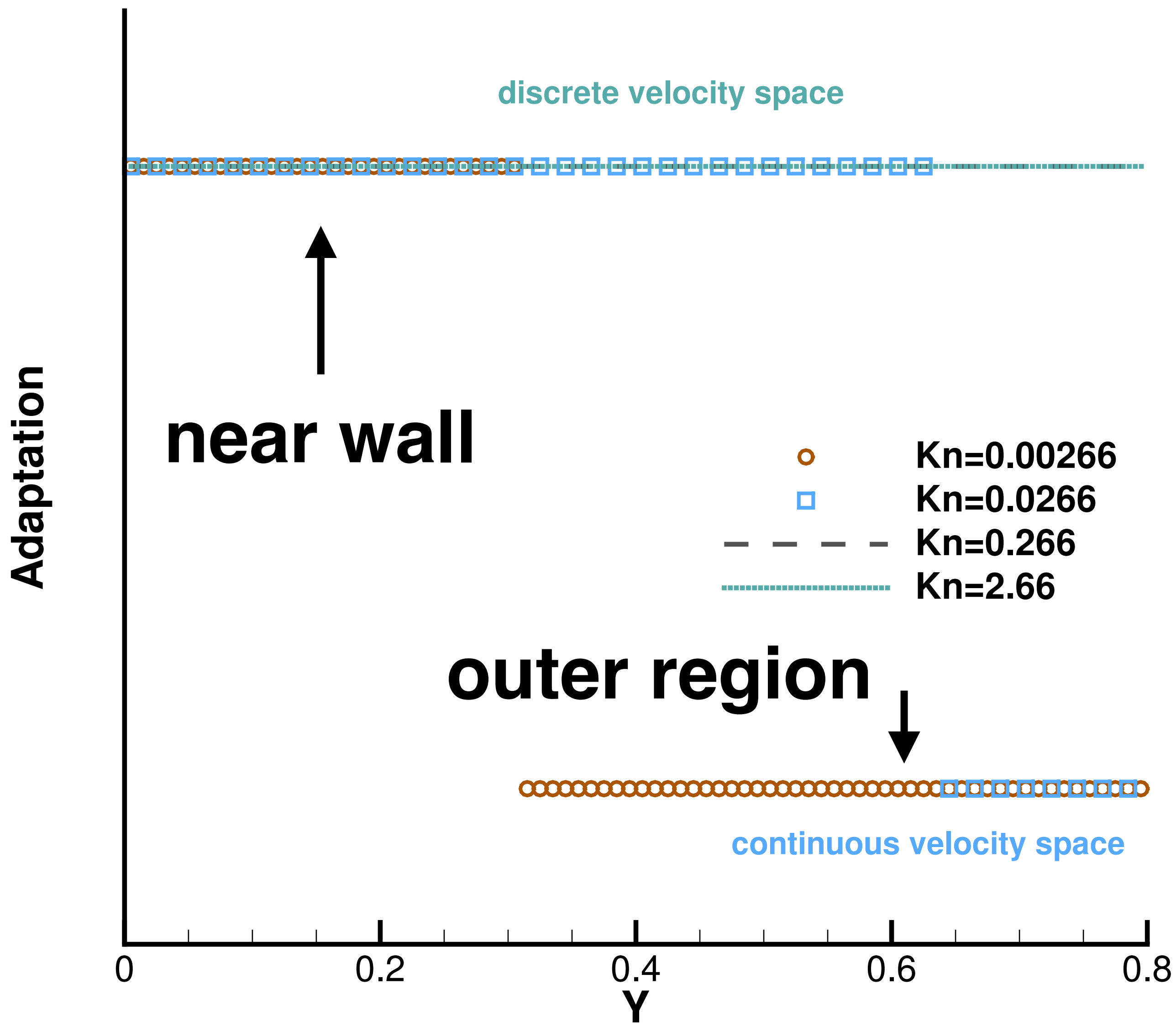
Also further coupled with quadtree mesh in phase space

[1] Levermore, C. D. (1996)
[2] Frank, M., Hauck C. D., Olbrant, E. (2013)
[3] Chen, S., Xu, K., Lee, C., and Cai, Q. (2012)

Rayleigh problem

Suddenly moving plate



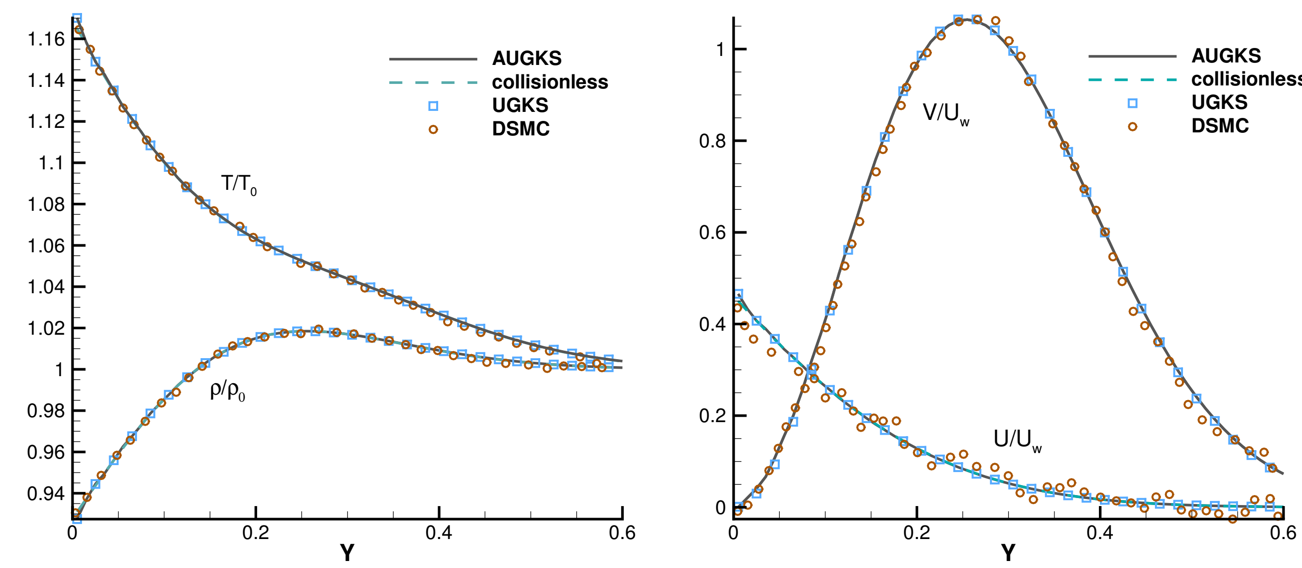


	AUGKS	UGKS
Kn=0.00266	1003.59	7477.10
Kn=0.0266	2223.62	7460.21
Kn=0.266	3751.75.	7438.06
Kn=2.66	4637.19	7457.87

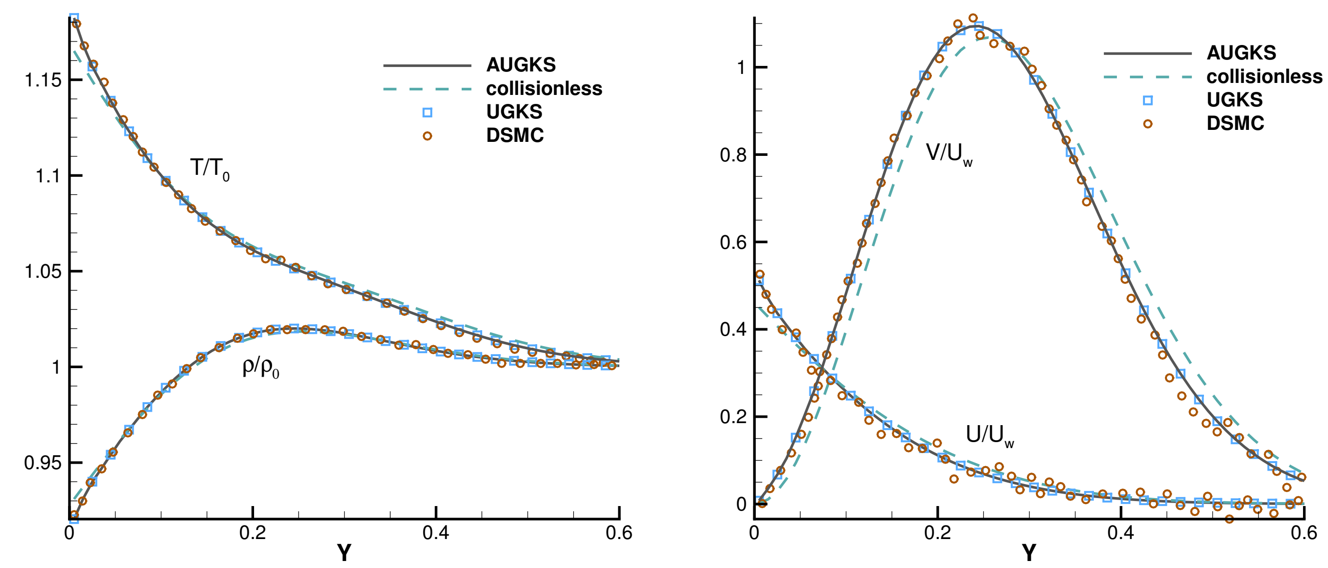
up to 7.45x faster

Figure: Computational cost and velocity space adaptation in the Rayleigh problem

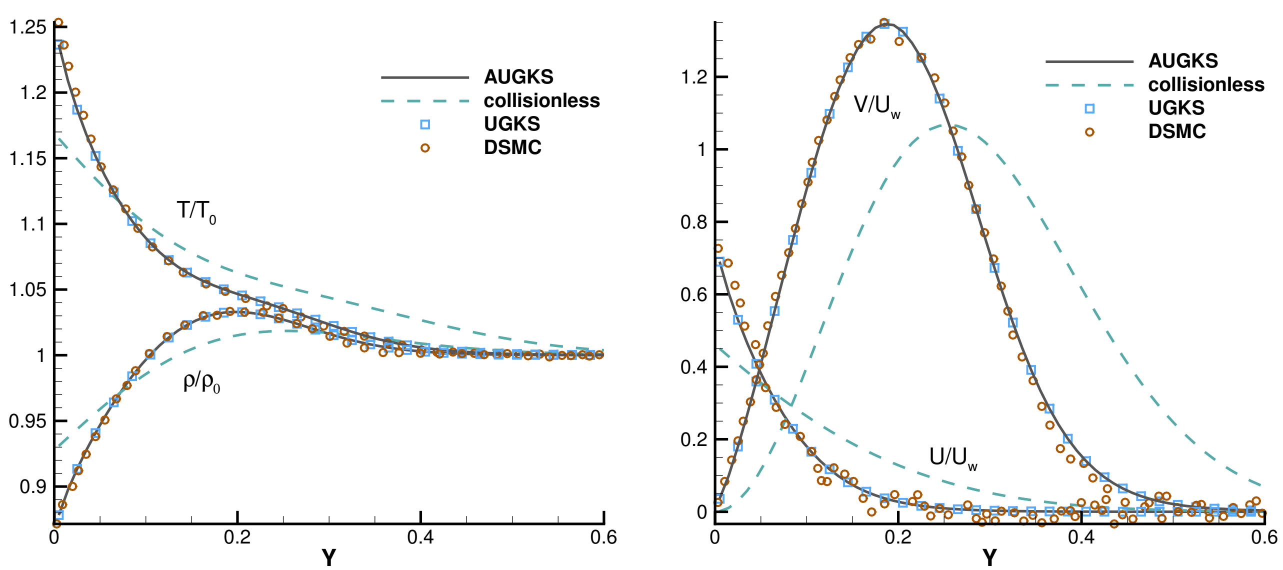
Rayleigh problem



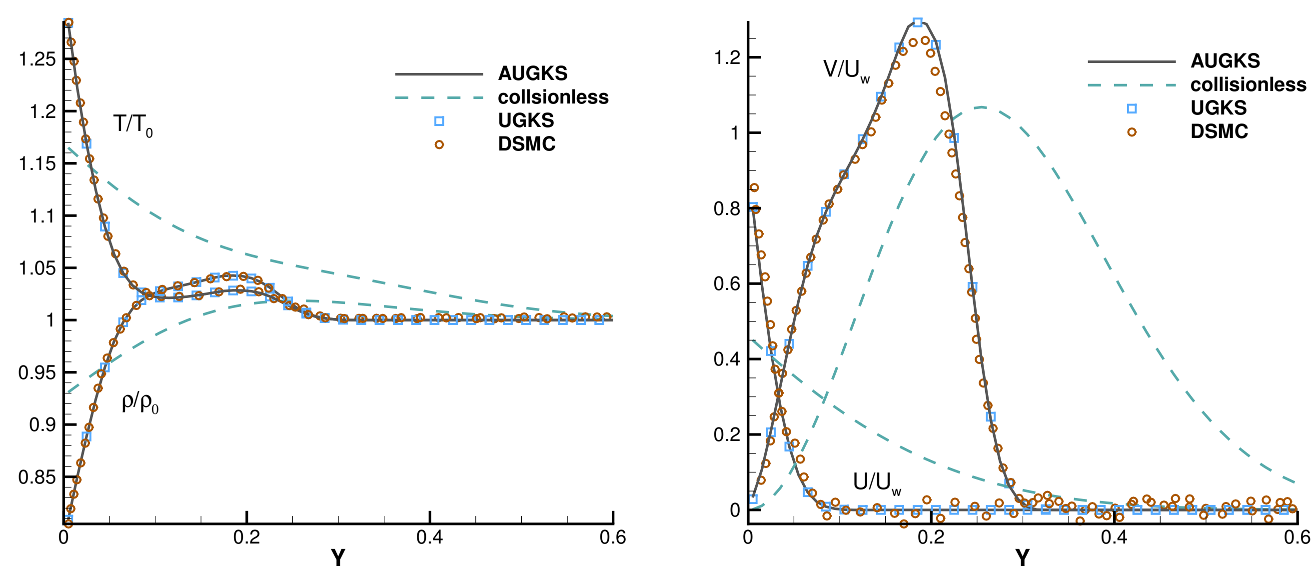
t=0.1 \tau_0, Kn=2.66



t=\tau_0, Kn=0.266



t=10 \tau_0, Kn=0.0266



t=100 \tau_0, Kn=0.00266

Figure: Solutions at different Knudsen number in the Rayleigh flow

Ma5 cylinder

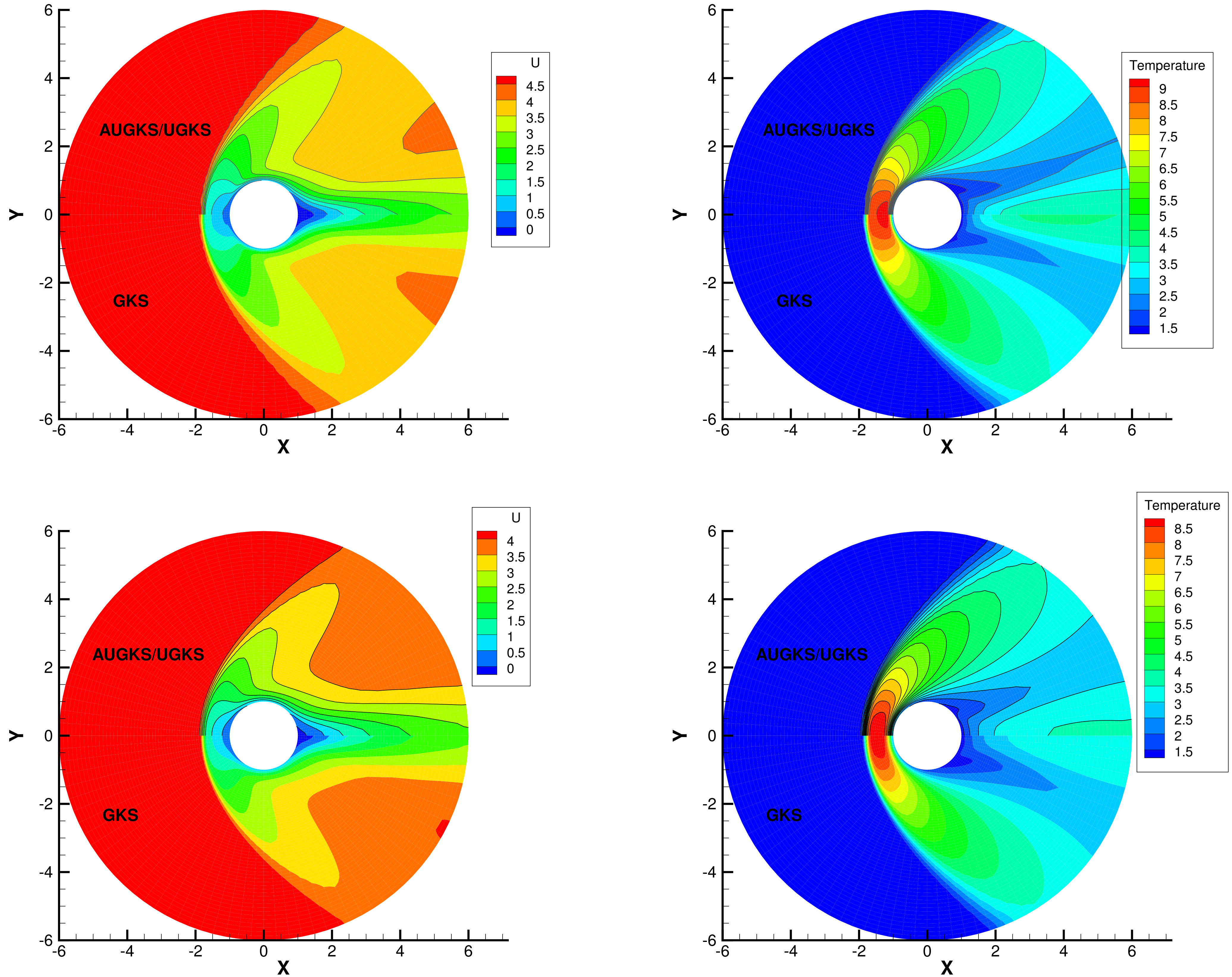


Figure: U-velocity and Temperature contours at Kn=0.001 and 0.01

Ma5 cylinder

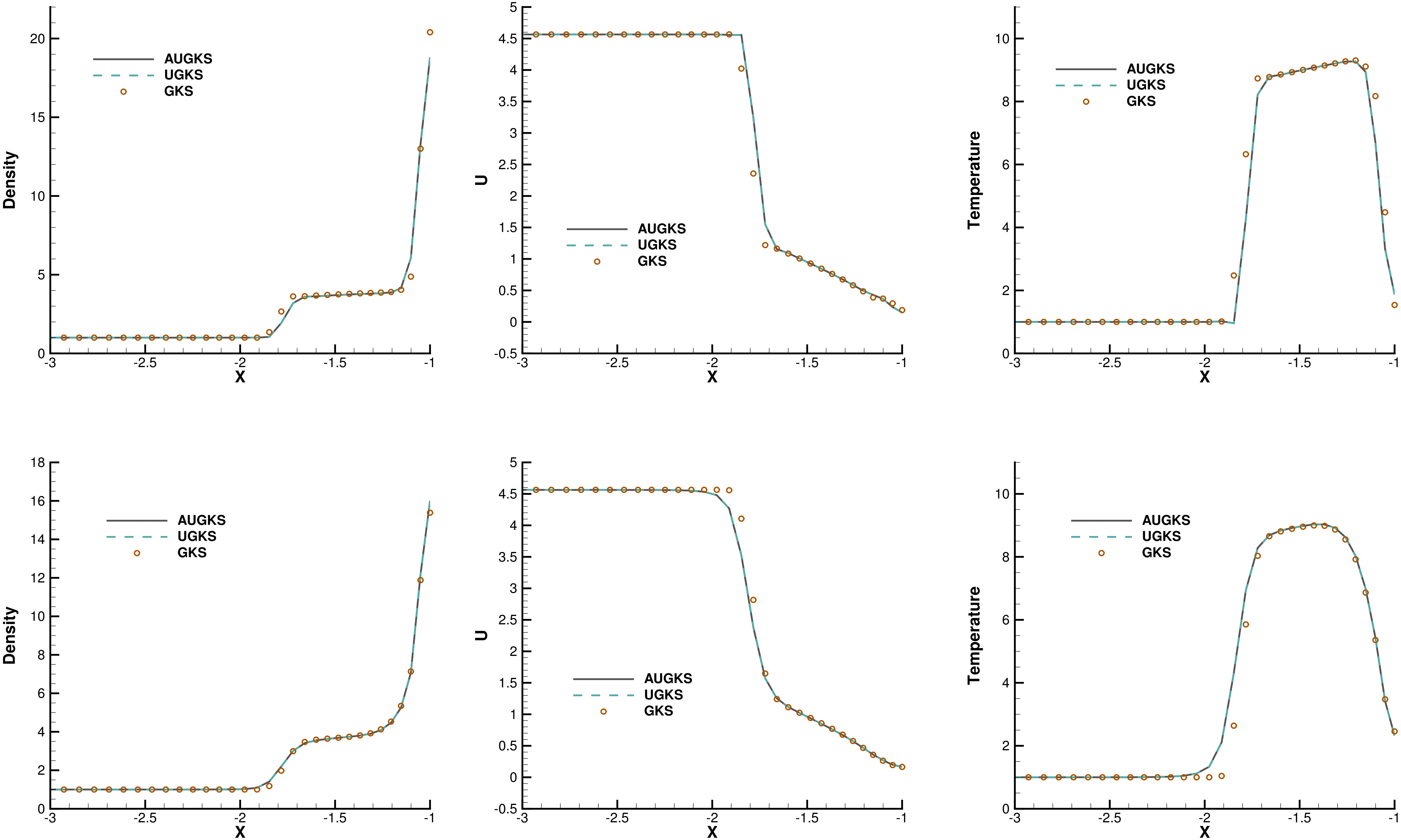


Figure: Solutions along the horizontal central line in front of cylinder at Kn=0.001 and 0.01

Ma5 cylinder

	AUGKS	UGKS	GKS
CPU time (s)	36130.68	117371.67	2975.07
Memory (KB)	452508	857520	14652

Kn=0.001
3.25x faster
52% memory

	AUGKS	UGKS	GKS
CPU time (s)	22145.10	75510.33	2536.55
Memory (KB)	614542	856944	12636

Kn=0.01
3.41x speed
72% memory

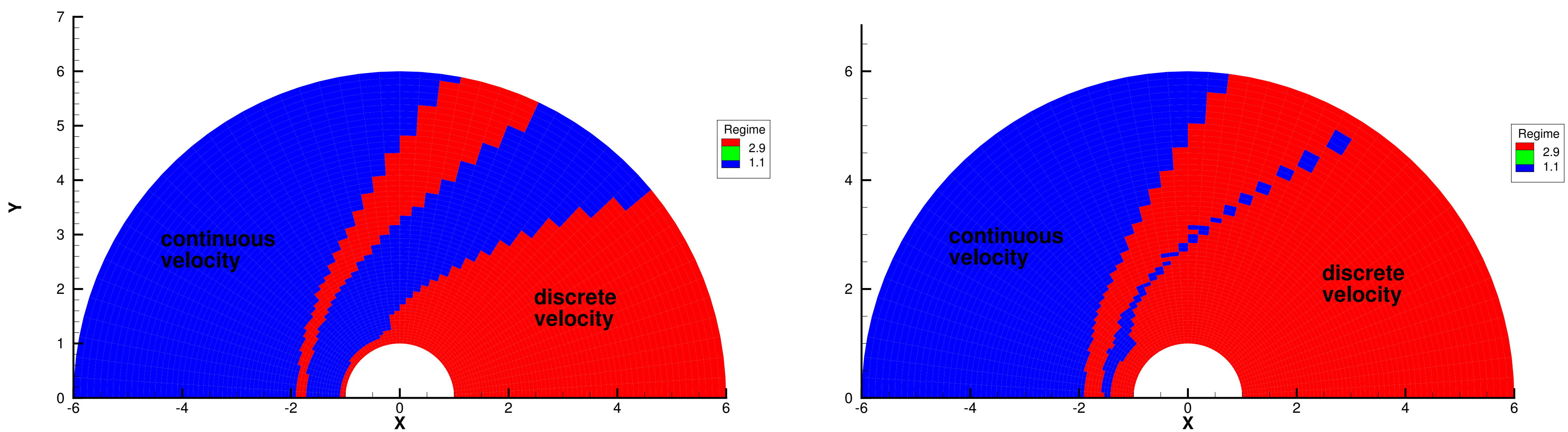
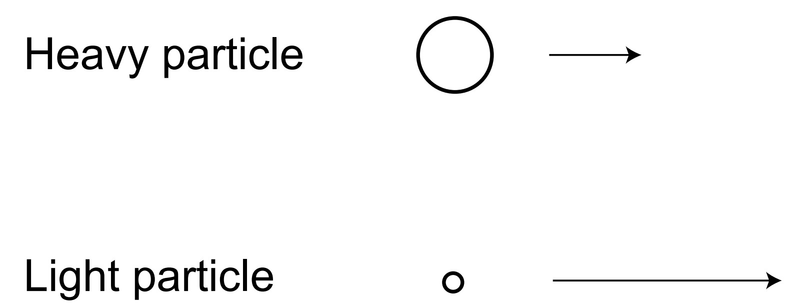


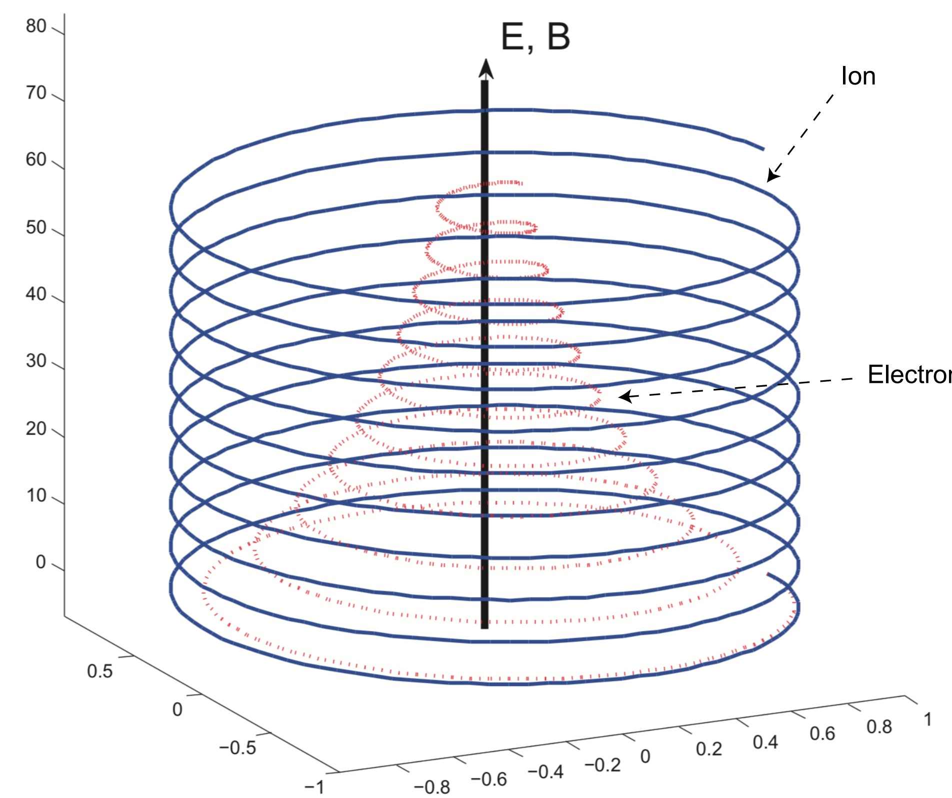
Figure: Computational cost and velocity space adaptation for cylinder flow at Kn=0.001 and 0.01

3. Multicomponent Gas and Plasma

- Additional degree of freedom
- Boltzmann equation: consider interspecies collision
- Fluid dynamic equations: additional equations for volume fraction, mass fraction or ratio of specific heat

“Plasma applications: a wide range of **n(10^6 ~ 10^{34} m^{-3})** and **kTe(0.1 ~ 10^6 eV)**.
...
Plasmas behave sometimes like fluids, and sometimes like a collection of individual particles.”





[1] Chen, F. F. (2012). *Introduction to plasma physics*. Springer Science & Business Media.

UGKS for multicomponent gas dynamics

Finite volume framework for gas mixture

$$\mathbf{W}_{\alpha}^{n+1} = \mathbf{W}_{\alpha}^{n} + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r} \Delta \mathbf{S}_r \cdot \mathbf{F}_{\alpha,r}^{W} dt + \int_{t^n}^{t^{n+1}} \mathbf{Q}_{\alpha}^{W} dt + \int_{t^n}^{t^{n+1}} \mathbf{G}_{\alpha}^{W} dt,$$

$$f_{\alpha}^{n+1} = f_{\alpha}^{n} + \frac{1}{\Omega_{\mathbf{x}}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_{\alpha,r}^{f} dt + \int_{t^n}^{t^{n+1}} Q_{\alpha}^{f} dt + \int_{t^n}^{t^{n+1}} G_{\alpha}^{f} dt$$

Flux: from BGK model for multicomponent gas interaction[1]

$$f_{\alpha}^{+} = n_{\alpha} \left(\frac{m_{\alpha}}{2\pi k_B \overline{T}_{\alpha}} \right)^{\frac{3}{2}} \exp\left(-\frac{m_{\alpha}}{2 k_B \overline{T}_{\alpha}} \left(\mathbf{u}_{\alpha} - \overline{\mathbf{U}}_{\alpha} \right)^2 \right)$$

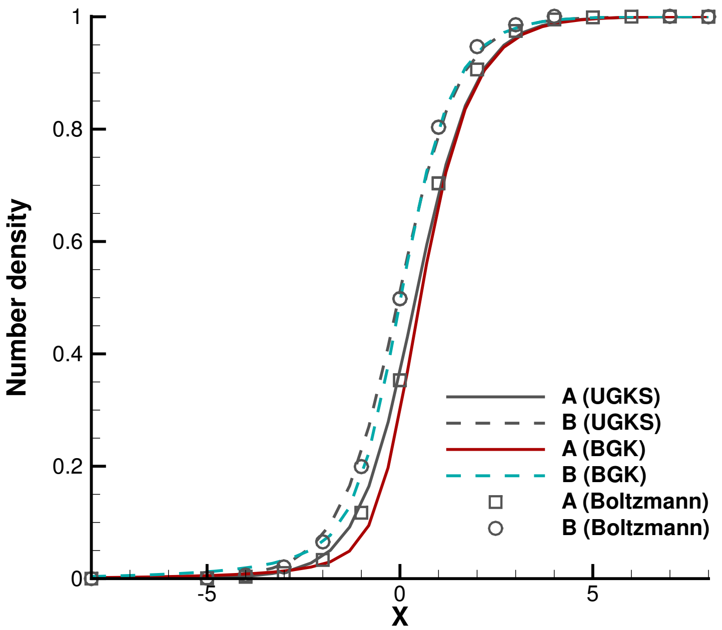
Fictitious variables

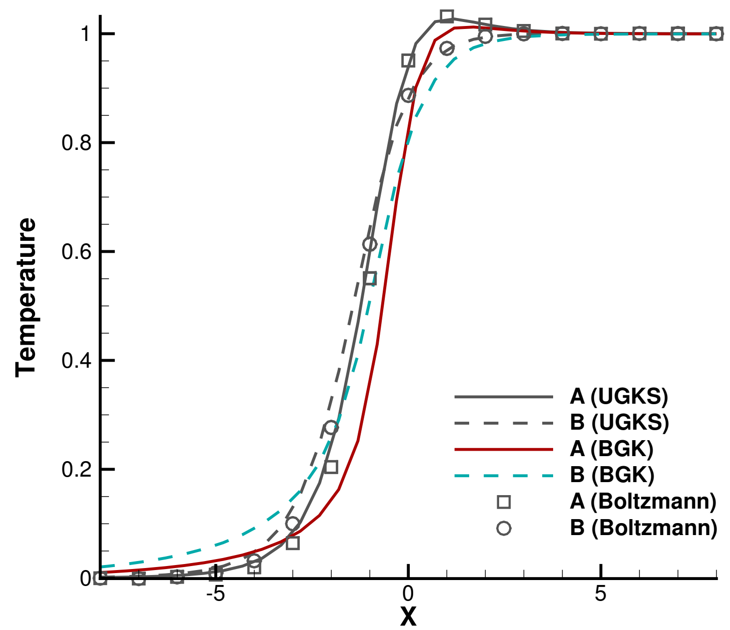
$$\begin{aligned}
&\overline{\mathbf{U}}_{\alpha} = \mathbf{U}_{\alpha} + \tau_{\alpha} \textstyle\sum_r \frac{2 m_r}{m_{\alpha} + m_r} \nu_{\alpha r} \left(\mathbf{U}_r - \mathbf{U}_{\alpha} \right) \\
&\tfrac{3}{2} k_B \overline{T}_{\alpha} = \tfrac{3}{2} k_B T_{\alpha} - \tfrac{m_{\alpha}}{2} \left(\overline{\mathbf{U}}_{\alpha} - \mathbf{U}_{\alpha} \right)^2 \\
&+\tau_{\alpha} \textstyle\sum_r \frac{4 m_{\alpha} m_r}{(m_{\alpha} + m_r)^2} \nu_{\alpha r} \left[\tfrac{3}{2} k_B T_r - \tfrac{3}{2} k_B T_{\alpha} + \tfrac{m_r}{2} \left(\mathbf{U}_r - \mathbf{U}_{\alpha} \right)^2 \right]
\end{aligned}$$

[1] Andries, P., Aoki, K., and Perthame, B. (2002). A consistent BGK-type model for gas mixtures. *Journal of Statistical Physics*, *106*(5-6), 993-1018.

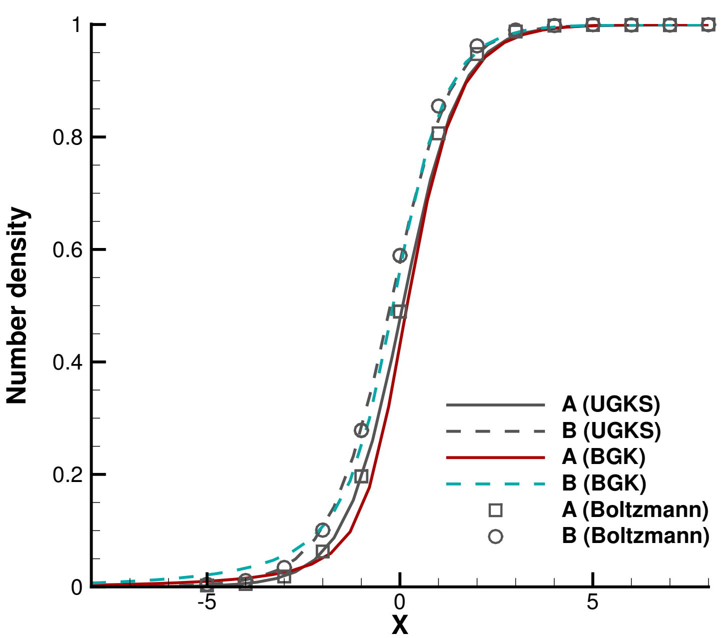
Neutral gas solutions: normal shock structure

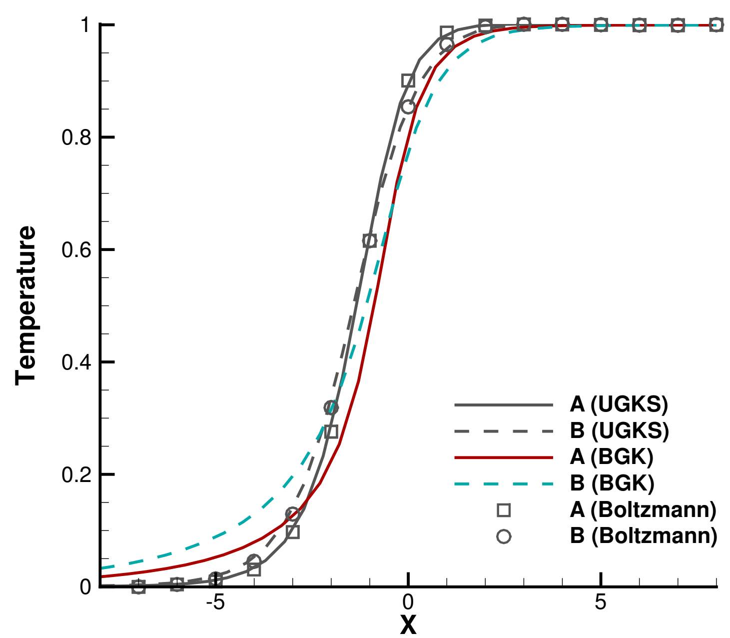
Ma=3.0, $m_B/m_A=0.5$





$n_A/(n_A+n_B)=0.1$





$n_A/(n_A+n_B)=0.9$

UGKS for plasma dynamics

Coupled evolution of electromagnetic field: Maxwell's equations

$$\mathbf{W}_\alpha^{n+1} = \mathbf{W}_\alpha^n + \frac{1}{\Omega_\mathbf{x}} \int_{t^n}^{t^{n+1}} \sum_r \Delta \mathbf{S}_r \cdot \mathbf{F}_{\alpha,r}^W dt + \int_{t^n}^{t^{n+1}} \mathbf{Q}_\alpha^W dt + \int_{t^n}^{t^{n+1}} \mathbf{G}_\alpha^W dt,$$

$$f_\alpha^{n+1} = f_\alpha^n + \frac{1}{\Omega_\mathbf{x}} \int_{t^n}^{t^{n+1}} \sum_{r=1} \Delta \mathbf{S}_r \cdot \mathbf{F}_{\alpha,r}^f dt + \int_{t^n}^{t^{n+1}} Q_\alpha^f dt + \int_{t^n}^{t^{n+1}} G_\alpha^f dt$$

$$\mathbf{M}_\alpha^{n+1} = \mathbf{M}_\alpha^n + \frac{1}{\Omega_\mathbf{x}} \int_{t^n}^{t^{n+1}} \sum_r \Delta \mathbf{S}_r \cdot \mathbf{F}_{\alpha,r}^M dt + \int_{t^n}^{t^{n+1}} \mathbf{S}_\alpha dt$$

$$\begin{aligned} &\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla_\mathbf{x} \times \mathbf{B} = -\frac{1}{\varepsilon_0}\mathbf{j} \\ &\frac{\partial \mathbf{B}}{\partial t} + \nabla_\mathbf{x} \times \mathbf{E} = 0 \\ &\nabla_\mathbf{x} \cdot \mathbf{E} = \frac{\sigma}{\varepsilon_0} \\ &\nabla_\mathbf{x} \cdot \mathbf{B} = 0 \end{aligned} \longrightarrow \begin{aligned} &\frac{\partial \mathbf{E}}{\partial t} - c^2 \nabla_\mathbf{x} \times \mathbf{B} + \chi c^2 \nabla_\mathbf{x} \phi = -\frac{1}{\varepsilon_0}\mathbf{j}, \\ &\frac{\partial \mathbf{B}}{\partial t} + \nabla_\mathbf{x} \times \mathbf{E} + \gamma \nabla_\mathbf{x} \psi = 0, \\ &\frac{1}{\chi}\frac{\partial \phi}{\partial t} + \nabla_\mathbf{x} \cdot \mathbf{E} = \frac{\sigma}{\varepsilon_0}, \\ &\frac{\varepsilon_0 \mu_0}{\gamma}\frac{\partial \psi}{\partial t} + \nabla_\mathbf{x} \cdot \mathbf{B} = 0, \end{aligned}$$

[1] Munz, C. D. et al. (2000)

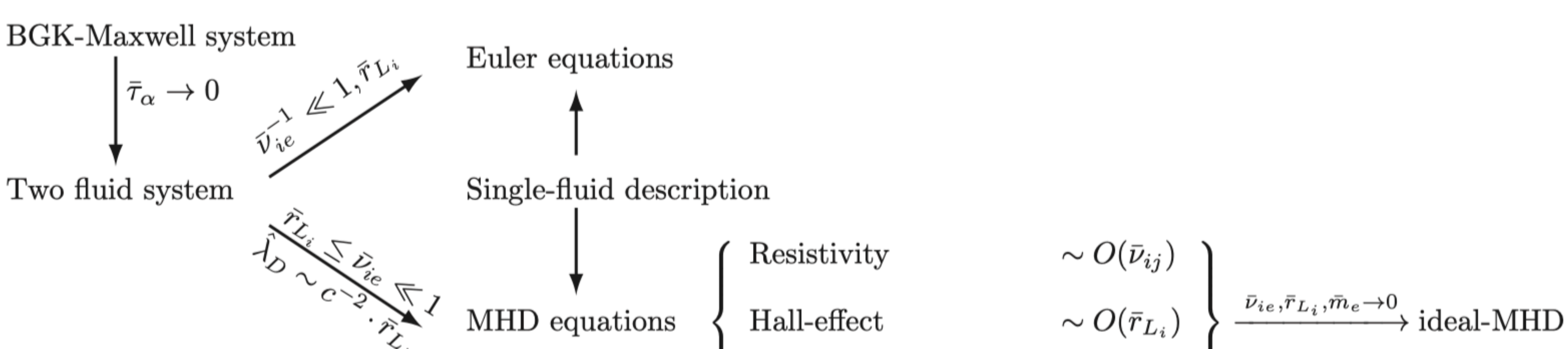
Asymptotic behaviors of UGKS

Kinetic equation

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{u}_\alpha \cdot \nabla_{\mathbf{x}} f_\alpha + \frac{q_\alpha}{m_\alpha}\left(\mathbf{E} + \mathbf{u}_\alpha \times \mathbf{B}\right) \cdot \nabla_{\mathbf{u}} f_\alpha = C_\alpha$$

Asymptotic limits in magnetohydrodynamic regime: ideal MHD, resistive MHD, Hall MHD, Two fluids, **…**

$$\frac{\partial n_\alpha}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_\alpha \mathbf{U}_\alpha) = 0$$
$$\frac{\partial(\rho_\alpha \mathbf{U}_\alpha)}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_\alpha \mathbf{U}_\alpha \mathbf{U}_\alpha) = \nabla_{\mathbf{x}} \cdot \mathbf{P}_\alpha + n_\alpha q_\alpha (\mathbf{E} + \mathbf{U}_\alpha \times \mathbf{B}) + \mathbf{R}_\alpha$$
$$\frac{\partial(\rho_\alpha \mathcal{E}_\alpha)}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_\alpha \mathcal{E}_\alpha \mathbf{U}_\alpha) = \nabla_{\mathbf{x}} \cdot (\mathbf{P}_\alpha \mathbf{U}_\alpha) - \nabla_{\mathbf{x}} \cdot \mathbf{q}_\alpha + \mathbf{U}_\alpha \cdot (n_\alpha q_\alpha \mathbf{E} + \mathbf{R}_\alpha) + H_\alpha$$



MHD regime:

- MHD, resistive MHD, Hall MHD, Two fluid, **…**
- Macroscopic fluid solver

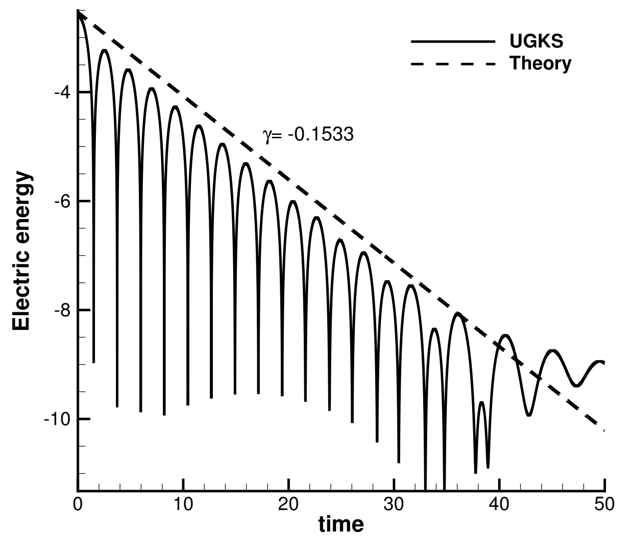
Kinetic regime:

- Fokker-Planck, Vlasov, BGK, **…**
- Gyrokinetic code, PIC, FP solver, **…**

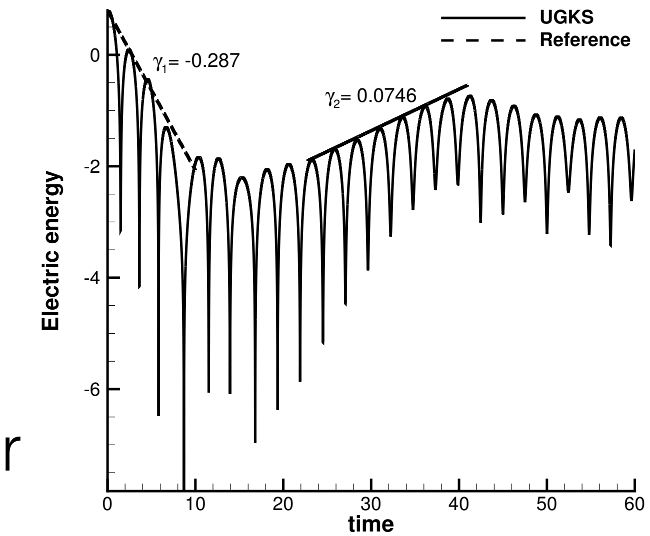
Vlasov solutions

Landau damping

$$f_0(x,u) = \frac{1}{\sqrt{2\pi}}[1+\alpha\cos(kx)]\exp\left(-\frac{u^2}{2}\right)$$



linear

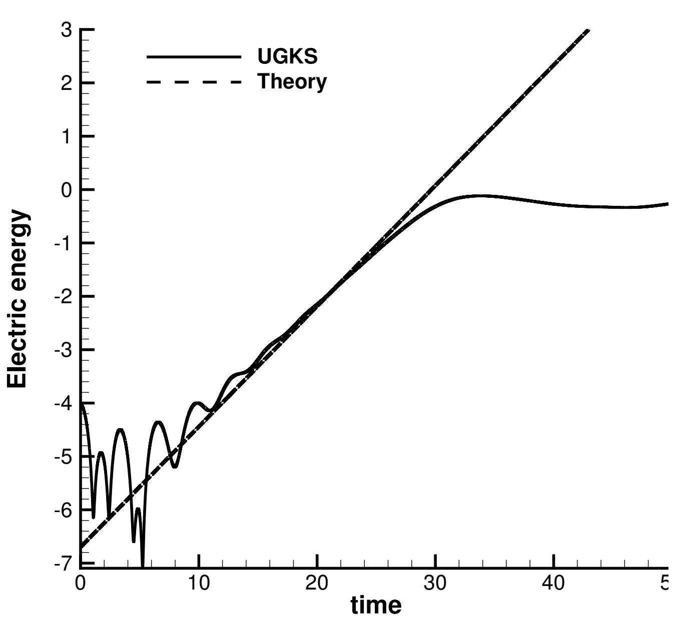


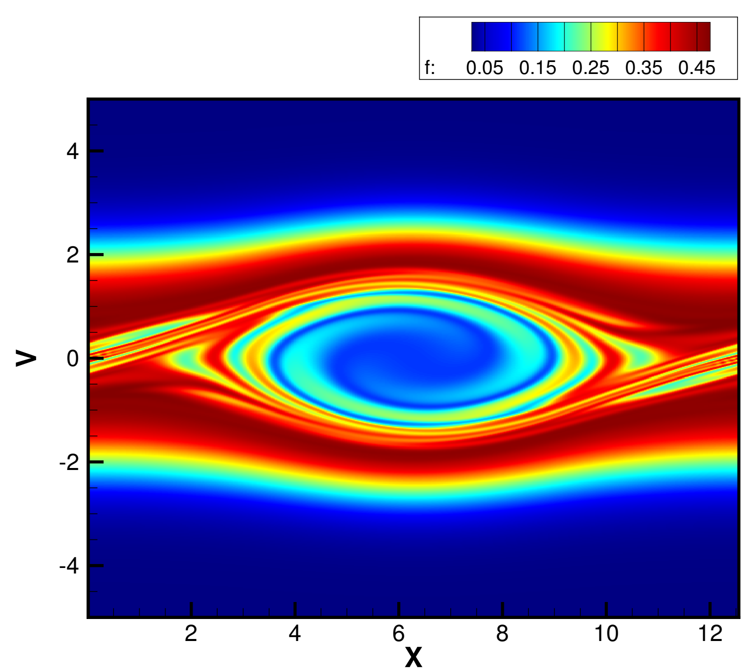
nonlinear

Two-stream instability

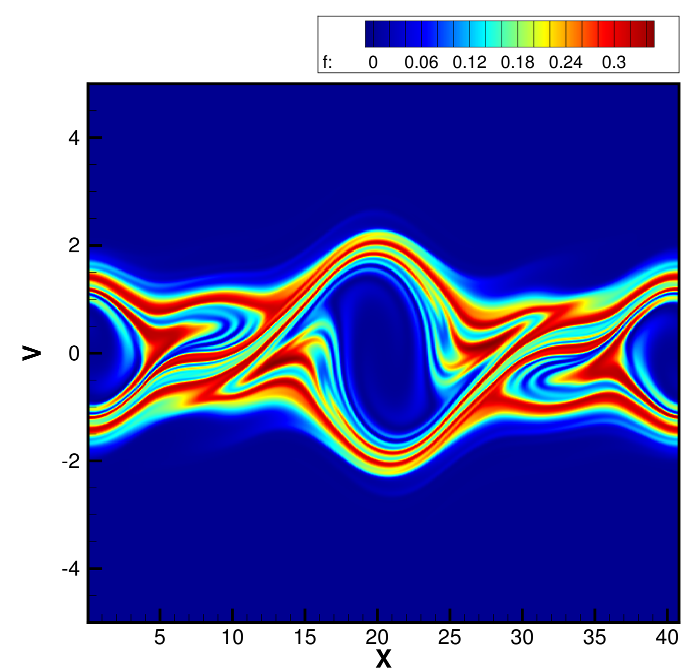
$$f_0(x,u) = \frac{2}{7\sqrt{2\pi}}\left(1+5u^2\right)\left[1+\alpha\left(\frac{\cos(2kx)+\cos(3kx)}{1.2}+\cos(kx)\right)\right]\exp\left(-\frac{u^2}{2}\right)$$

$$f_0(x,u) = \frac{1}{2u_{th}\sqrt{2\pi}}\left[\exp\left(-\frac{(u-U)^2}{2u_{th}^2}\right)+\exp\left(-\frac{(u+U)^2}{2u_{th}^2}\right)\right][1+\alpha\cos(kx)]$$





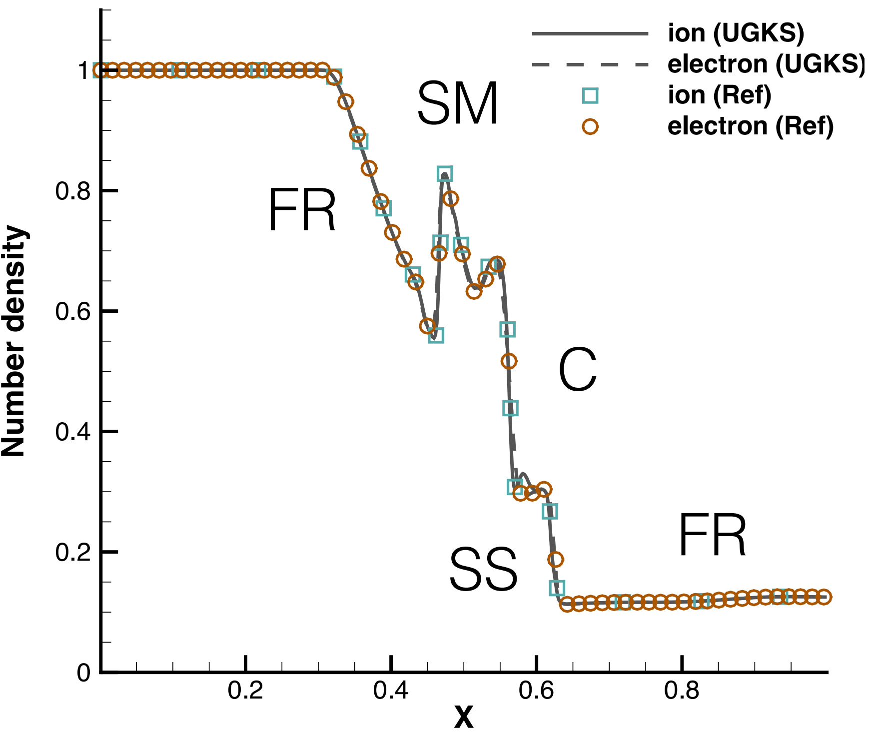
linear

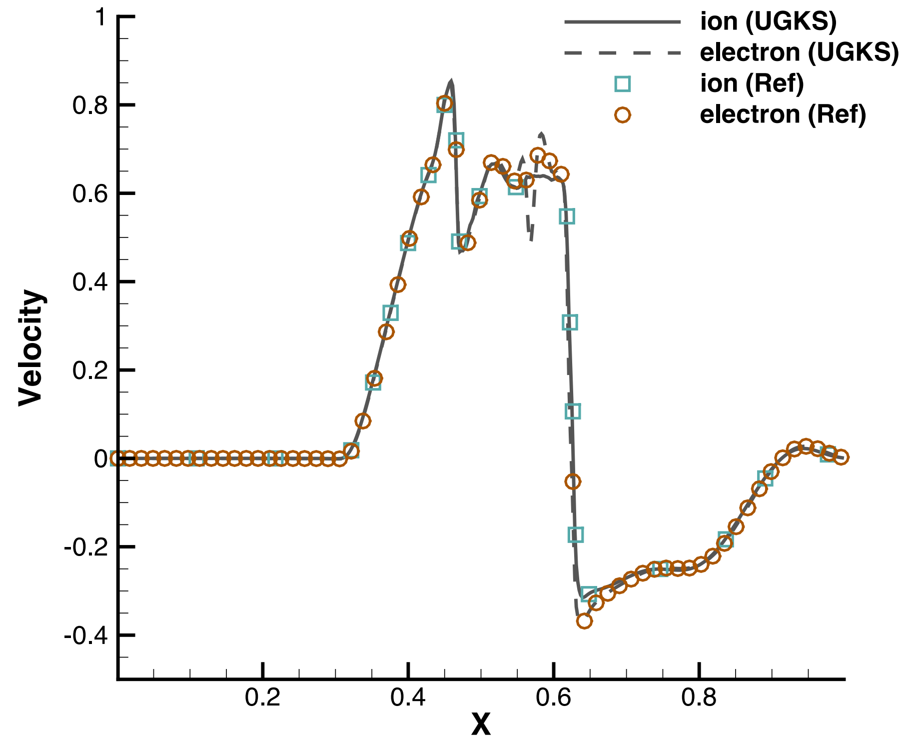


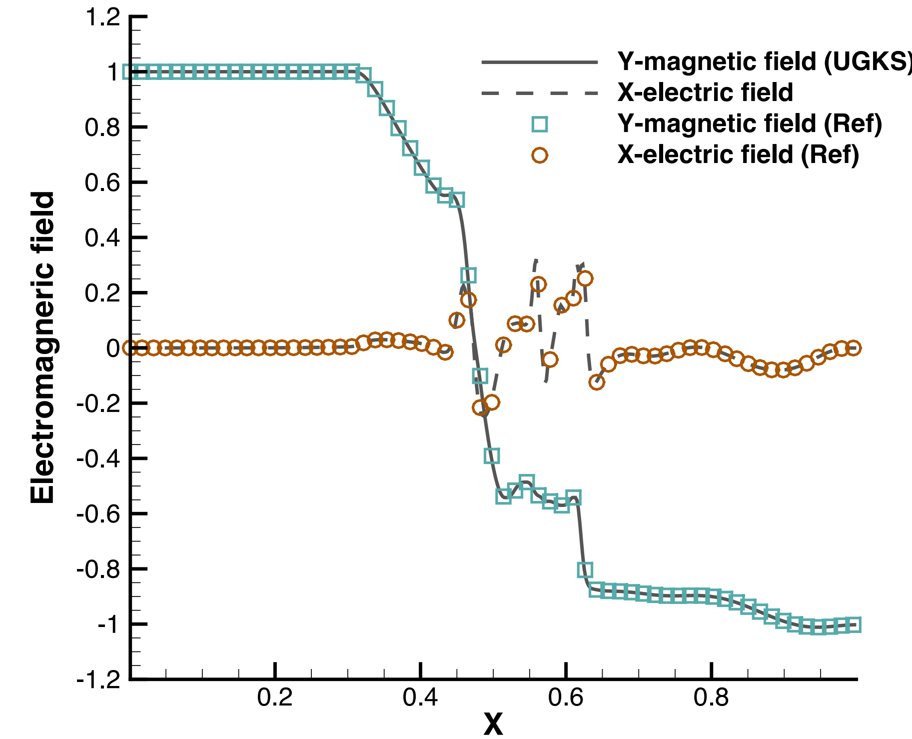
nonlinear

MHD solutions: Brio-Wu shock tube

mi/me=25, Kn=0.01, rL=0.001, t=0.1





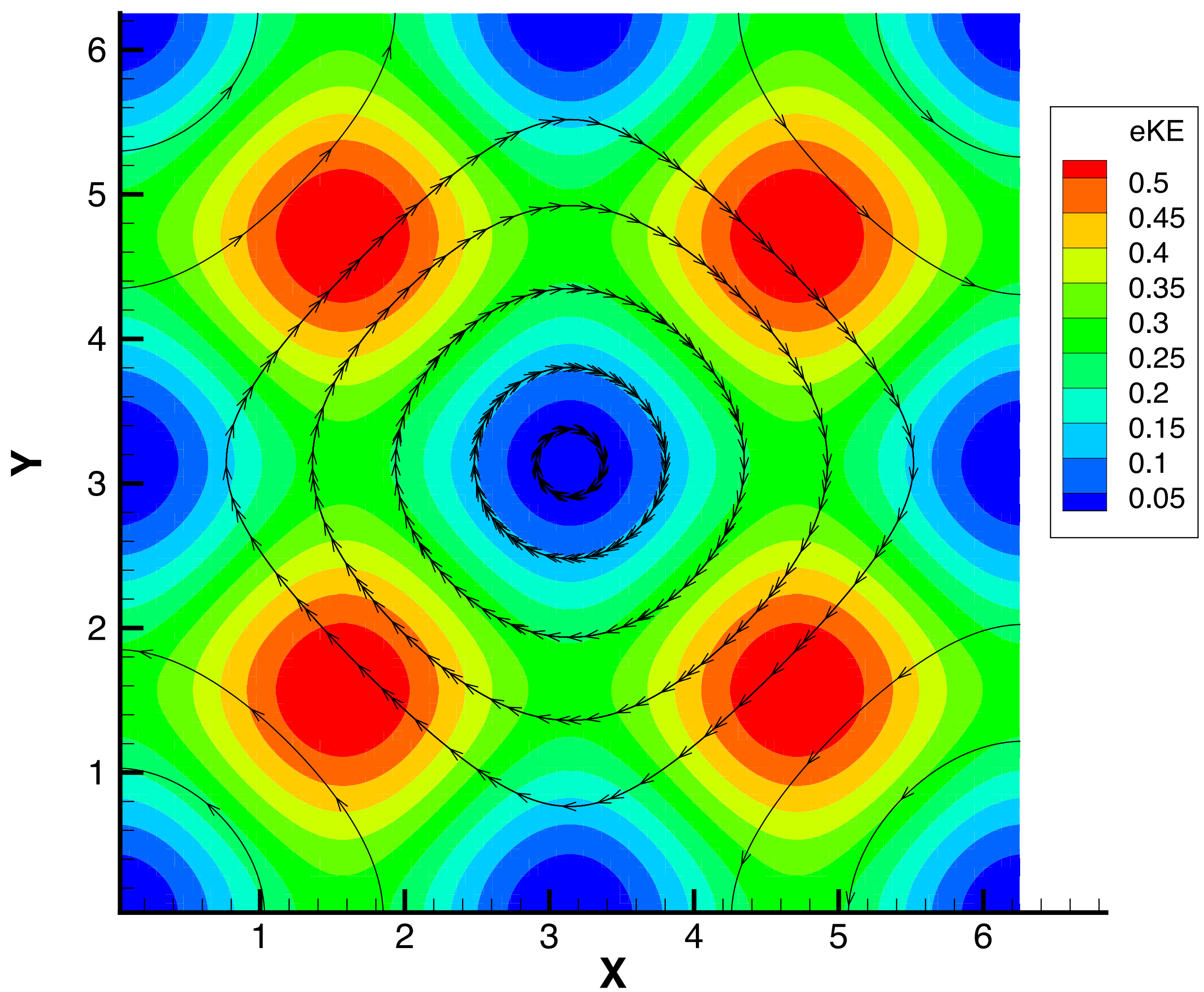


FR: fast rarefaction wave
C: contact discontinuity
SS: slow shock
SM: slow compound wave

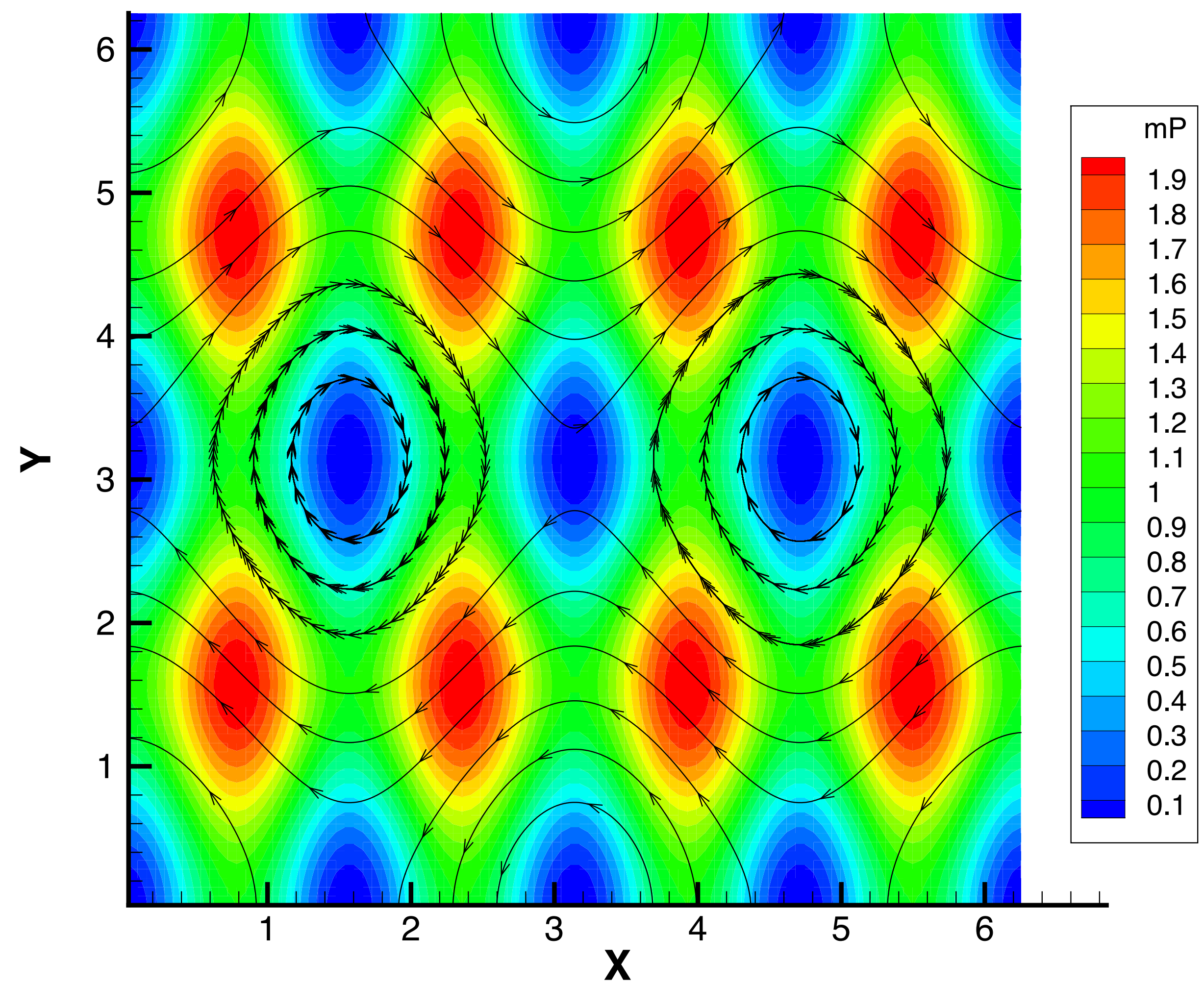
[1] Brio, M., and Wu, C. C. (1988). An upwind differencing scheme for the equations of ideal magnetohydrodynamics. *Journal of computational physics*, *75*(2), 400-422.

MHD solutions: Orszag-Tang turbulence model

Ni=Ne=Gamma^2, T=1.2, P=Gamma, Mi/Me=5, Kn=0.0001,r=0.05



Initial velocity and kinetic energy

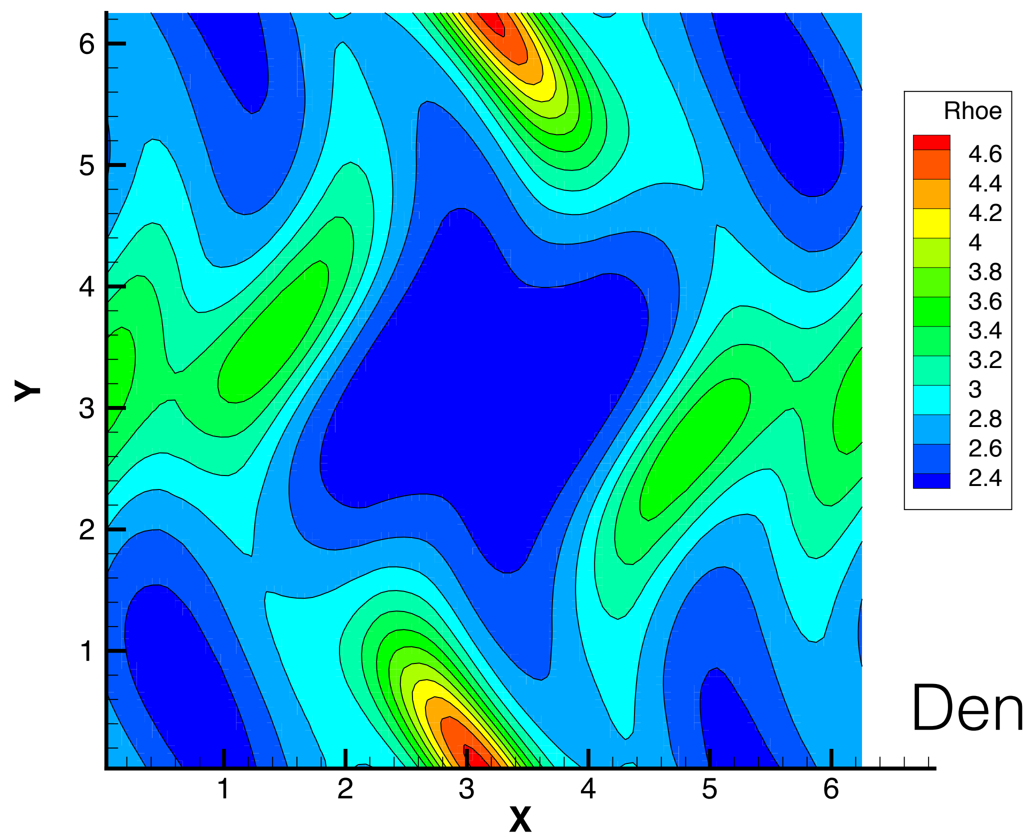


Initial electromagnetic field

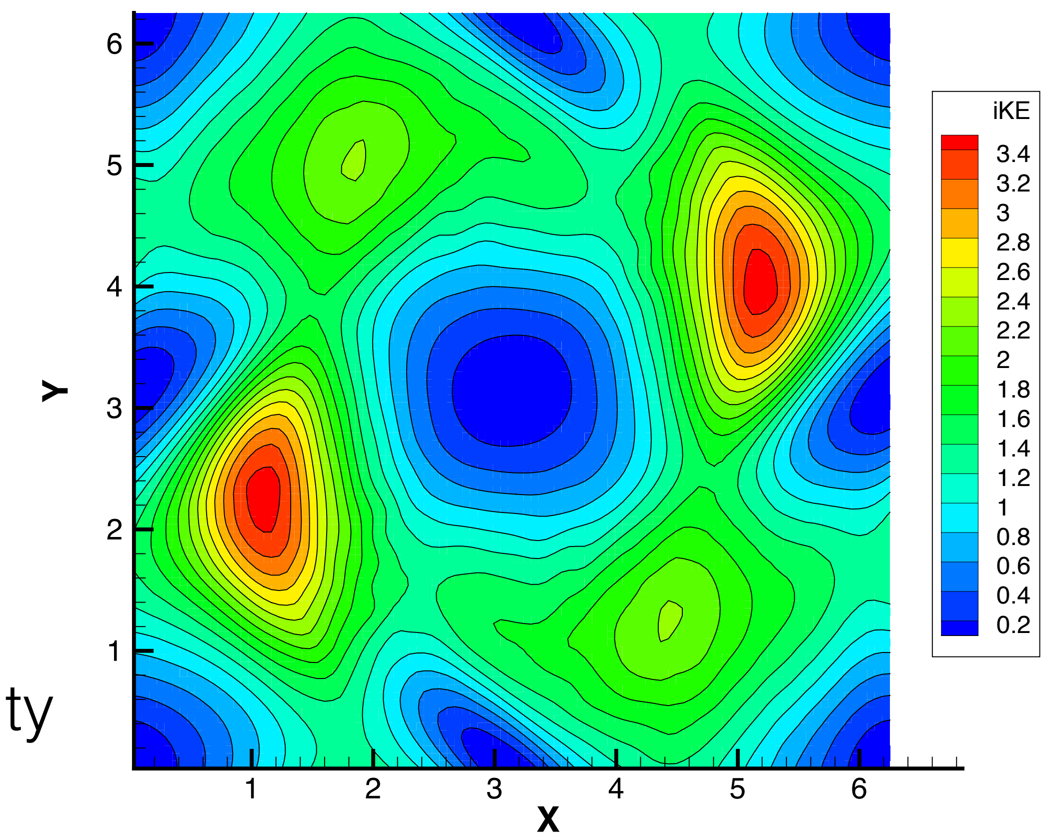
[1] Orszag, S. A., & Tang, C. M. (1979). Small-scale structure of two-dimensional magnetohydrodynamic turbulence. *Journal of Fluid Mechanics*, *90*(1), 129-143.

MHD solutions: Orszag-Tang turbulence model

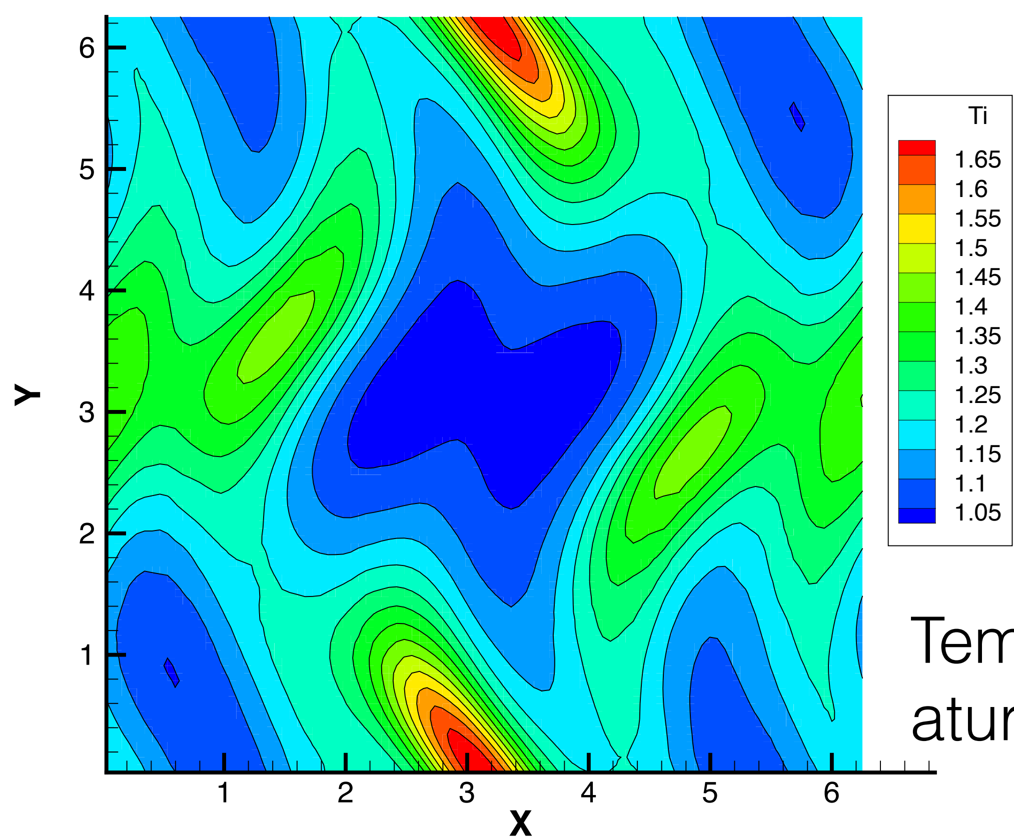
t=0.5



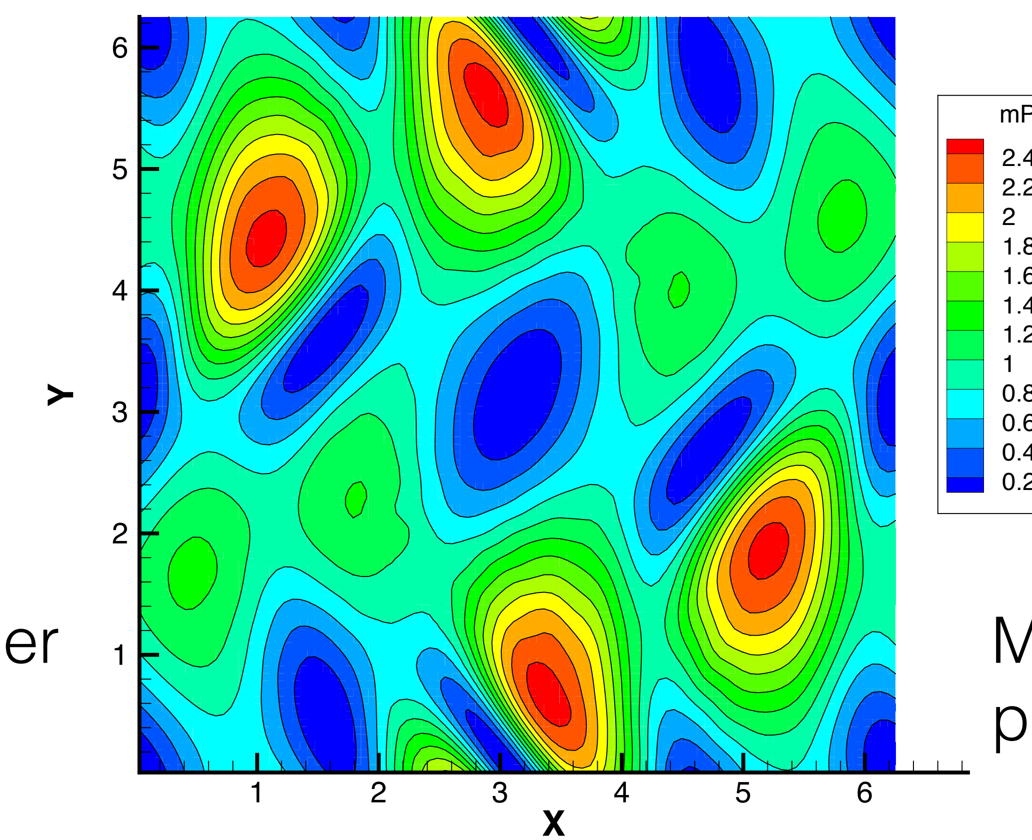
Density



Kinetic energy



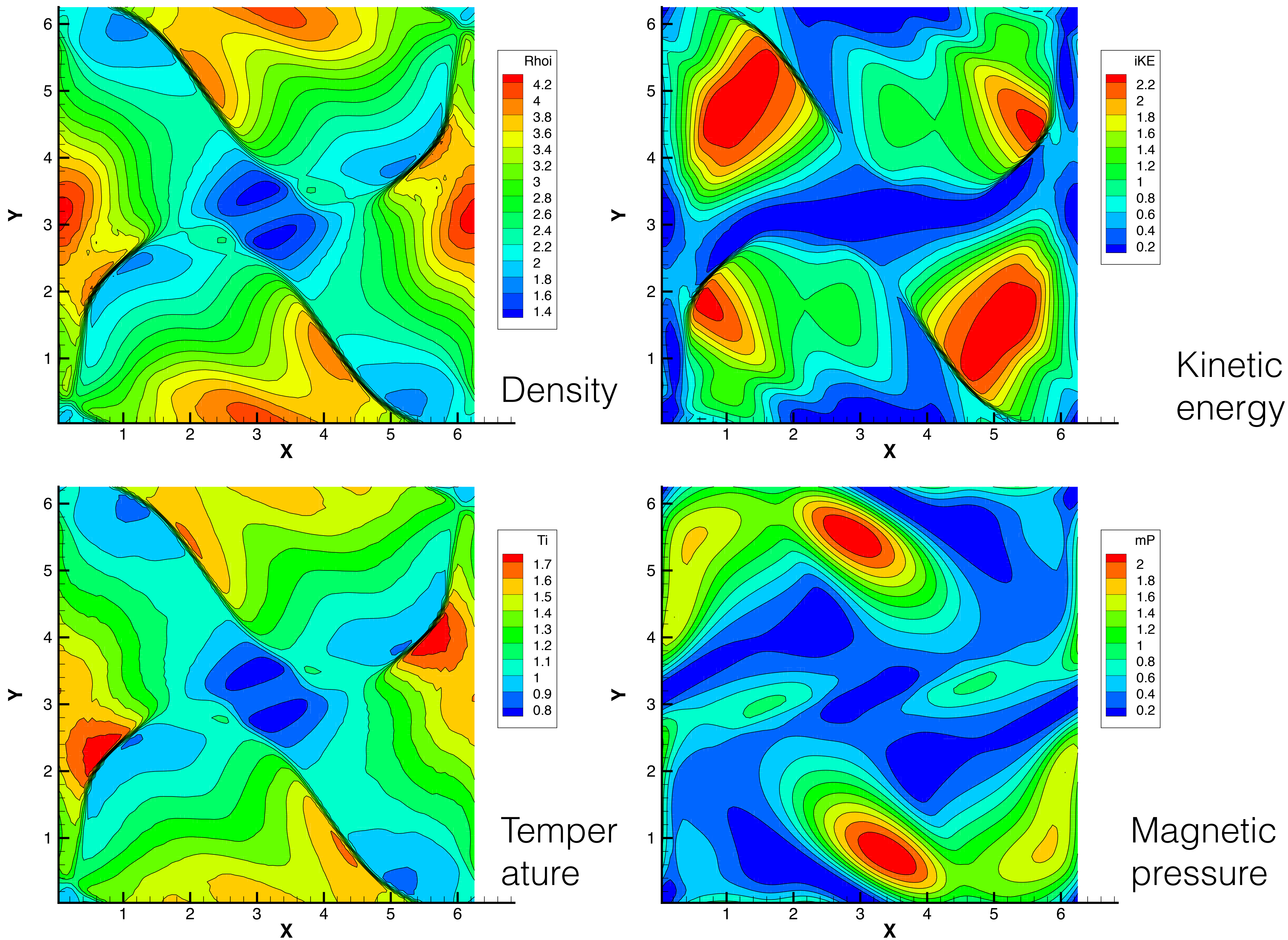
Temper ature



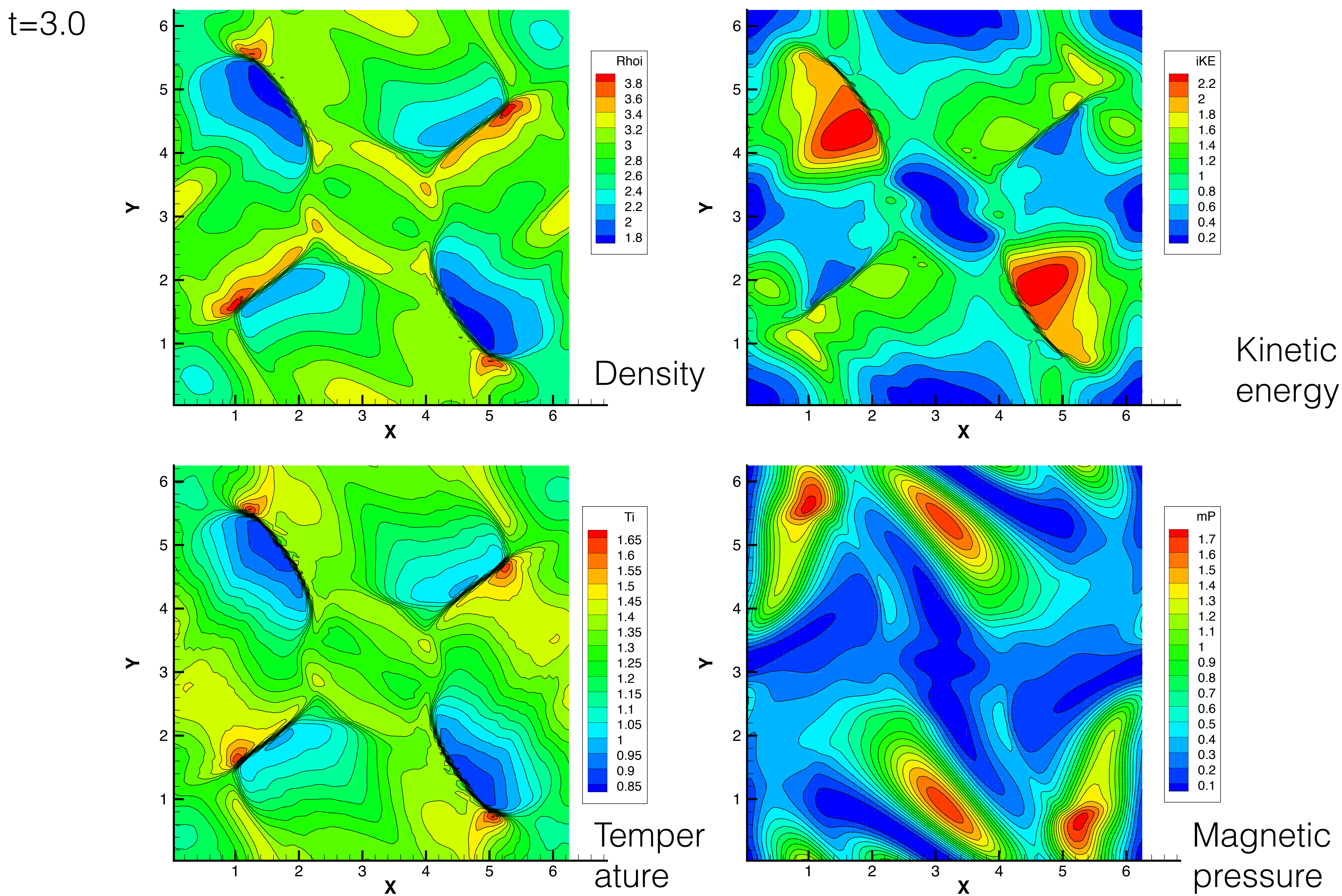
Magnetic pressure

MHD solutions: Orszag-Tang turbulence model

t=2.0



MHD solutions: Orszag-Tang turbulence model



Conclusion

UGKS: a preliminary attempt for multiscale modeling and simulation

Three typical scenarios of multiscale transport problems

- Forcing gas dynamics and well-balanced scheme
- High speed flow and velocity-space adaptive method
- Multicomponent gas and plasma dynamics

Outlook

- Mathematics: entropy-closure methodology
- Algorithm: particle formulation, data driven
- Physics: plasma, turbulence, complex systems

Publications

Xiao, T., Cai, Q., and Xu, K. (2017). A well-balanced unified gas-kinetic scheme for multiscale flow transport under gravitational field. *Journal of Computational Physics, 332*, 475-491.

Xiao, T., Xu, K., Cai, Q., and Qian, T. (2018). An investigation of non-equilibrium heat transport in a gas system under external force field. *International Journal of Heat and Mass Transfer, 126*, 362-379.

Xiao, T., Xu, K., and Cai, Q. (2019). A unified gas-kinetic scheme for multiscale and multicomponent flow transport. *Applied Mathematics and Mechanics*, accepted.

Xiao, T., Xu, K., and Cai, Q. (2018). A velocity-space adaptive unified gas kinetic scheme for continuum and rarefied flows. arXiv:1802.04972v1 [physics.comp-ph], submitted to *Journal of Computational Physics*.

Xiao, T., Liu, C. , Xu, K., and Cai, Q. A unified gas-kinetic scheme for partially ionized plasmas, in preparation.

Thanks!

Any questions are welcome :)