

# Unified Gas-kinetic Scheme for Multiscale Transport

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**Hong Kong University of Science and Technology**

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

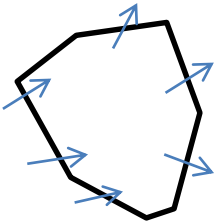


# Contents

- Modeling, PDEs, and Computation
- Direct modeling for multiscale transport processes
  - Unified Gas-kinetic Scheme (UGKS)**
    - rarefied gas dynamics
    - radiative transfer
    - plasma
    - ...
- **Conclusion**

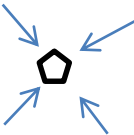
# Current CFD Methodology

dynamic description  
on a specific modeling scale

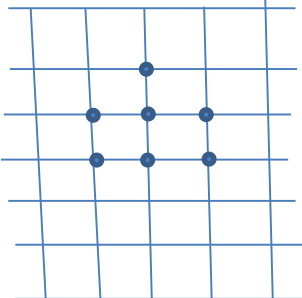


PDEs

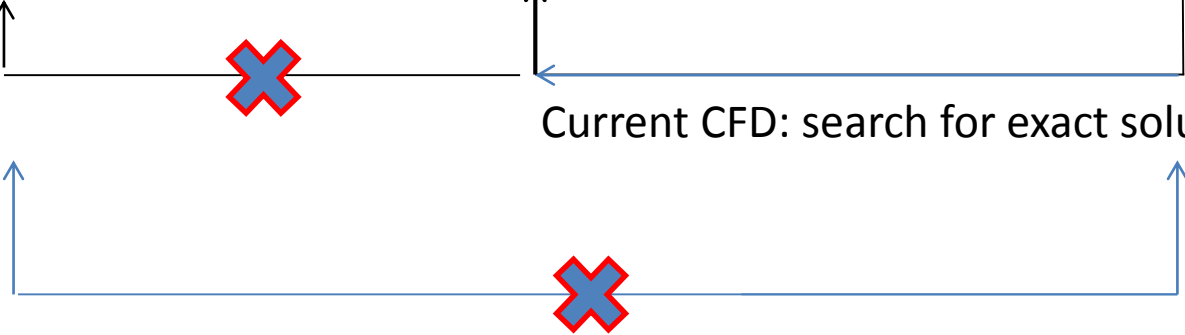
Euler, NS, ..., Boltzmann



Computation



Current CFD: search for exact solution of PDE



No direct connection between the **mesh size scale** and the **physical modeling scale**

# The 10 orders of magnitude hierarchy

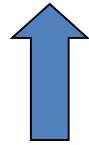
(air under standard conditions, 1 atm, 0°C)  $n_0 = 2.687 \times 10^{25} \text{ m}^{-3}$



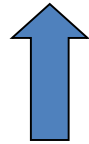
**HYDRODYNAMIC**  
**NAVIER-STOKES**

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{\nabla P}{\rho} + \nu \Delta \mathbf{u}$$

(continuum description)



**KINETIC**  
**BOLTZMANN EQUATION**



• Mean free-path:  $\lambda_0 = (\sqrt{2} \pi d^2 n_0)^{-1} = 6.1 \times 10^{-8} \text{ m}$



**MICROSCOPIC**  
**MOLECULAR DYNAMICS**

• Effective molecular diameter (via C-E formulas):  $d \approx 3.7 \times 10^{-10} \text{ m}$





Having failed to obtain any CFL picture, we have switched to a CLL one: Richard Courant, Hans Lewy, and Jean Leray at the Arden Conference Center around 1950. It may be thought as a first order approximation... (From Peter Lax files)



Richard Courant, Kurt Friedrichs, and Hans Lewy

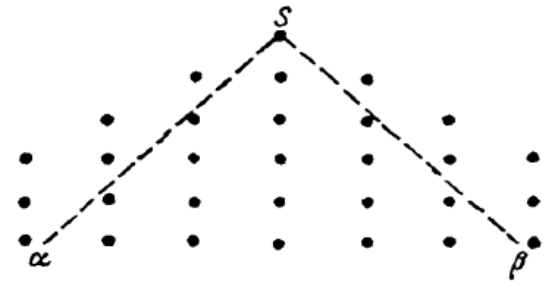


Fig. 9.

1928

# Über die partiellen Differenzengleichungen der mathematischen Physik.

Von

R. Courant, K. Friedrichs und H. Lewy in Göttingen,

English Translation:

**On the partial difference equations of mathematical physics**

IBM JOURNAL • MARCH 1967

Problems involving the classical linear partial differential equations of mathematical physics can be reduced to algebraic ones of a very much simpler structure by replacing the differentials by difference quotients on some (say rectilinear) mesh. This paper will undertake an elementary discussion of these algebraic problems, in particular of the behavior of the solution as the mesh width tends to zero. For present purposes we limit ourselves mainly to

cases. We will show by typical examples that the passage to the limit is indeed possible, i.e., that the solution of the difference equation converges to the solution of the corresponding differential equation; in fact we will find

active. Nowhere do we assume the existence of the solution to the differential equation problem—on the contrary, we obtain a simple existence proof by using the limiting process.<sup>1</sup> For the case of elliptic equations convergence is

obtained independently of the choice of mesh, but we will find that for the case of the initial value problem for hyperbolic equations, convergence is obtained only if the ratio of the mesh widths in different directions satisfies certain inequalities which in turn depend on the position of the characteristics relative to the mesh.

(CFL condition)

力学丛书·典藏版—6

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# Current CFD principle -> Numerical PDEs

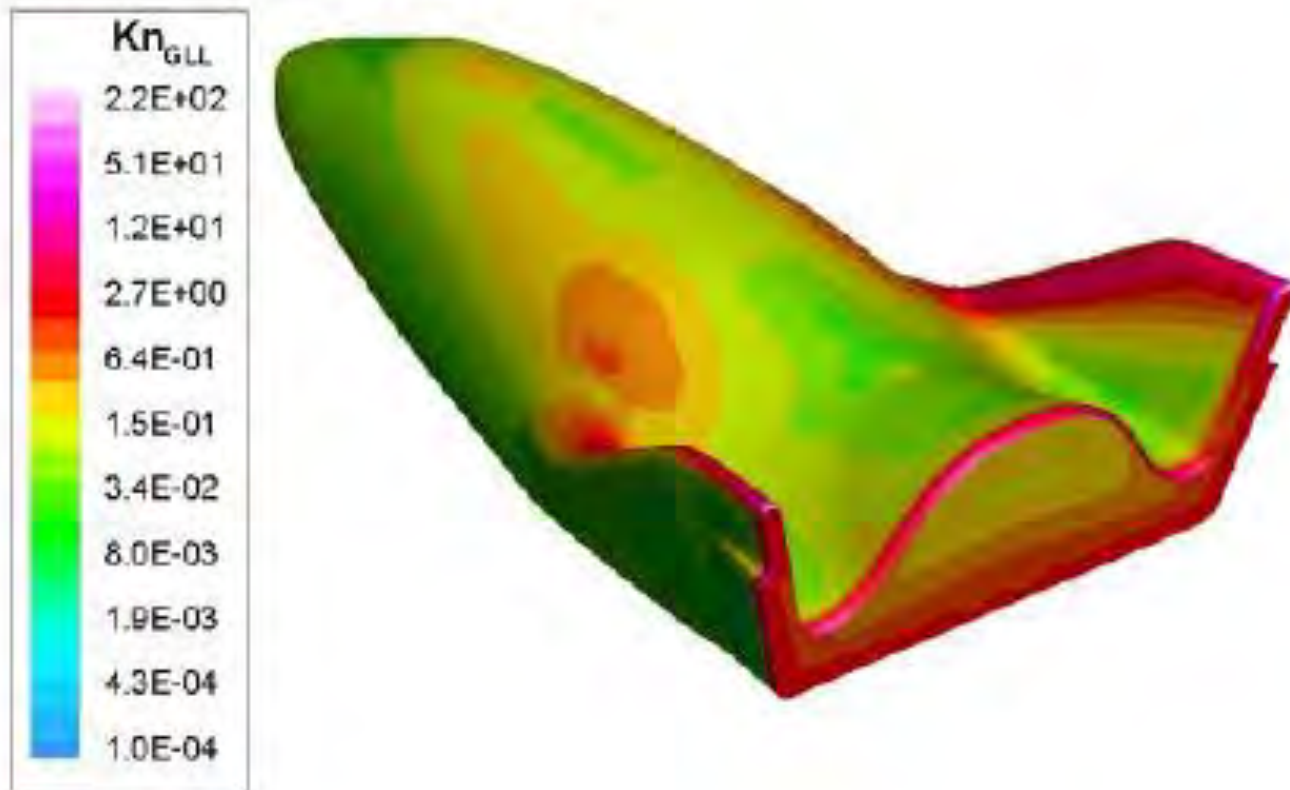
## Limitations:

1. To get convergent solution of the PDEs **as mesh size and time step go to zero**. With limited cell size and time step, theoretically never know the exact underlying governing equations.
2. All PDEs are valid in their modeling scales. It is hard to study **multiple scale** problem if there is no such a governing equation valid in all scales.
3. In certain scales, we don't have the corresponding PDEs at all.

$M_\infty = 4$  ,  $Re = 5937.3$

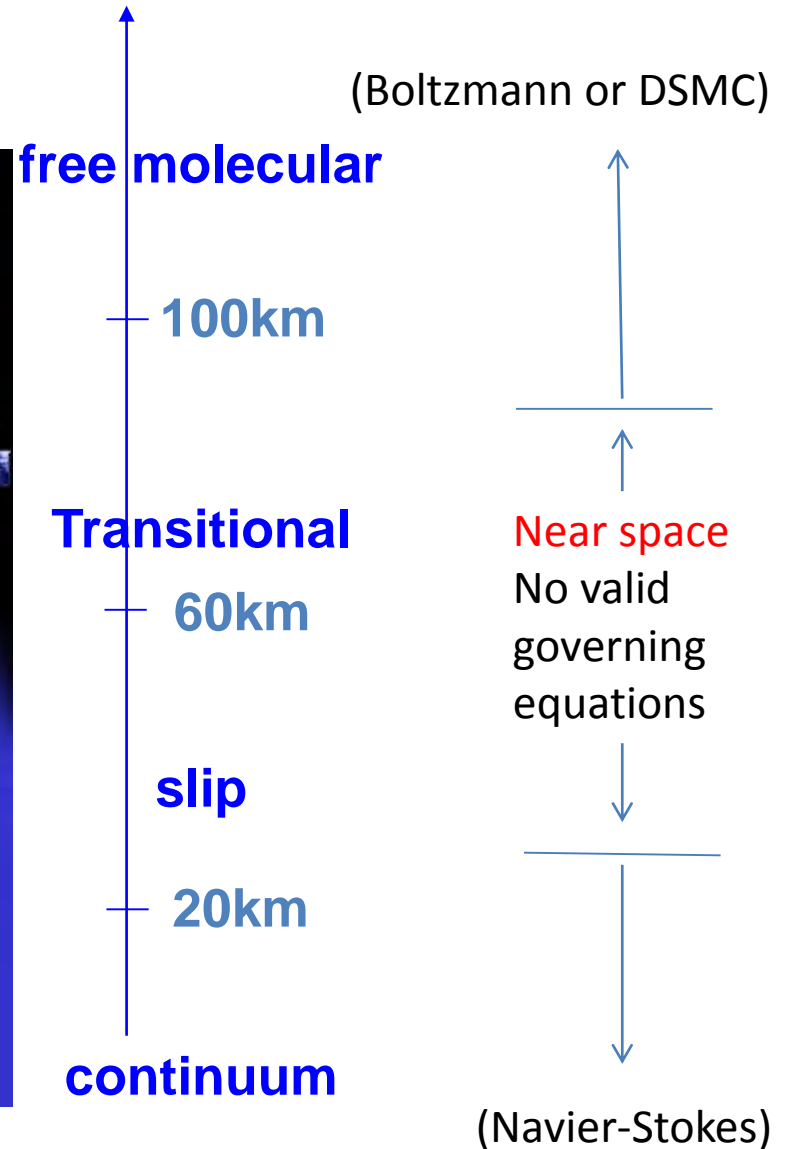
Minimum  $Kn_{GLL}$  is:  $8.81e-004$

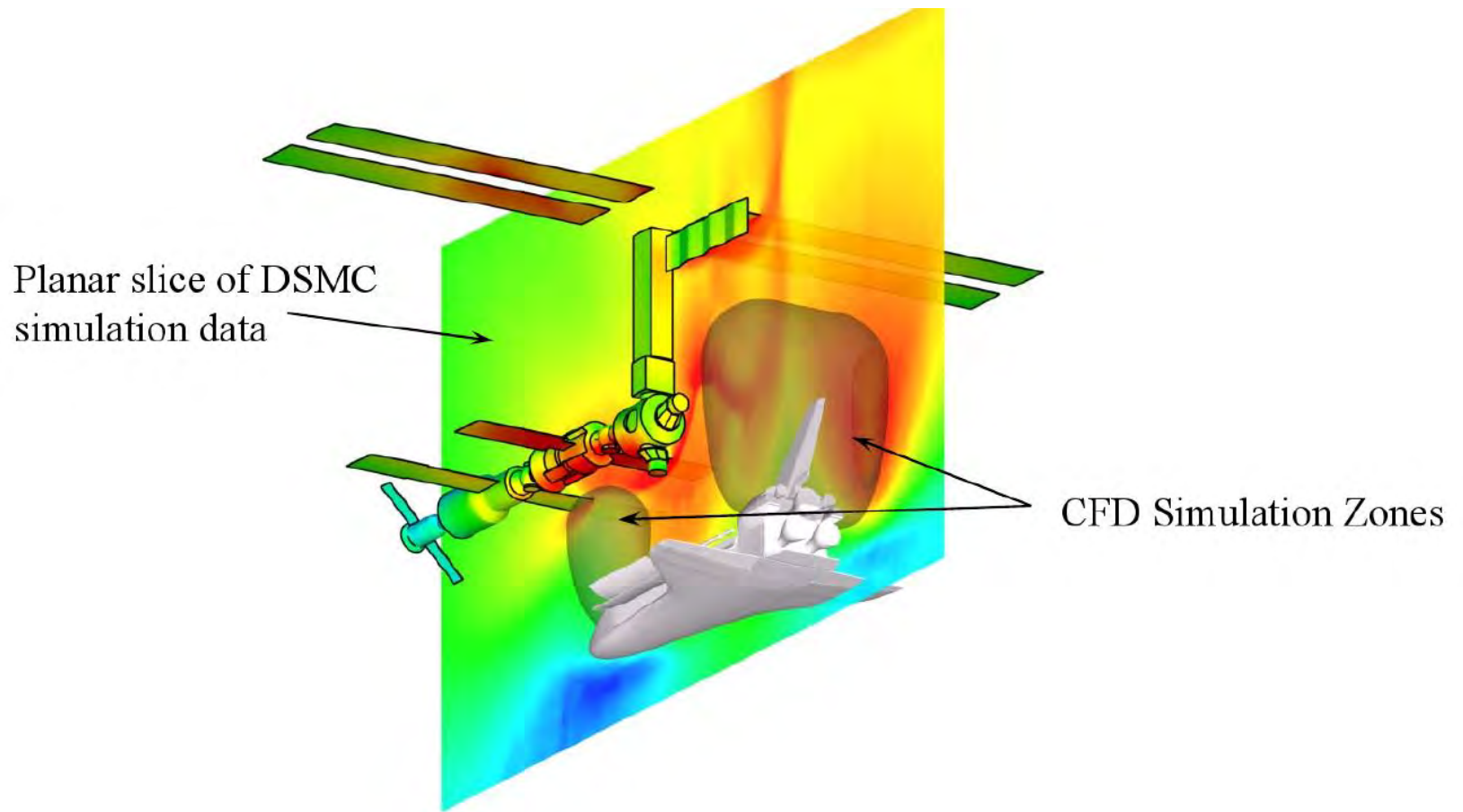
Maximum  $Kn_{GLL}$  is:  $2.29e+002$



D.W. Jiang

# Near Space flow modeling

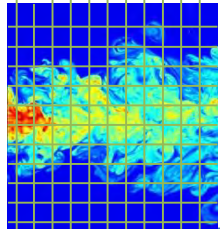




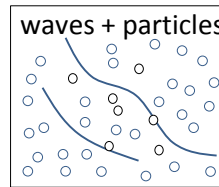
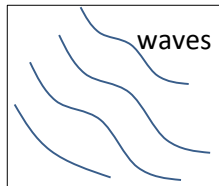
Turbulent modeling

<-> Navier-Stokes <-> ? ? <-> Boltzmann -> Molecular Dynamics

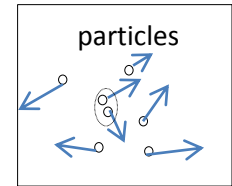
turbulence



NS



Boltzmann



***Hydrodynamic scale !***

Non-equilibrium  
irreversible hydrodynamics

?

***Kinetic scale***

NS

Boltzmann

Direct Physical Modeling

**unified description**



# Theoretical fluid dynamics

# Computational fluid dynamics

Euler equations



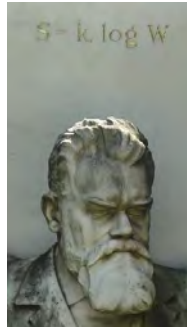
Navier-Stokes equations



...

...

Boltzmann equation



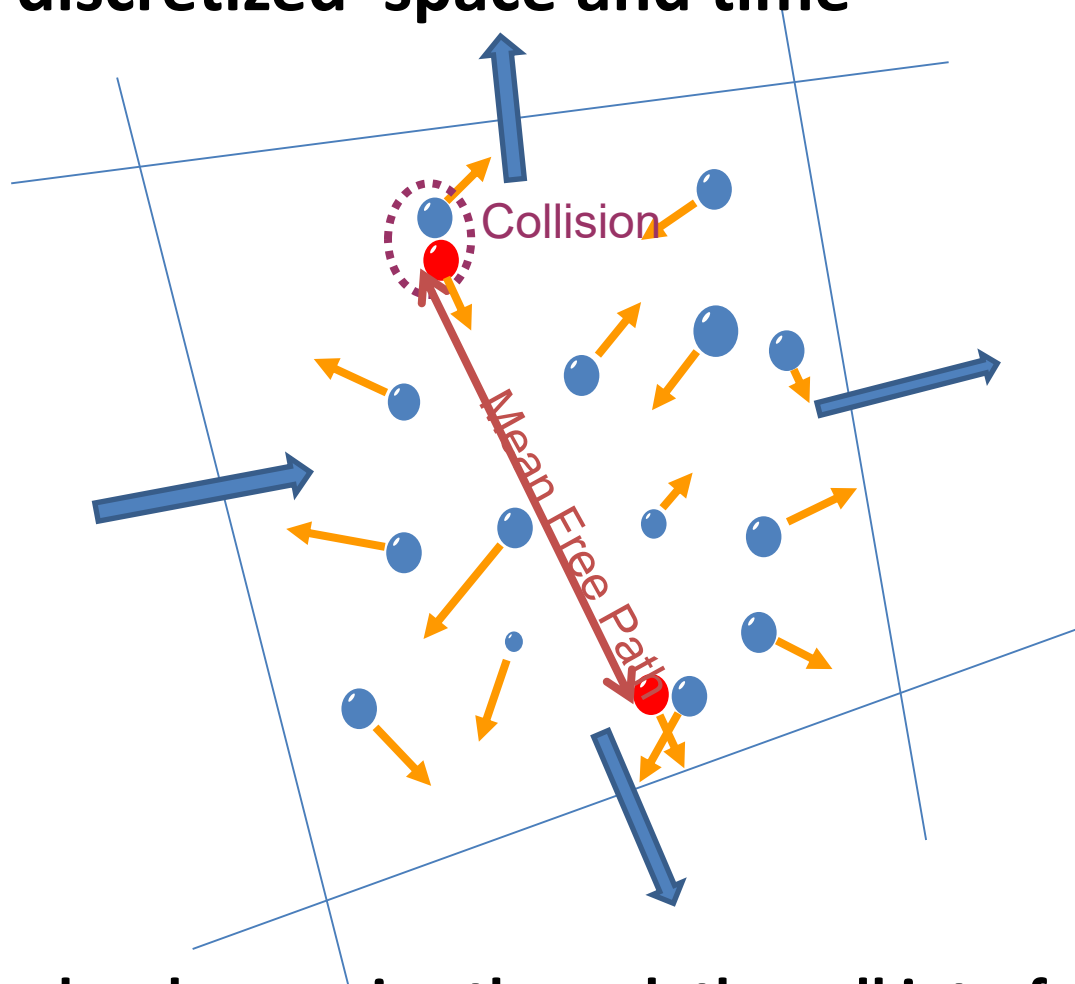
*Distinct governing equations in different scale modeling*

***Aim:***

***A continuous spectrum of governing Equations***

# Direct Modeling for CFD

# Computation: a description of flow motion in a discretized space and time



The way of gas molecules passing through the cell interface depends on the cell resolution and particle mean free path

# Direct modeling in discretized space

$f$  : gas distribution function,

$W$  : conservative macroscopic variables

## Fundamental Governing Equations

**Micro:**

$$f_j^{n+1} = f_j^n + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} [uf_{x_{j-1/2}}(t) - uf_{x_{j+1/2}}(t)] dt + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} Q(f, f) dx dt$$

**Marco:**

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int u \psi(f_{j-1/2} - f_{j+1/2}) du d\xi dt$$

**Modeling:**      **Interface distribution function**  
                     **Inner cell collision term**

# **Unified Gas-kinetic Scheme (UGKS)**

**(modeling for both continuum and rarefied flows)**



# General framework of Unified Gas-kinetic Scheme (UGKS)

Update of distribution function (micro):

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} [uf_{j-1/2,k}(t) - uf_{j+1/2,k}(t)] dt + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} Q(f, f) dx dt$$

Update of conservative variables (macro):

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int u_k \psi (f_{j-1/2,k} - f_{j+1/2,k}) du_k d\xi dt$$

Both **interface flux** and **inner cell collision term** need to be modeled

K. Xu and J.C. Huang

## Collision term treatment:

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} (u_k \hat{f}_{j-1/2,k} - u_k \hat{f}_{j+1/2,k}) dt \\ + A Q(f_j^n, f_j^n)_k + B \frac{\tilde{M}(f_j^{n+1})_k - f_{j,k}^{n+1}}{\tau_s^{n+1}},$$

1.  $A + B \sim \Delta t$  in order to have a consistent collision term treatment.
2. The scheme is stable in the whole flow regime.
3. In the rarefied flow regime, the scheme gives the Boltzmann solution.
4. In continuum regime, the scheme can efficiently recover the Navier-Stokes solutions.

$$Q(f, f) = \int_{R^3} \int_{S^2} (f'_* f' - f_* f) |u_r| \sigma d\Omega du_*.$$

# Interface flux modeling:

The flux evaluation is based on the integral solution of the kinetic model:

$$f_{j+1/2,k} = \frac{1}{\tau} \int_0^t g(x', t', u_k, \xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_{0,k}(x_{j+1/2} - u_k t)$$

Hydrodynamic evolution



Kinetic scale evolution



# UGKS: Evolution Processes

(micro-scale)

$$f_{j,k}^{n+1} = f_{j,k}^n + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} [uf_{j-1/2,k}(t) - uf_{j+1/2,k}(t)] dt + \frac{1}{\Delta X} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} Q(f, f) dx dt$$

taking conservative moments:

$$\psi = (1, u_k, \frac{1}{2}(u_k^2 + \xi^2))^T$$

mass, momentum and energy

(macro-scale)

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int u_k \psi (f_{j-1/2,k} - f_{j+1/2,k}) du_k d\xi dt$$

Scale  
up

Scale  
down

$g^{n+1}$

**Numerical path:**  $f^n \rightarrow W^{n+1} \rightarrow g^{n+1} \rightarrow f^{n+1}$

The update of gas distribution function becomes

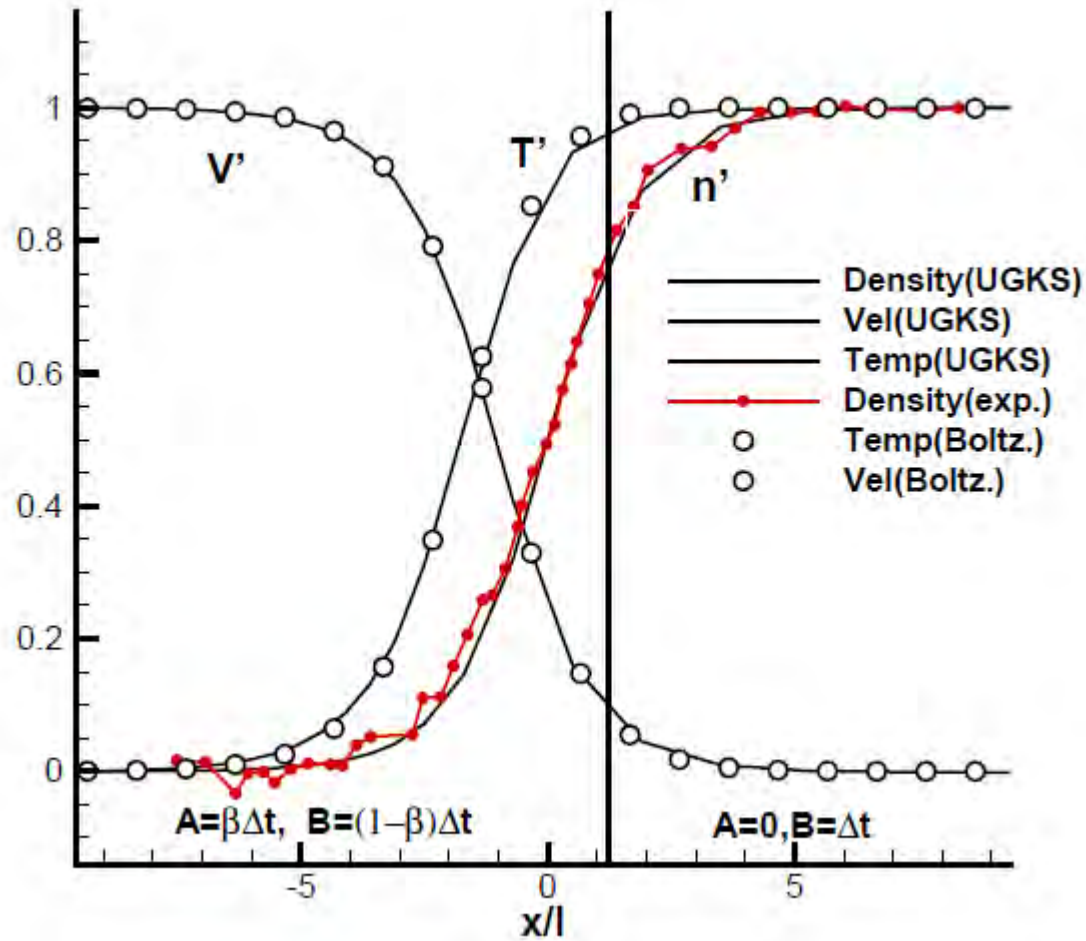
$$\begin{aligned}
 f_{j,k}^{n+1} &= f_{j,k}^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} [uf_{j-1/2,k}(t) - uf_{j+1/2,k}(t)] dt + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int_{x_{j-1/2}}^{x_{j+1/2}} \frac{g - f}{\tau} dx dt \\
 &= f_{j,k}^n + \frac{1}{\Delta x} \left( \int_{t^n}^{t^{n+1}} u_k (\tilde{g}_{j-1/2,k} - \tilde{g}_{j+1/2,k}) dt + \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) dt \right) \\
 &\quad + \frac{\Delta t}{2} \left( \frac{g_{j,k}^{n+1} - f_{j,k}^{n+1}}{\tau^{n+1}} + \frac{g_{j,k}^n - f_{j,k}^n}{\tau^n} \right)
 \end{aligned}$$

with the solution:

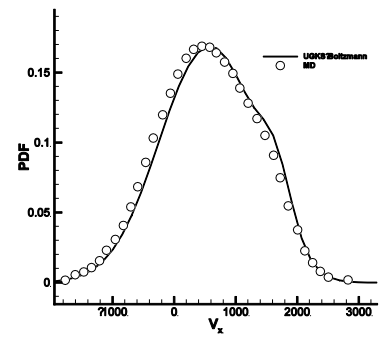
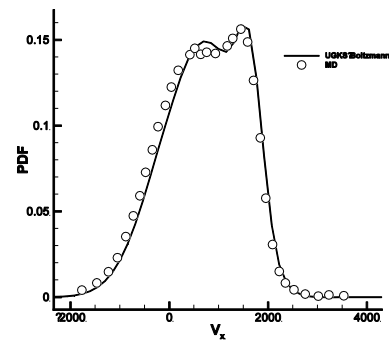
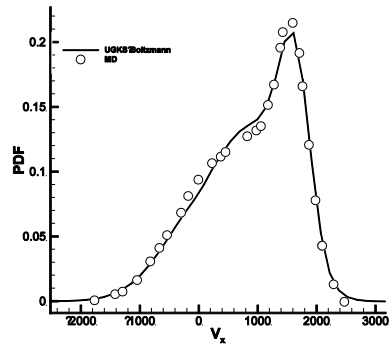
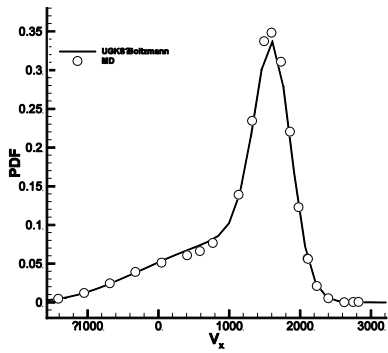
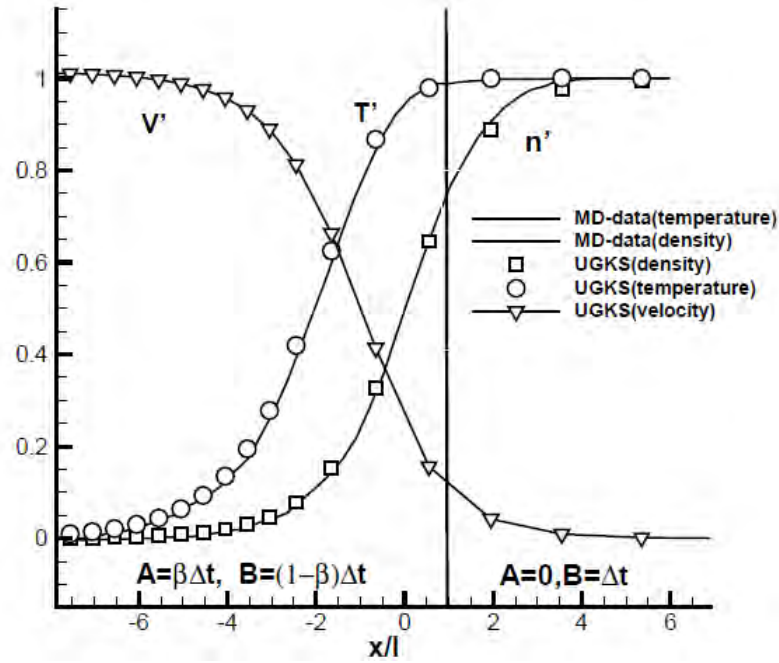
$$\begin{aligned}
 \left( 1 + \frac{\Delta t}{2\tau_j^{n+1}} \right) f_{j,k}^{n+1} &= f_{j,k}^n + \frac{1}{\Delta x} \left( \int_{t^n}^{t^{n+1}} u_k (\tilde{g}_{j-1/2,k} - \tilde{g}_{j+1/2,k}) dt + \int_{t^n}^{t^{n+1}} u_k (\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k}) dt \right) \\
 &\quad + \frac{\Delta t}{2} \left( \frac{g_{j,k}^{n+1}}{\tau_j^{n+1}} + \frac{g_{j,k}^n - f_{j,k}^n}{\tau_j^n} \right)
 \end{aligned}$$



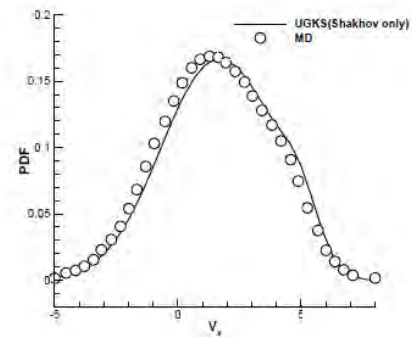
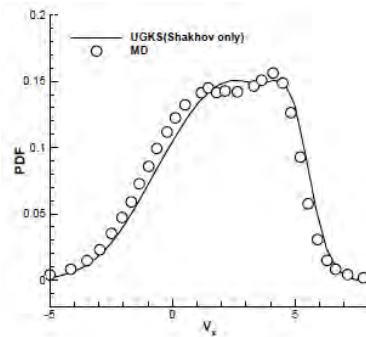
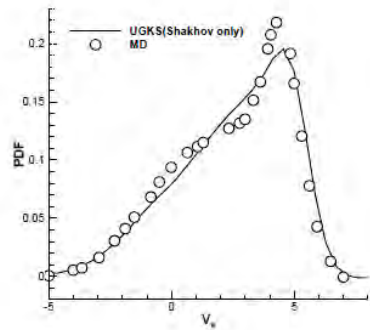
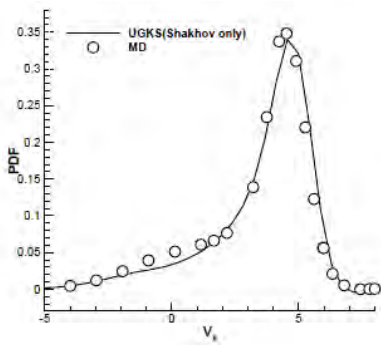
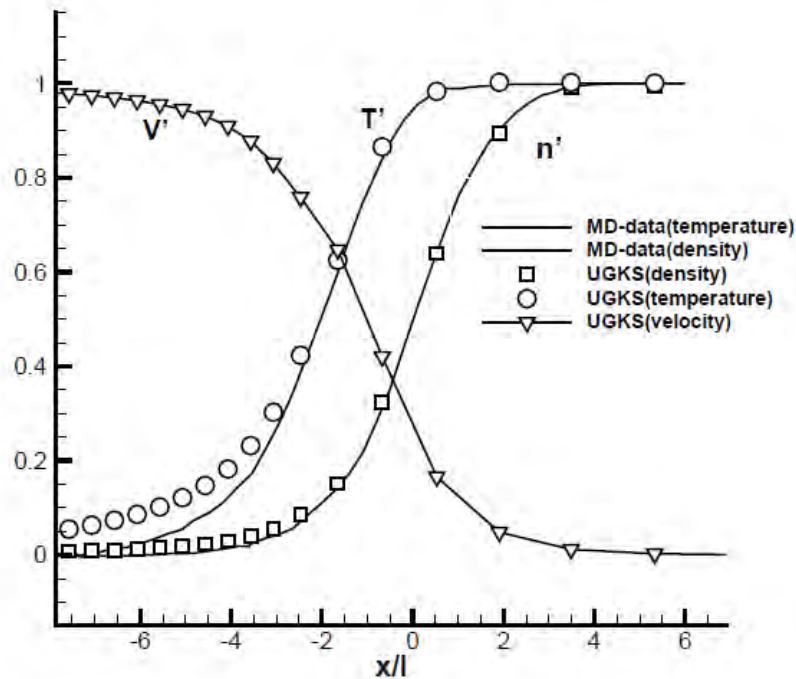
M=2.8 shock structure  
(UGKS vs Experiments)

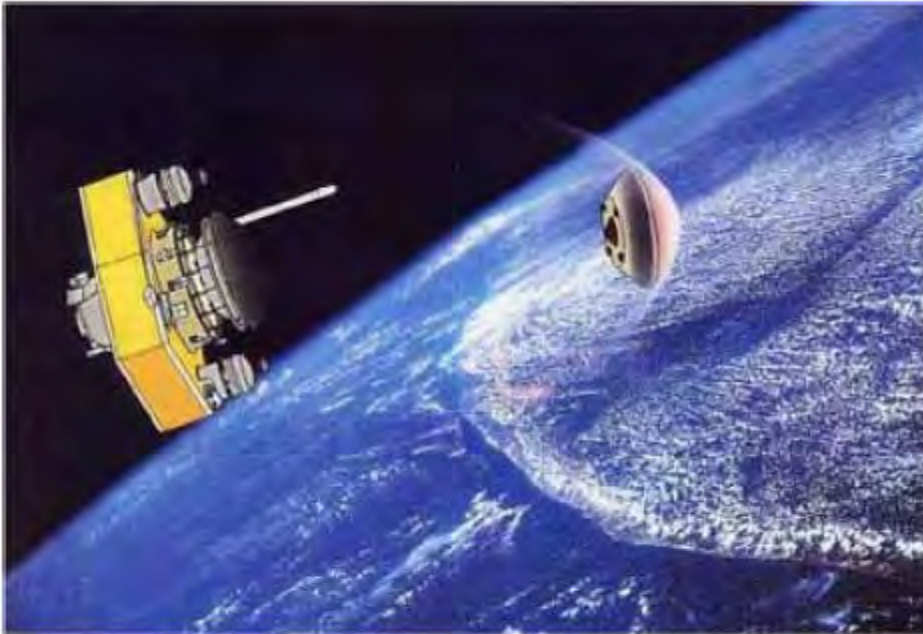


# M=5 shock structure: UGKS vs MD



# Shakhov model only:



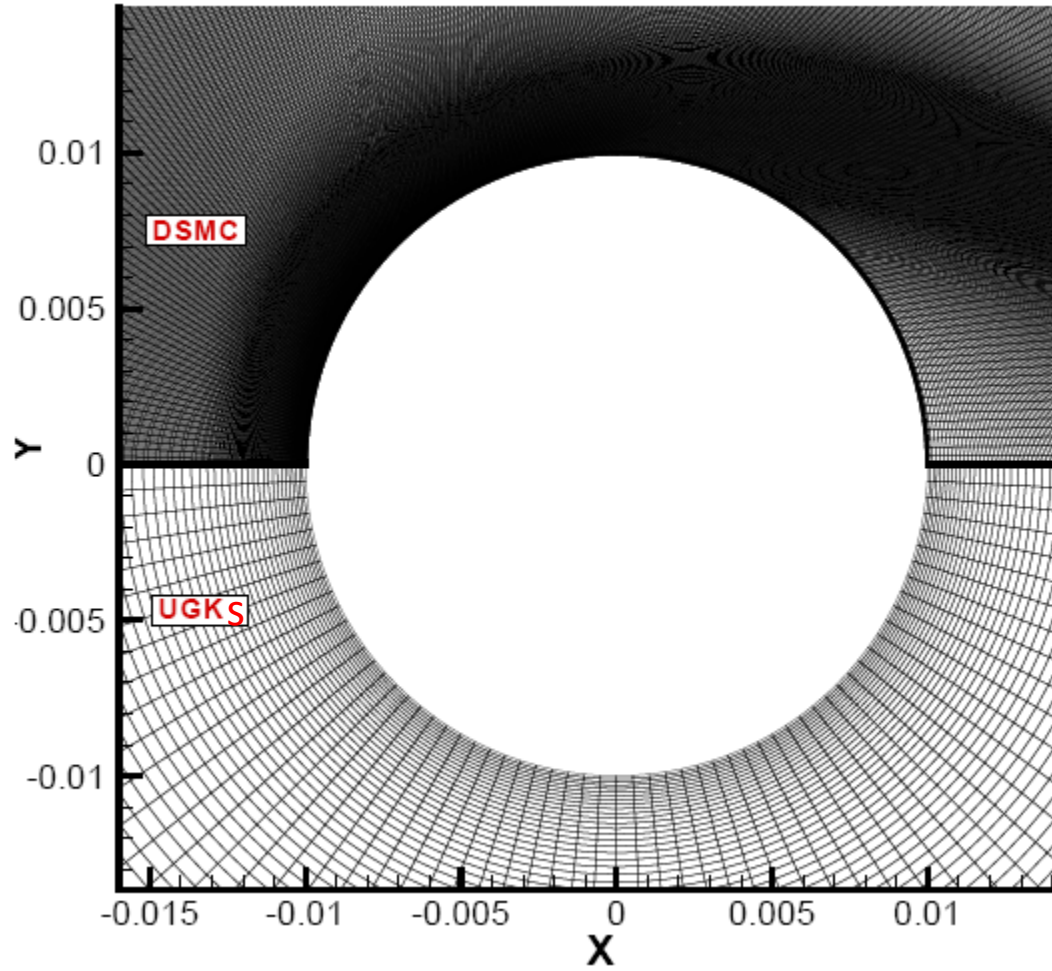


- Low-density gas dynamics



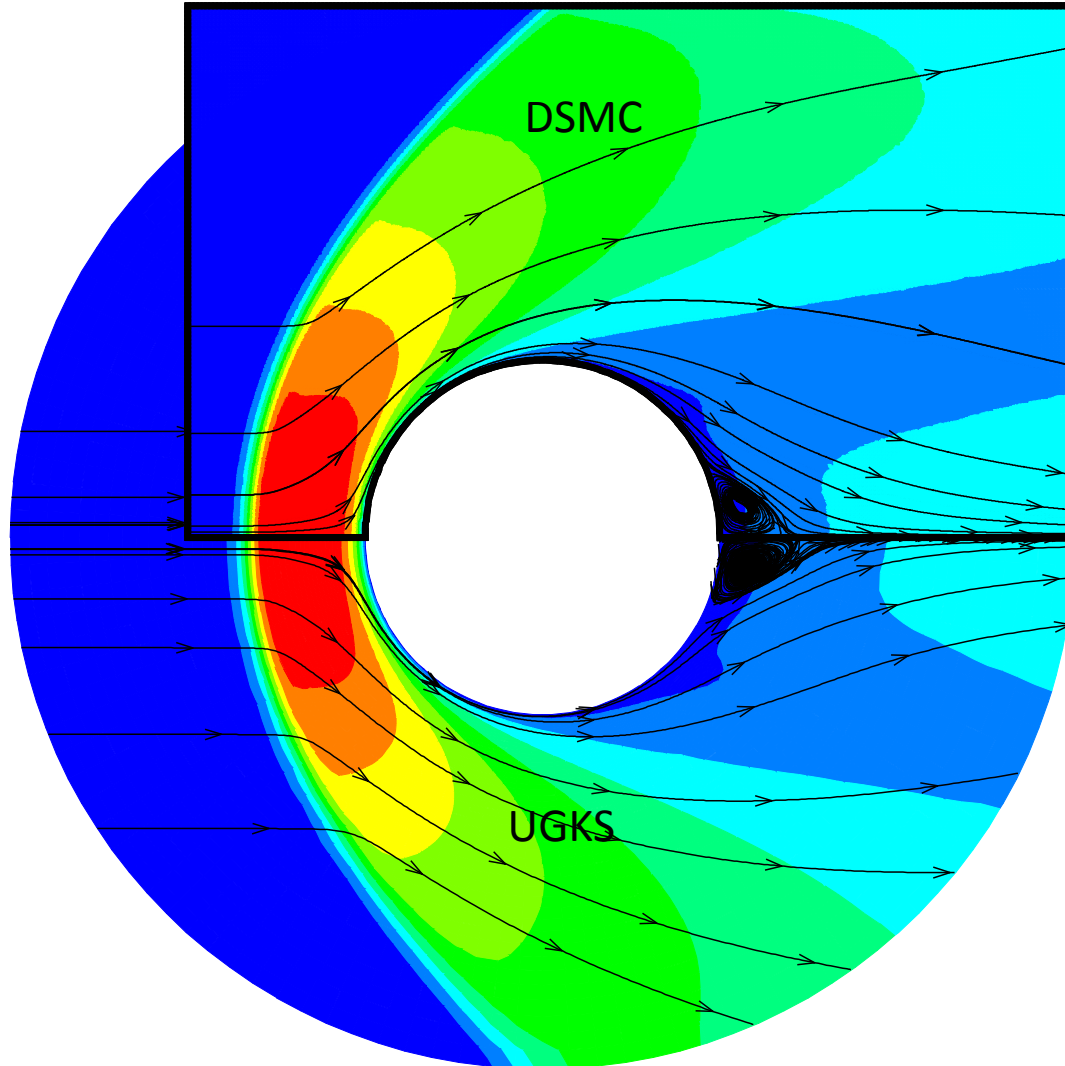
- Gas flows in micro-devices / nozzle

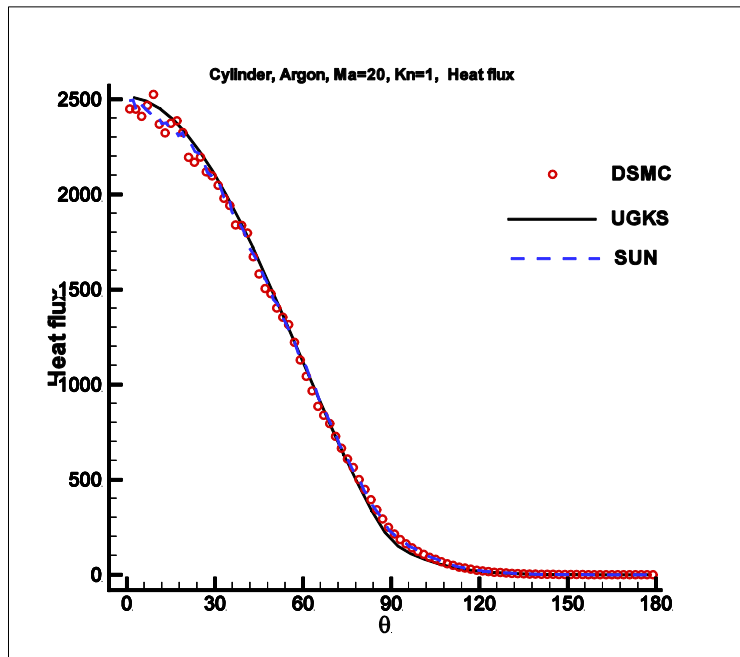
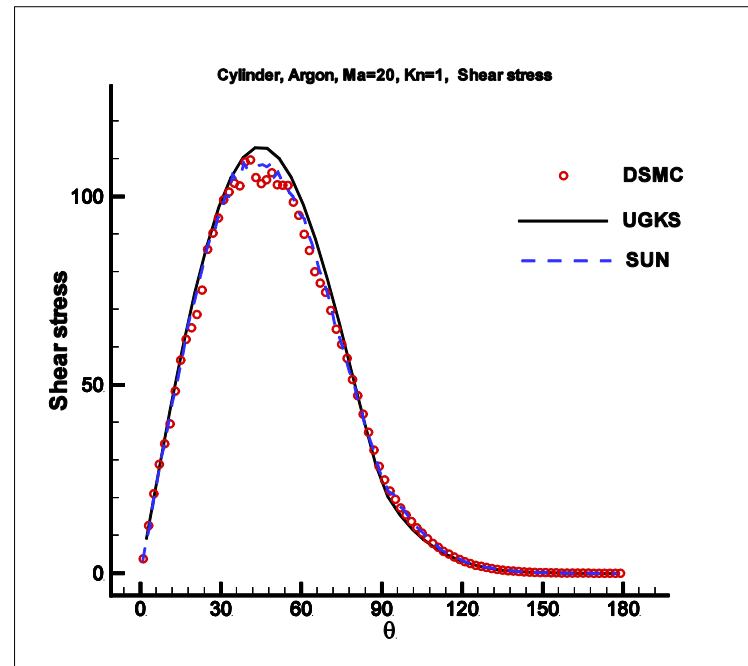
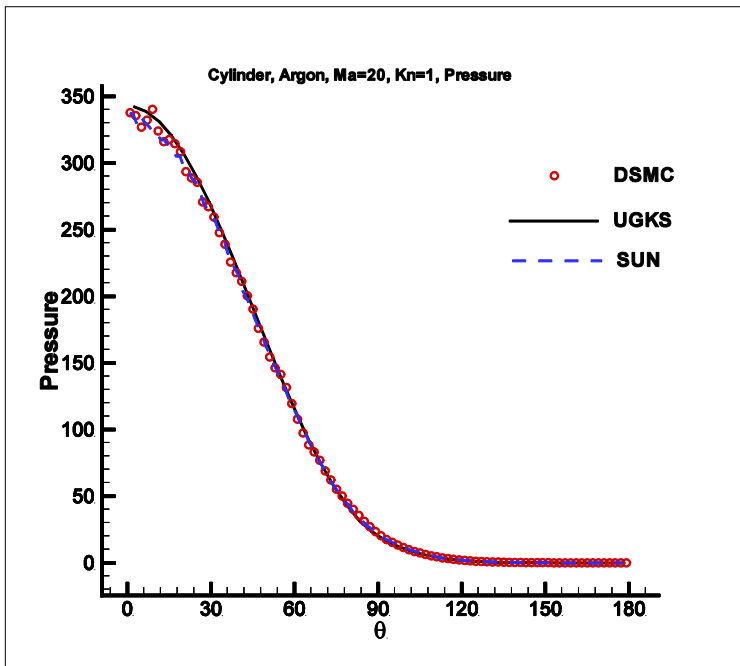
M=20, Kn=0.01



P.B. Yu

Cylinder, Argon,  $Ma=20, Kn=0.01$



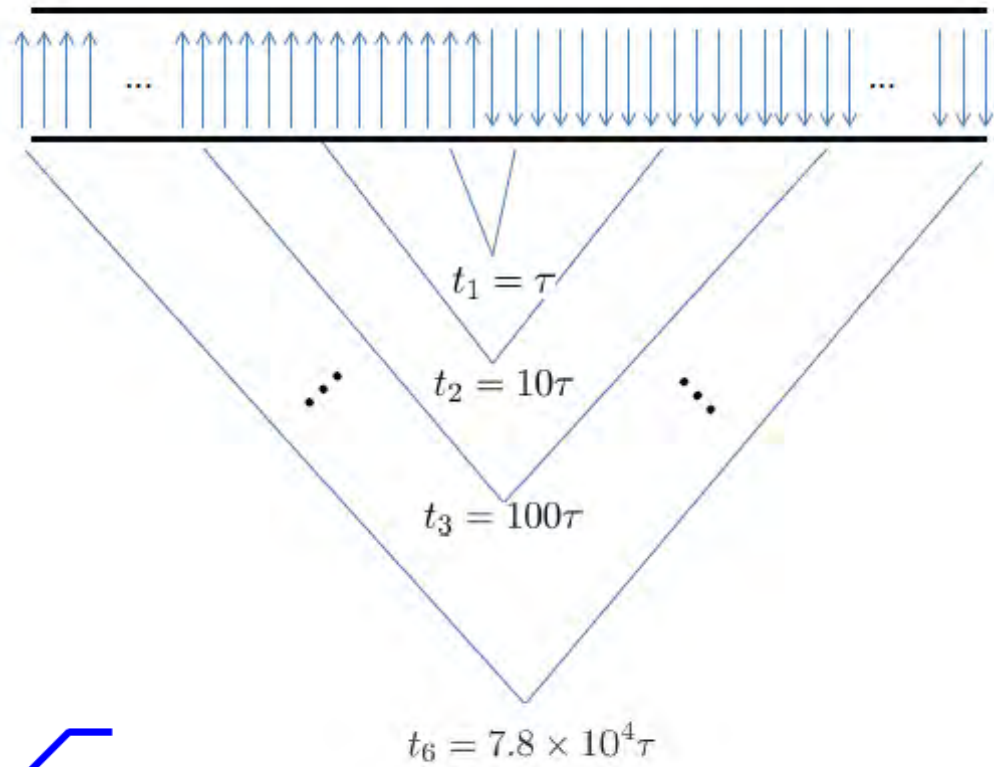


M=20, Kn=1

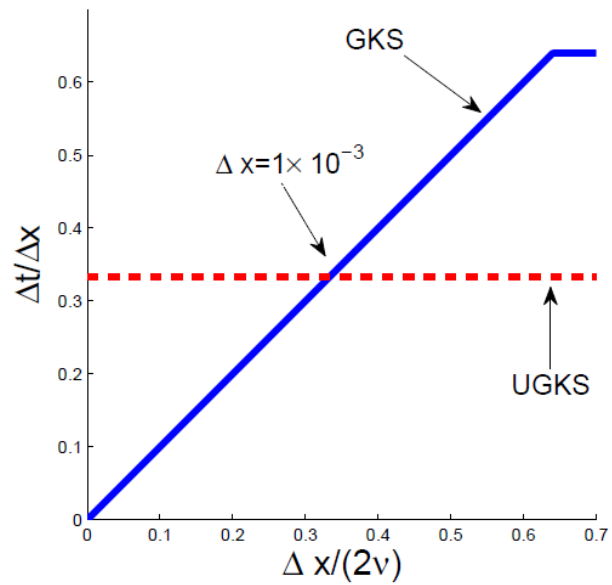
# **A continuous spectrum of gas dynamics description**



# Shear Layer

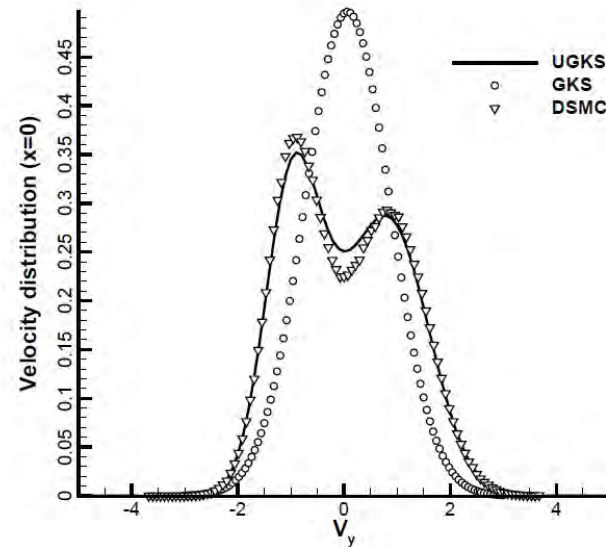
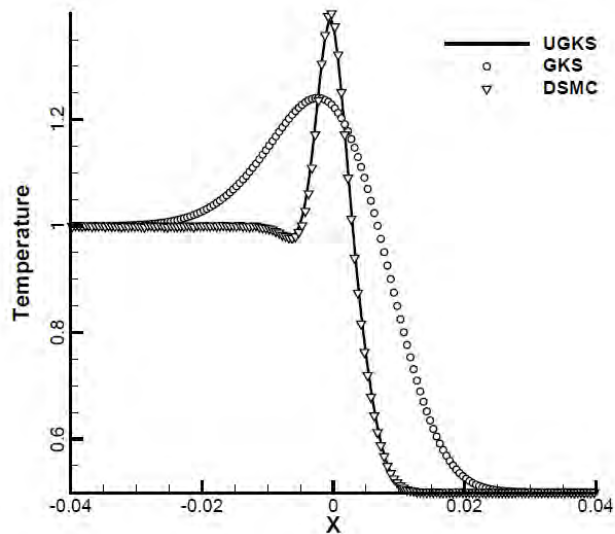
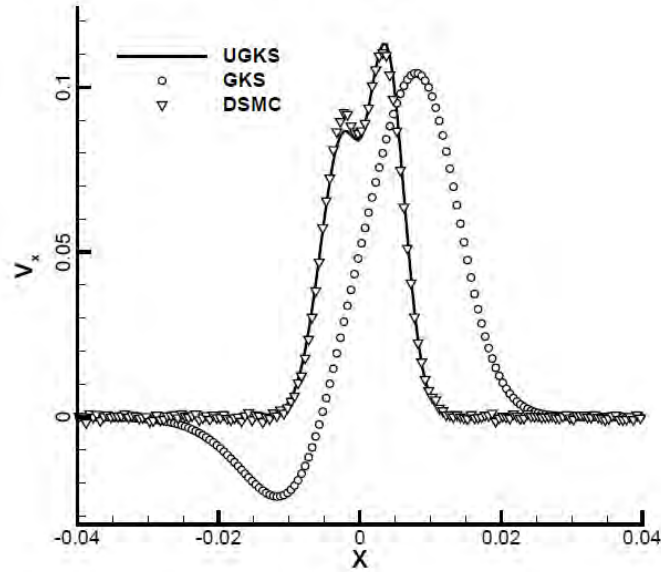
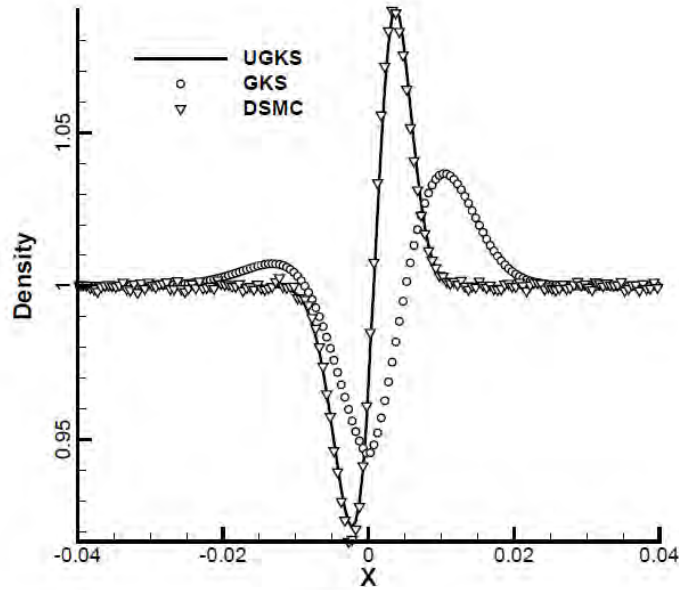


## Time step:



$t = 5.12 \times 10^{-3}$  ( $t = \tau_{ph}$ )

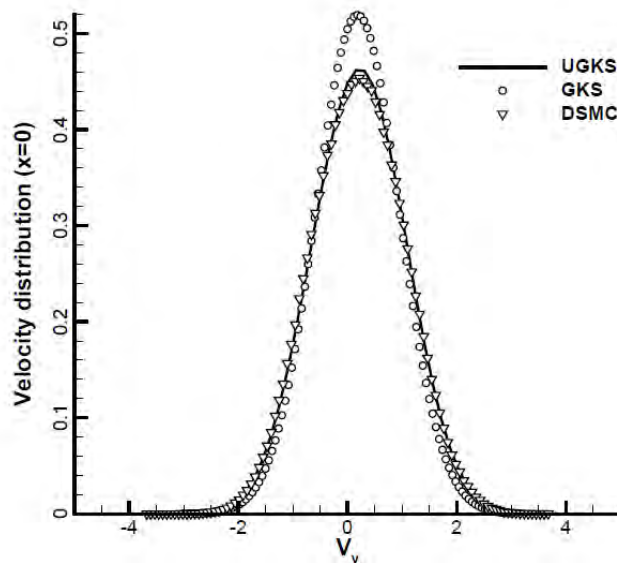
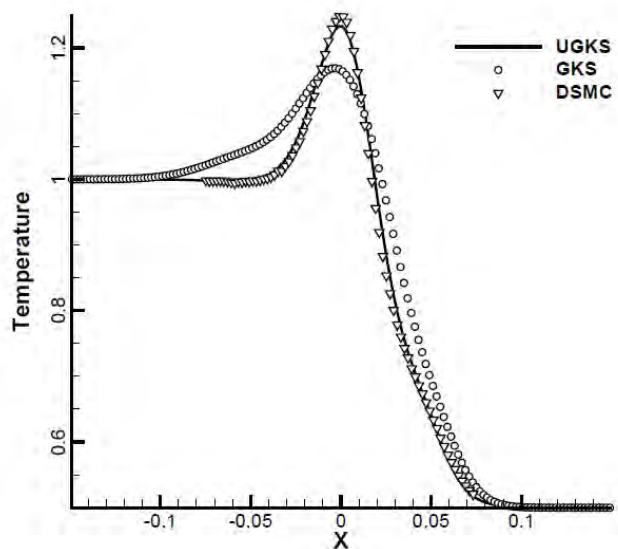
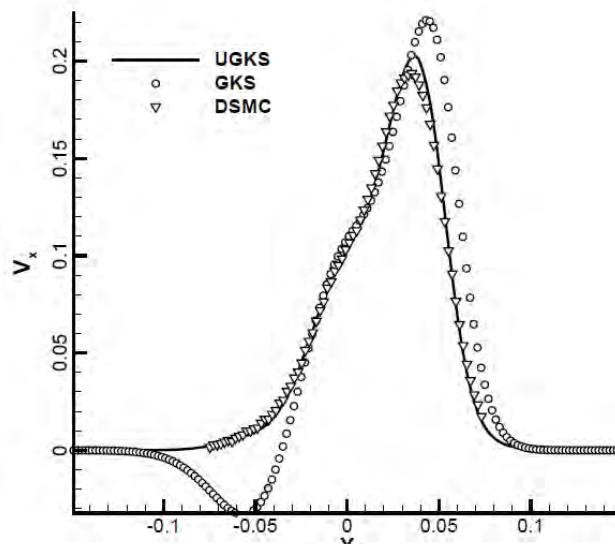
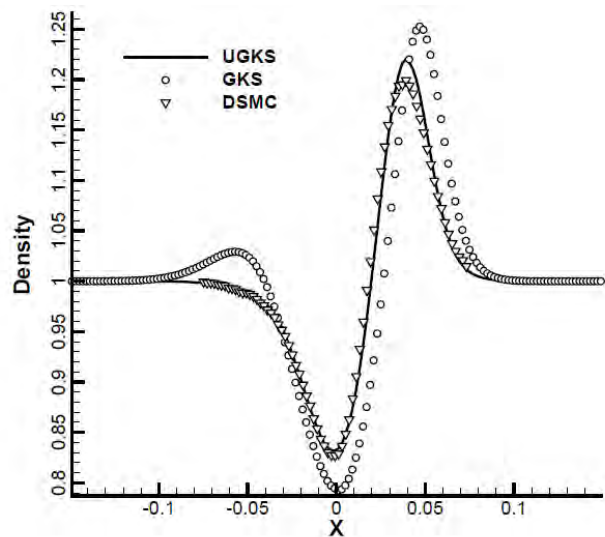
GKS  $dx/\ell = 0.1, dt = 1.96 \times 10^{-3} \tau_{ph}$   
UGKS  $dx/\ell = 0.1, dt = 1.65 \times 10^{-2} \tau_{ph}$



$$t = 5.12 \times 10^{-2} \quad (t = 10\tau_{ph})$$

$$\text{GKS } dx/\ell = 0.4, dt = 1.56 \times 10^{-2} \tau_{ph}$$

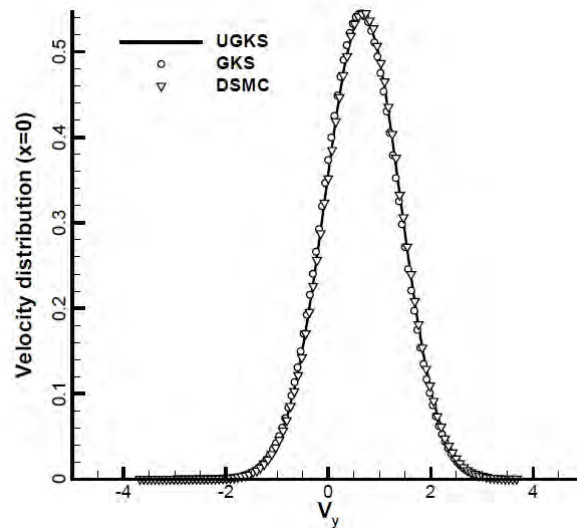
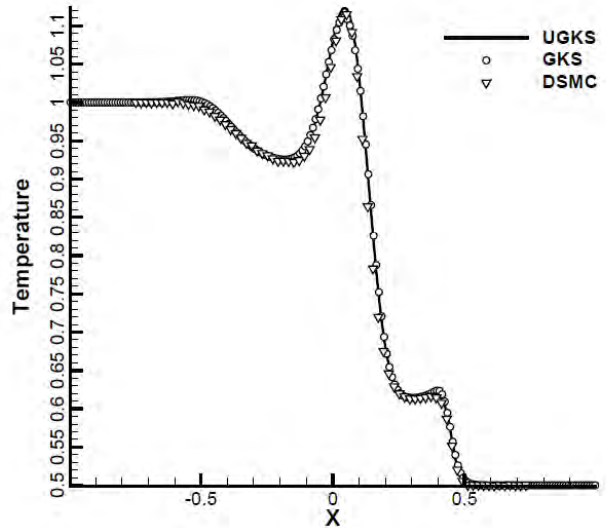
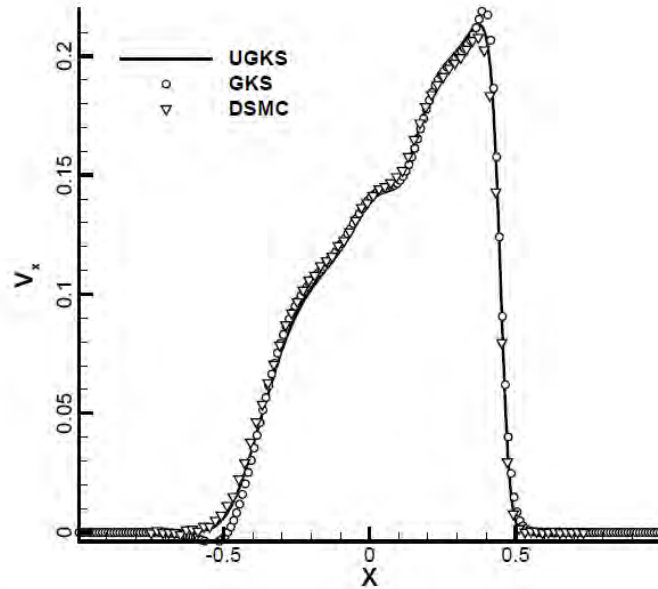
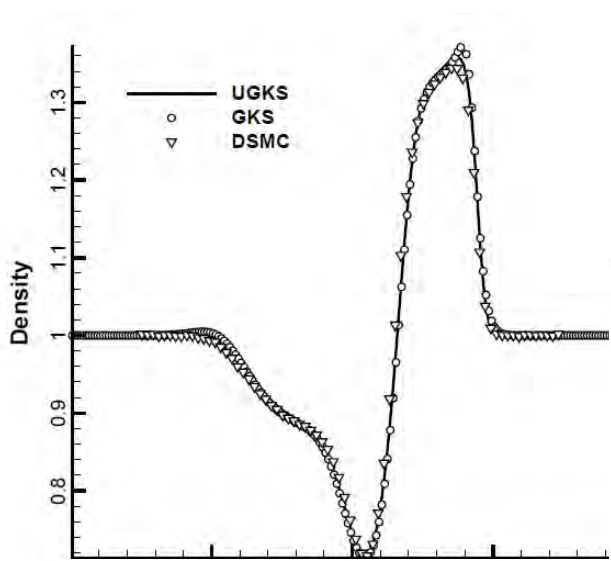
$$\text{UGKS } dx/\ell = 0.4, dt = 6.61 \times 10^{-2} \tau_{ph}$$



$t = 5.12 \times 10^{-1}$  ( $t = 100\tau_{ph}$ )

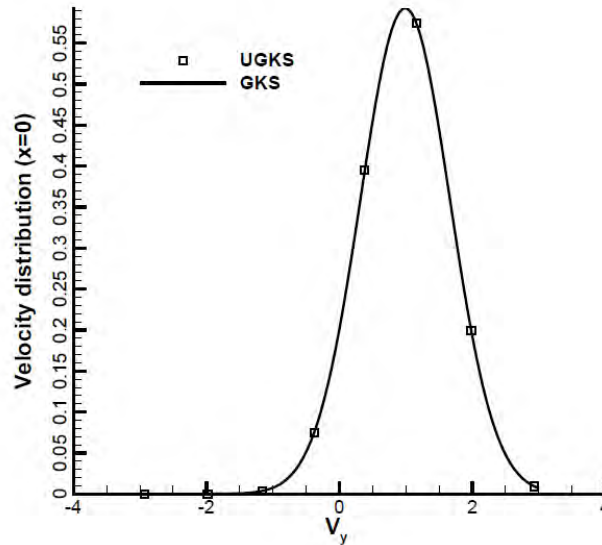
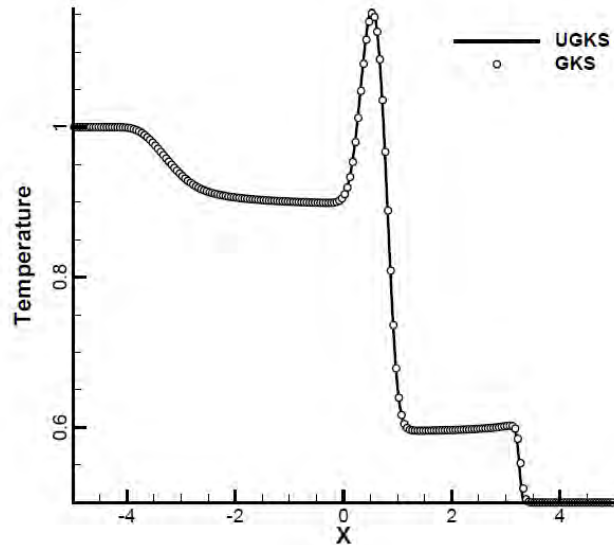
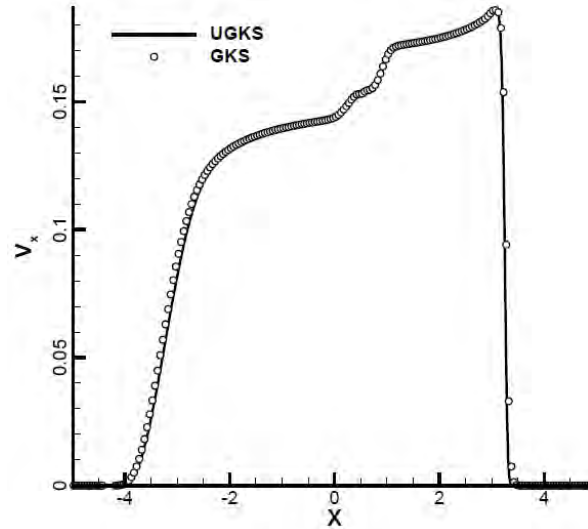
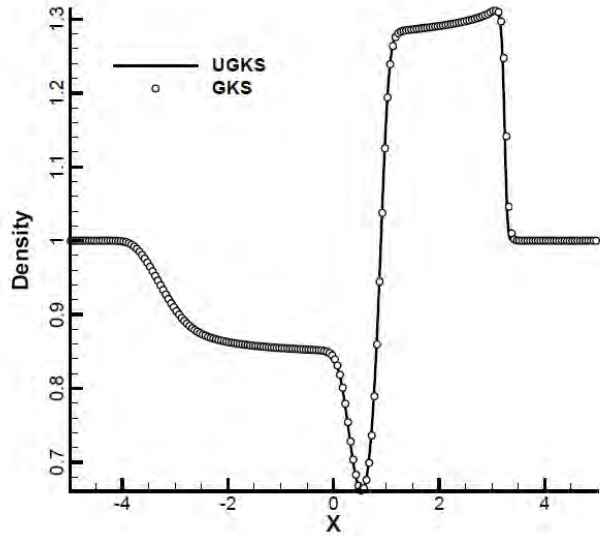
GKS  $dx/\ell = 2, dt = 3.91 \times 10^{-1}\tau_{ph}$

UGKS  $dx/\ell = 2, dt = 3.78 \times 10^{-1}\tau_{ph}$



$t = 4$  ( $t = 781.76\tau_{ph}$ )

GKS  $dx/\ell = 10, dt = 7.81\tau_{ph}$   
UGKS  $dx/\ell = 10, dt = 1.89\tau_{ph}$



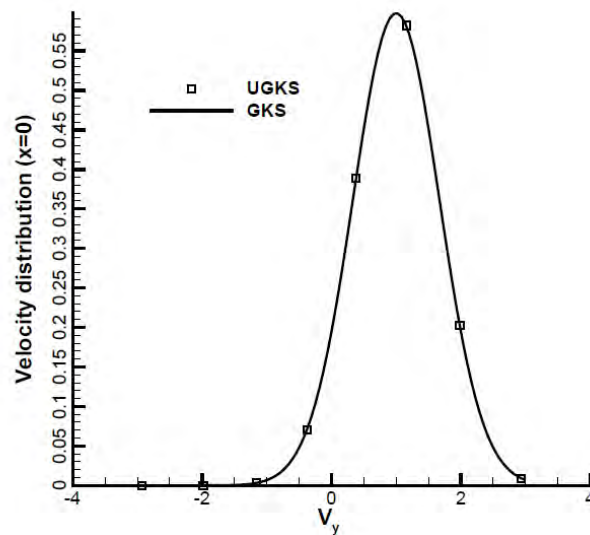
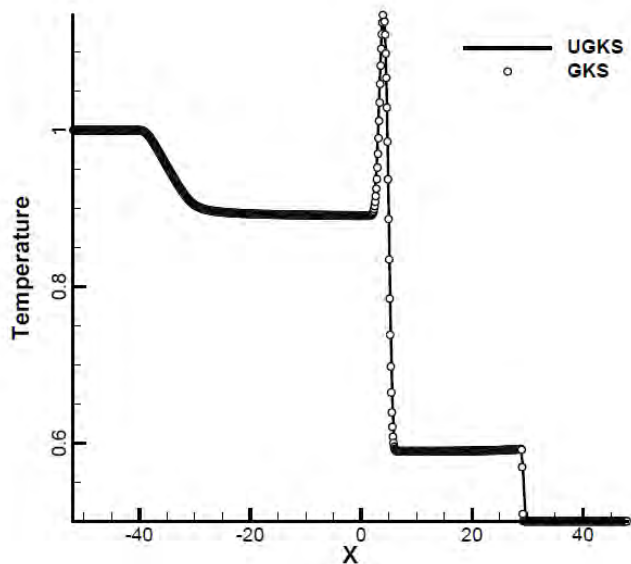
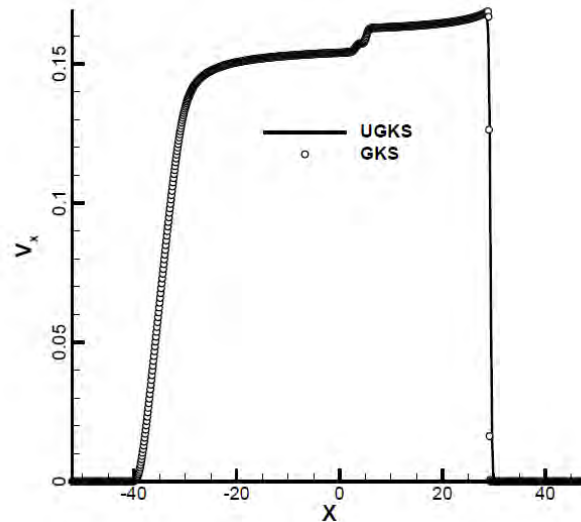
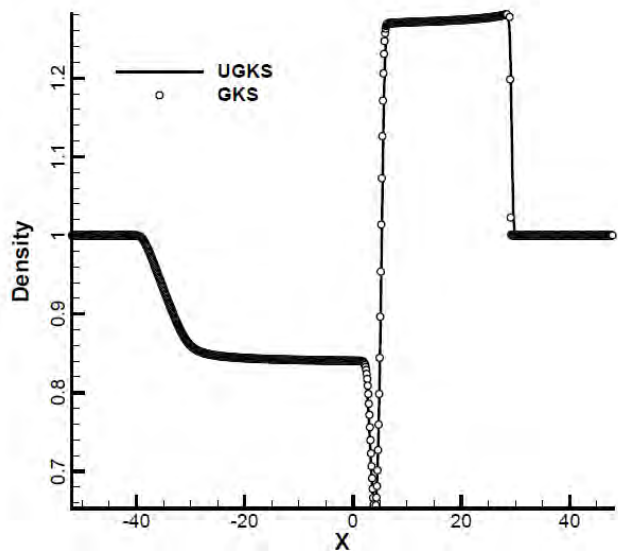
8x8 Gauss points



$t = 40$  ( $t = 7817.64\tau_{ph}$ )

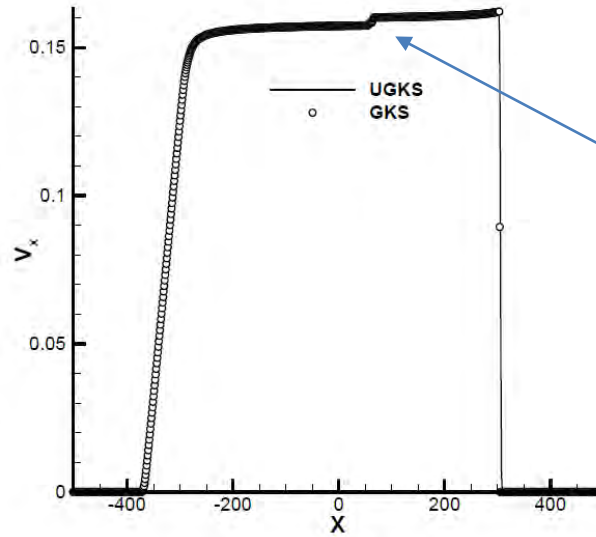
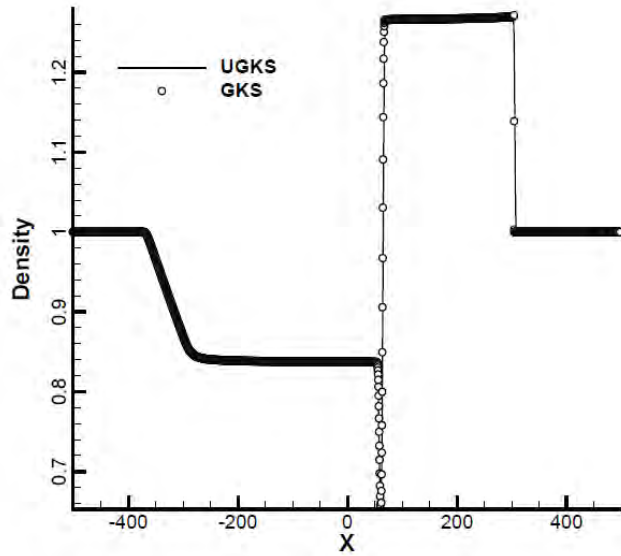
GKS  $dx/\ell = 10$ ,  $dt = 7.81\tau_{ph}$

UGKS  $dx/\ell = 50$ ,  $dt = 8.25\tau_{ph}$

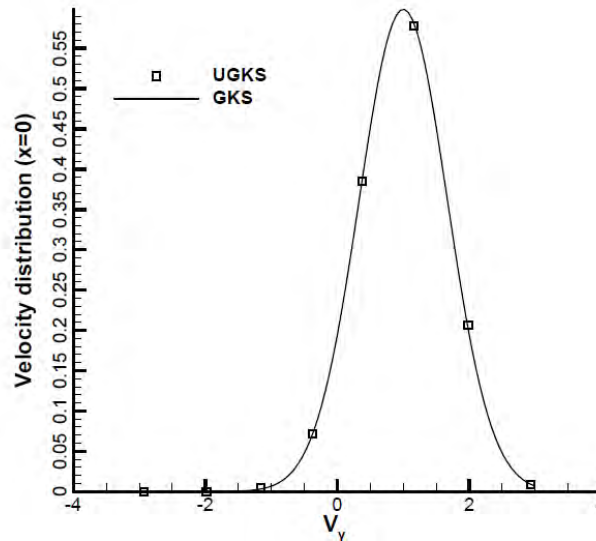
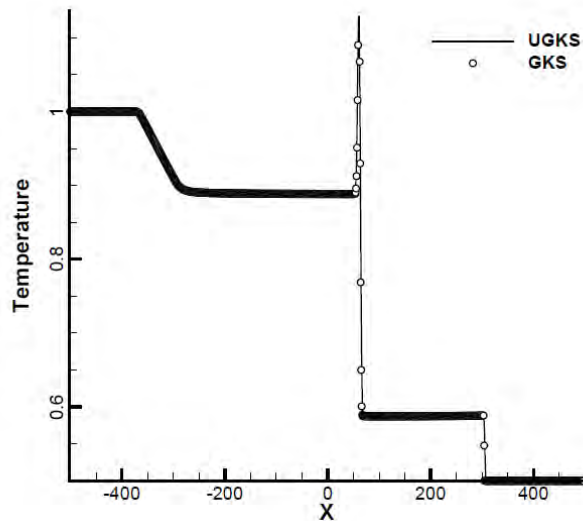


$t = 400$  ( $t = 78176.40\tau_{ph}$ )

GKS  $dx/\ell = 33.33$ ,  $dt = 26.06\tau_{ph}$   
UGKS  $dx/\ell = 250$ ,  $dt = 41.25\tau_{ph}$



Enlarged view  
on next page

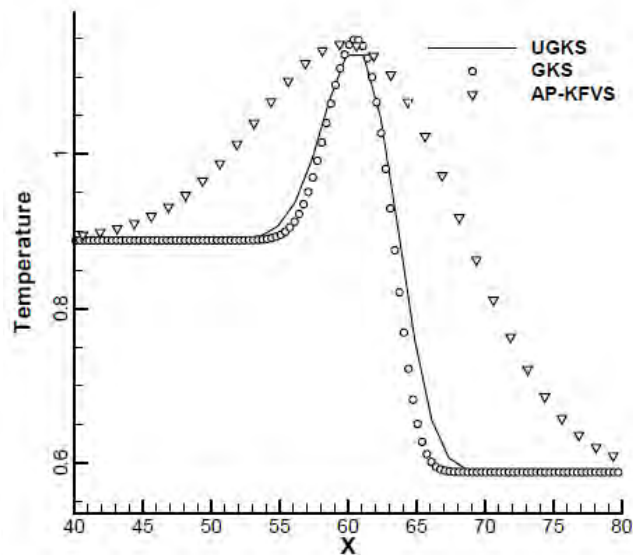
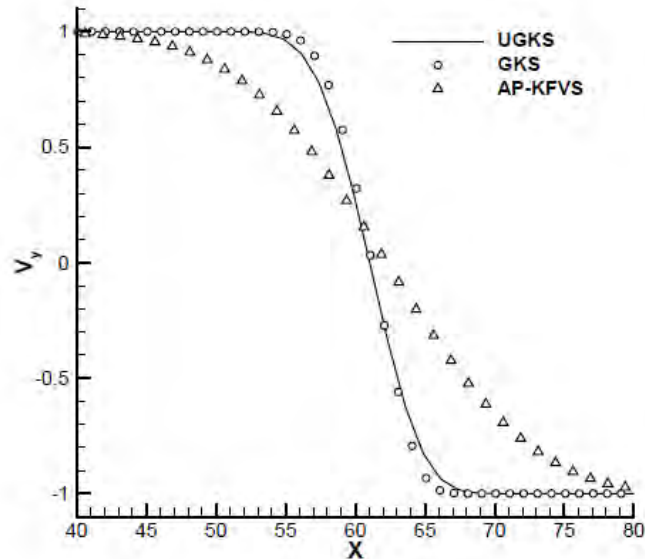
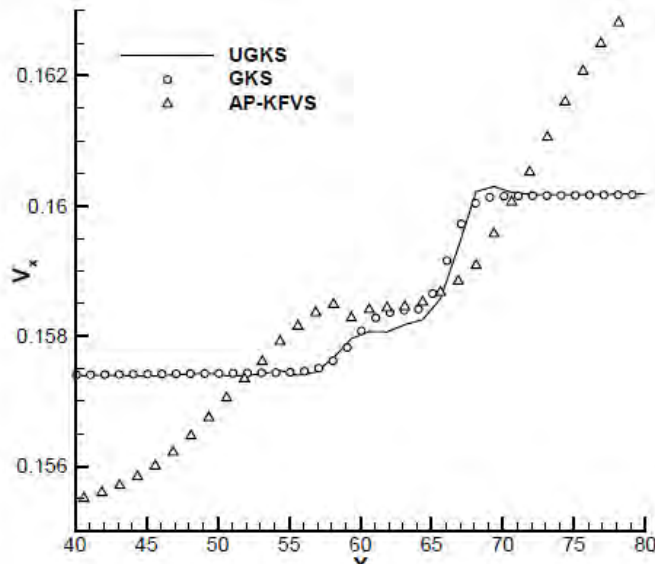
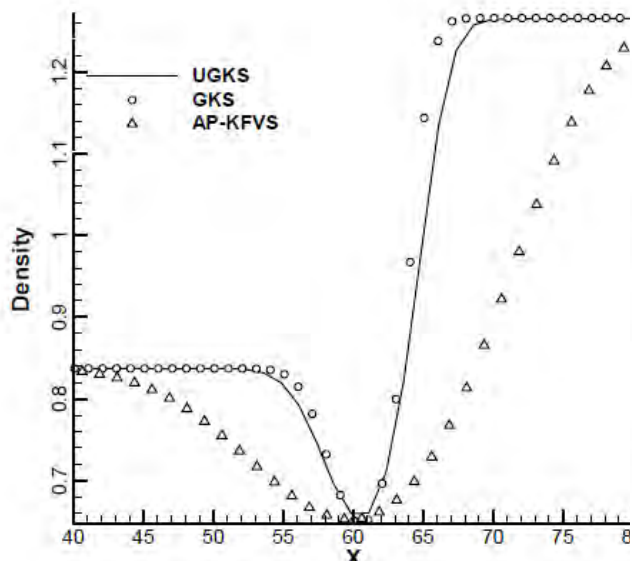


# Comparison with other schemes: GKS (NS), UGKS, AP-KFVS

AP-KFVS  $dx/\ell = 250, dt = 41.25\tau_{ph}$

GKS  $dx/\ell = 33.33, dt = 26.06\tau_{ph}$

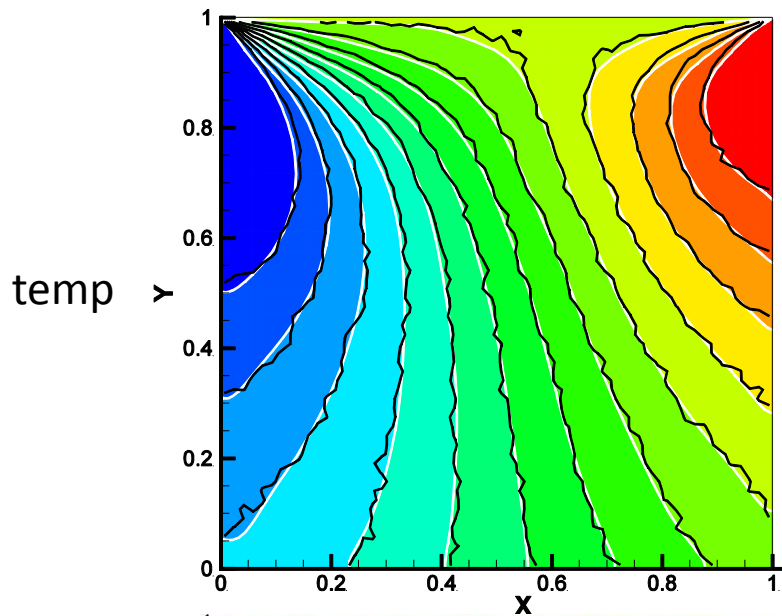
UGKS  $dx/\ell = 250, dt = 41.25\tau_{ph}$



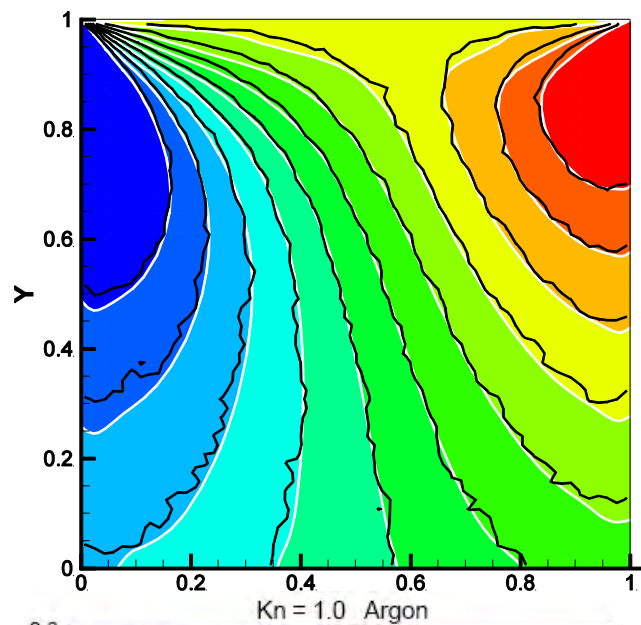


# UGKS vs DSMC

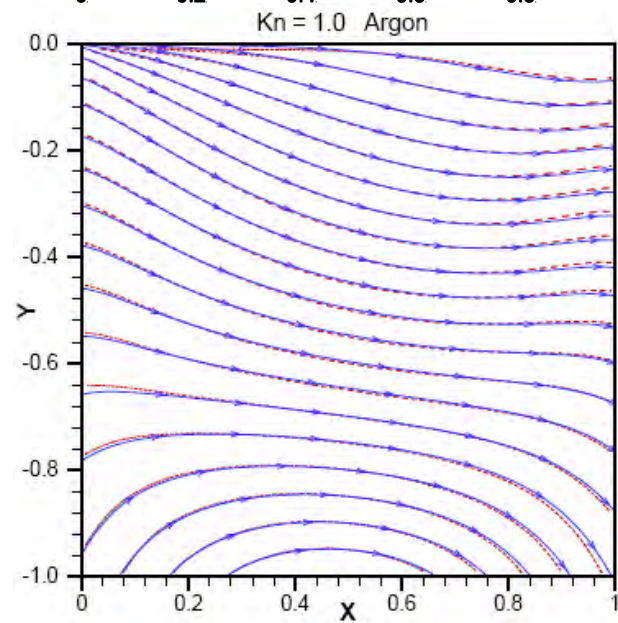
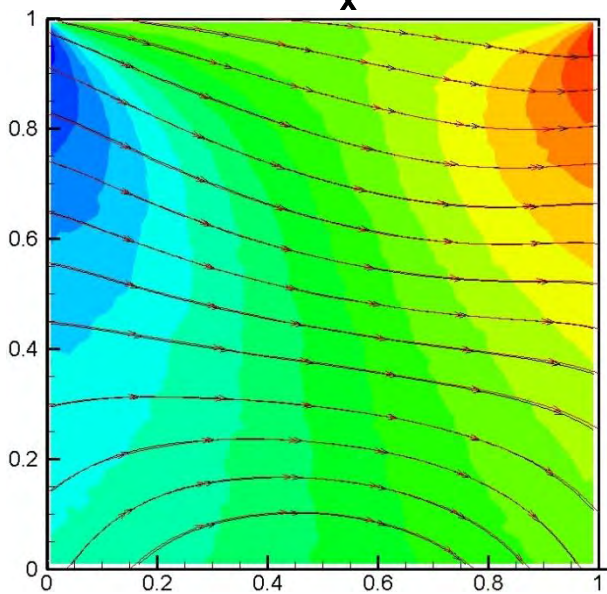
Kn=10



Kn=1

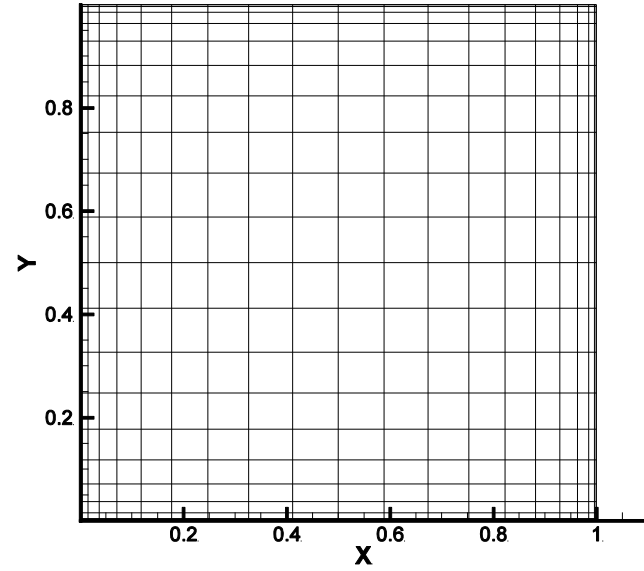
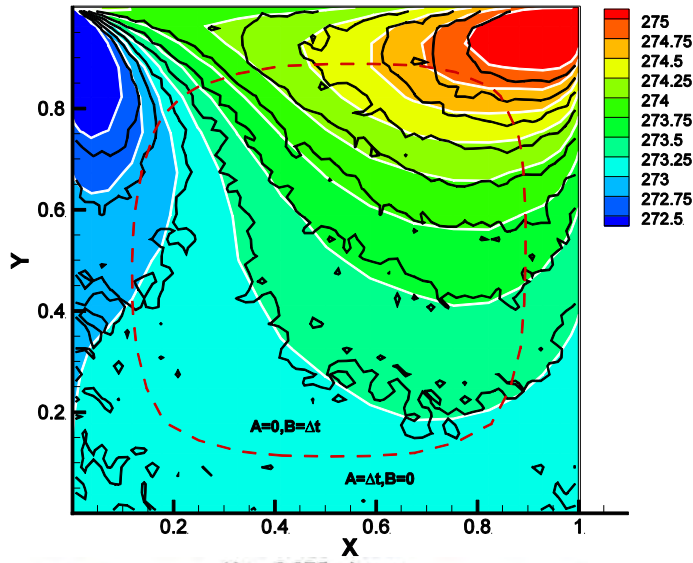


Heat flux

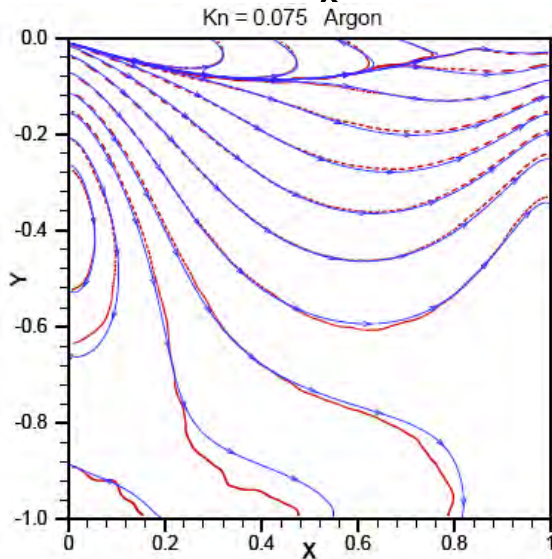


# Kn=0.075 cavity case

temp

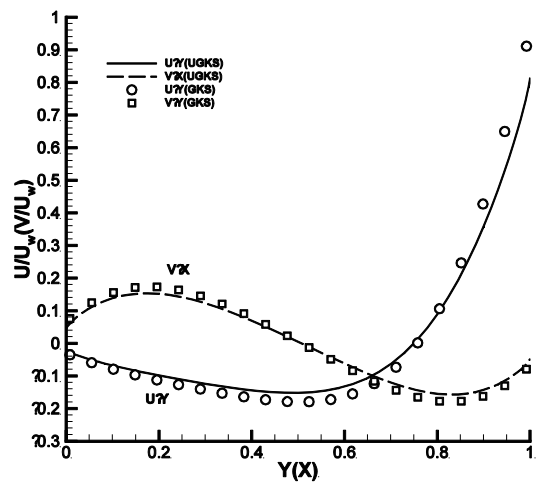
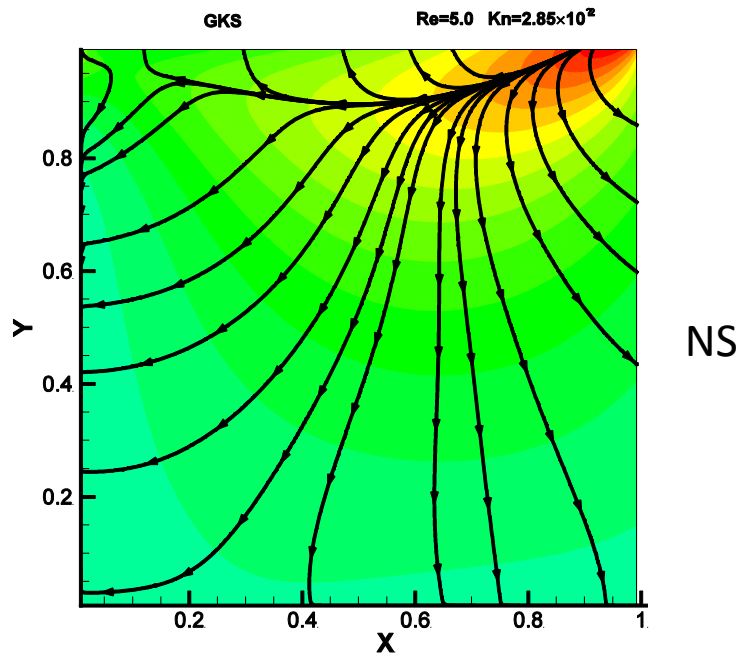
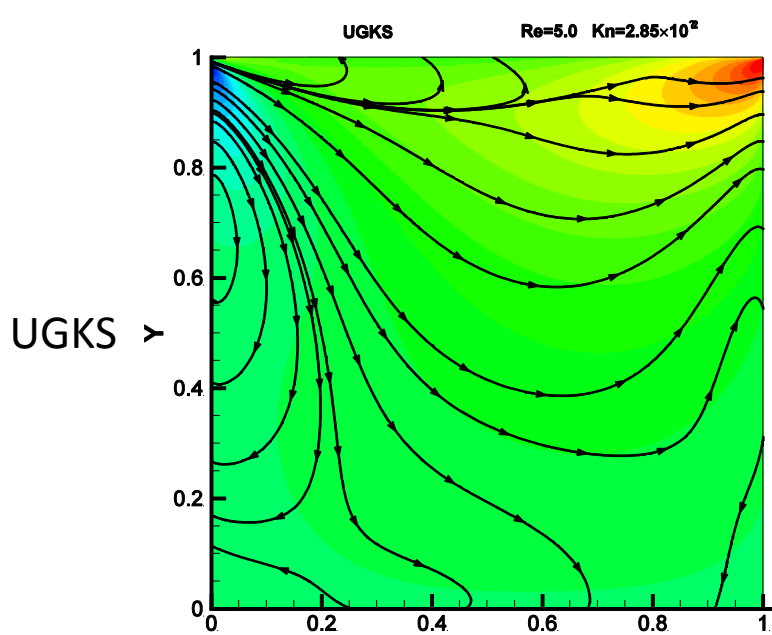


Heat flux

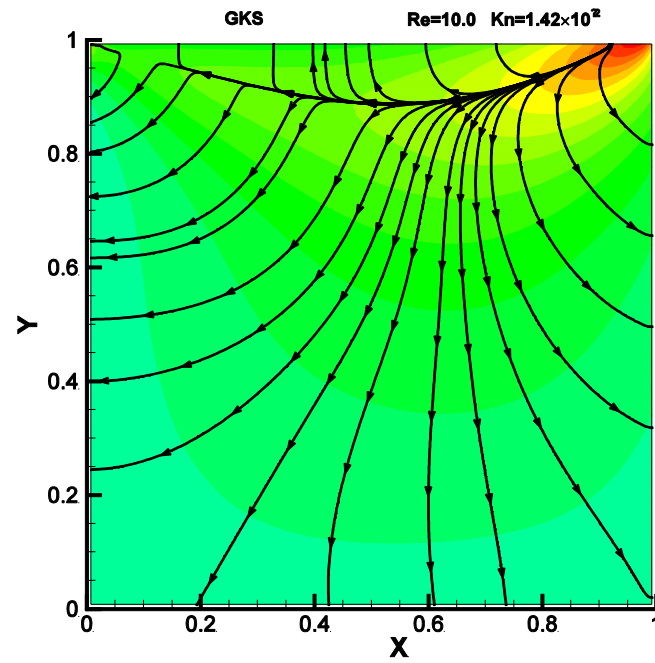
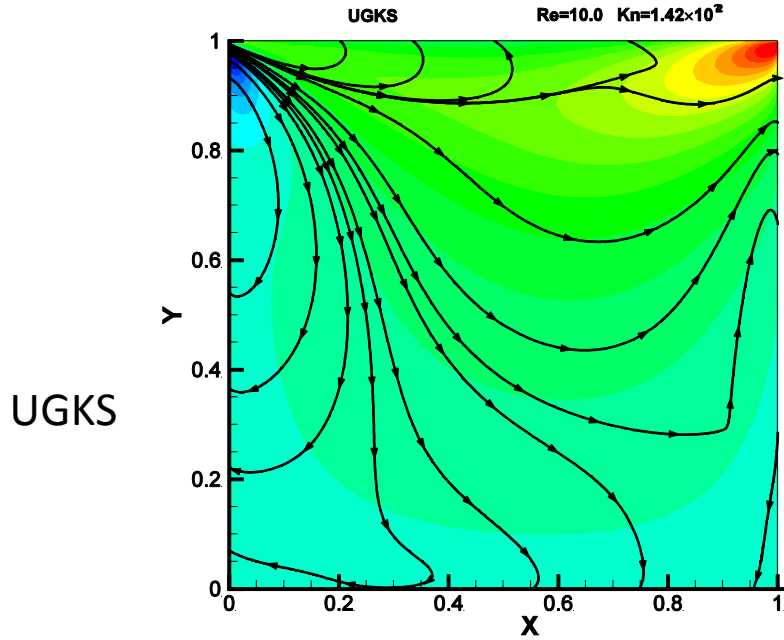


C. Liu

Re=5, Kn=0.0285

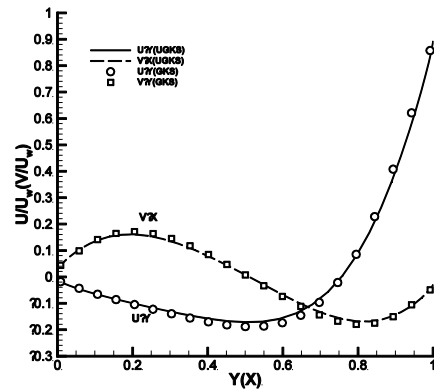


Re=10, Kn=0.0142

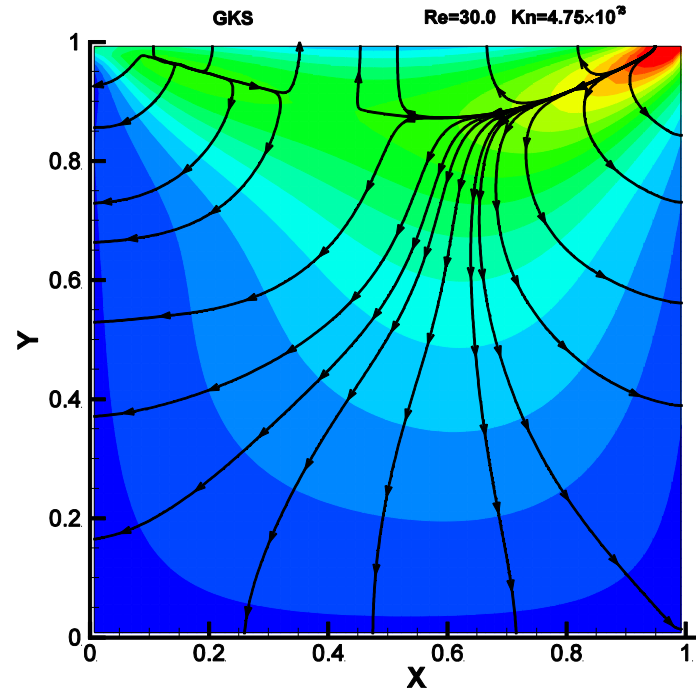
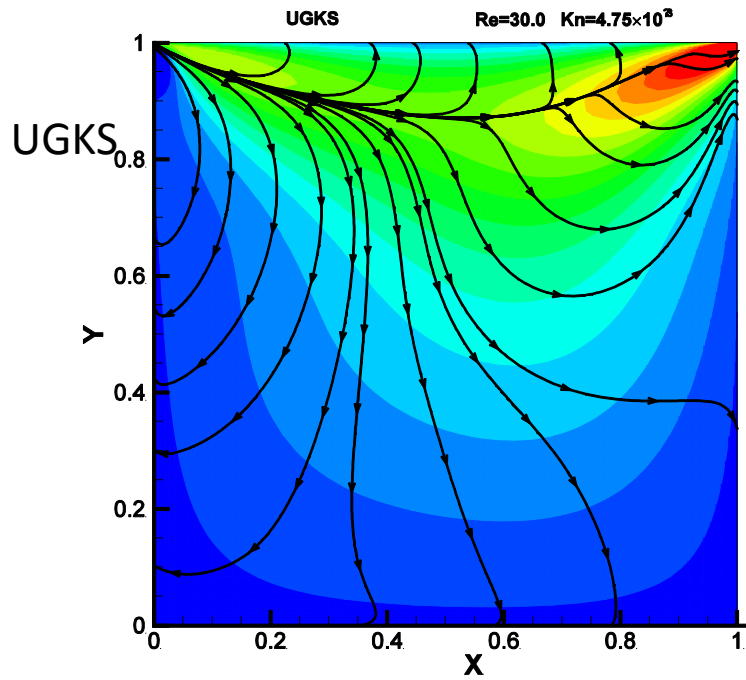


NS

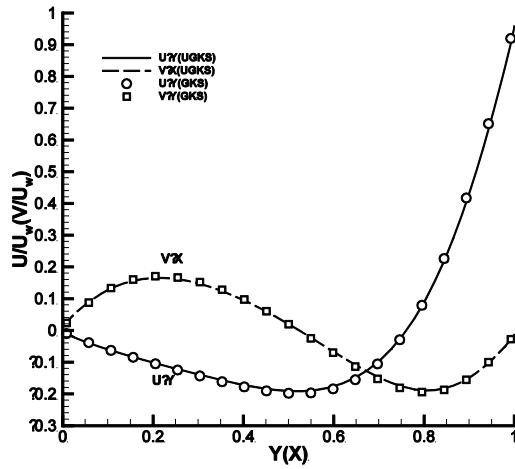
UGKS



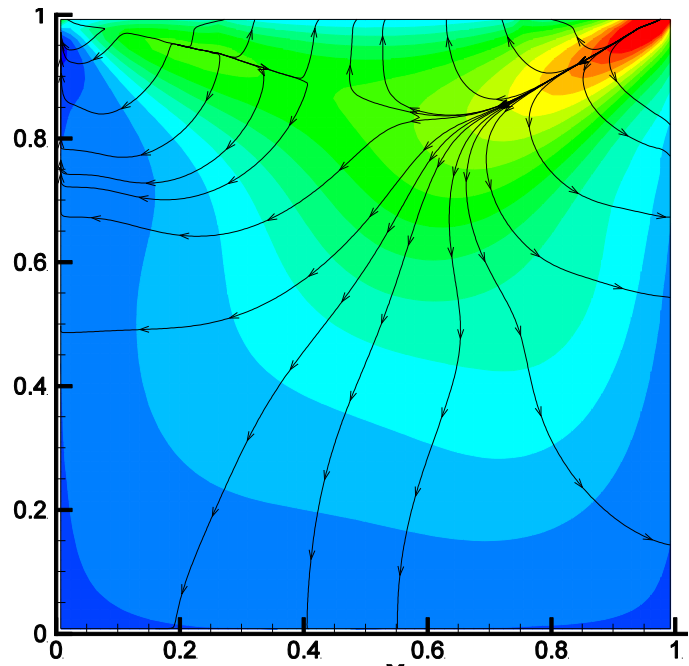
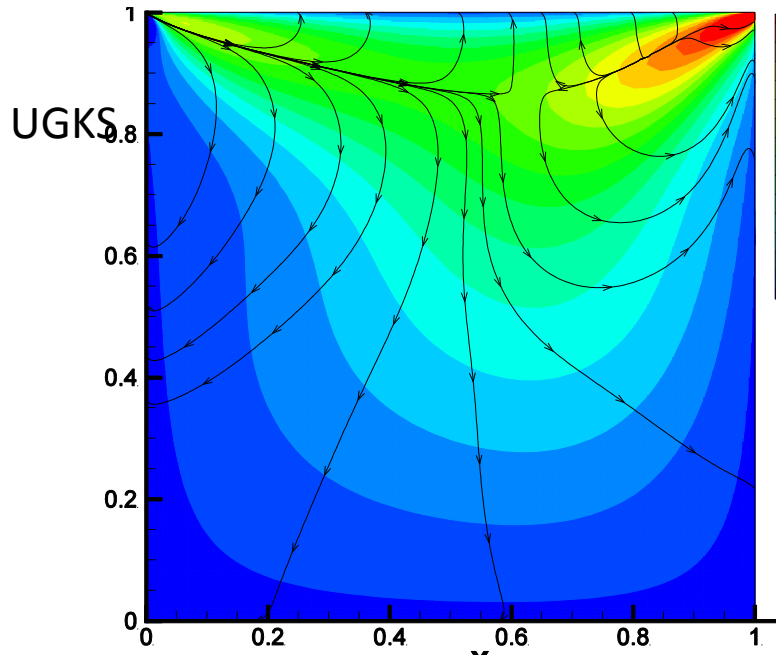
Re=30, Kn=0.00475



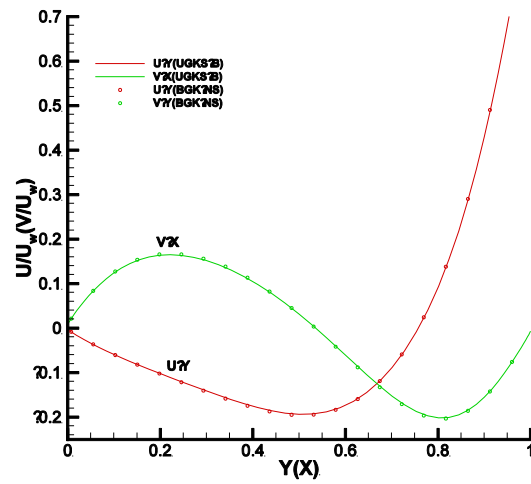
NS



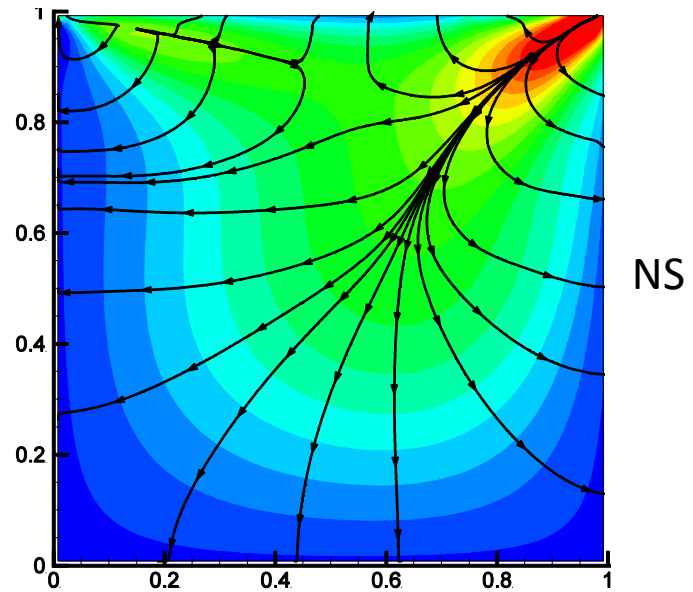
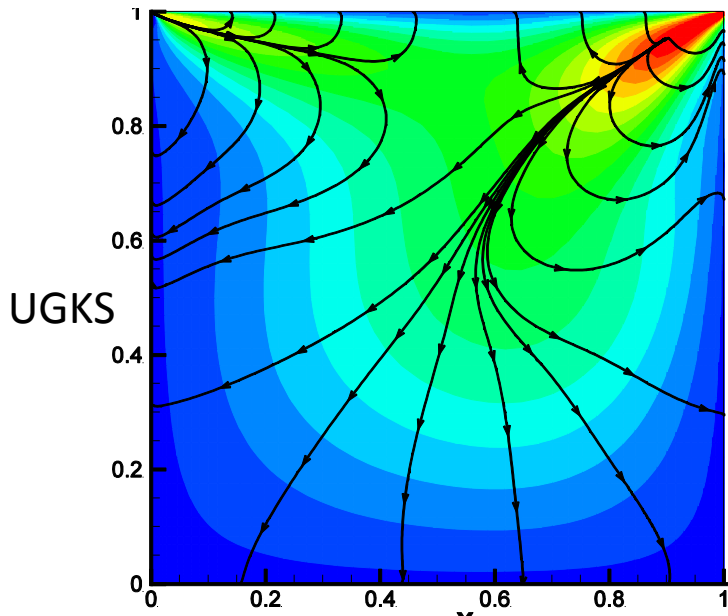
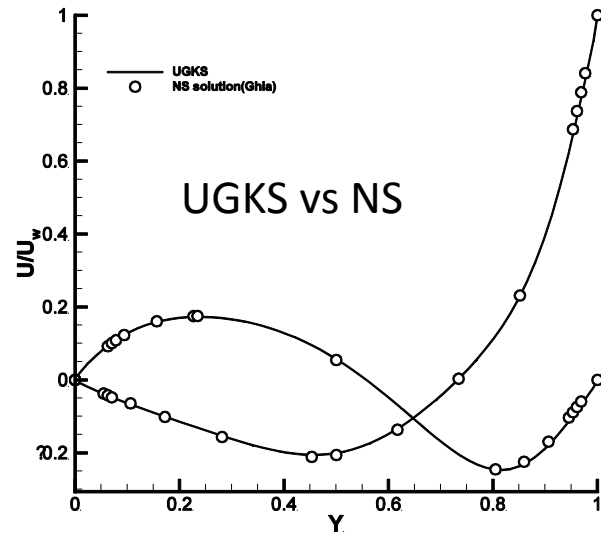
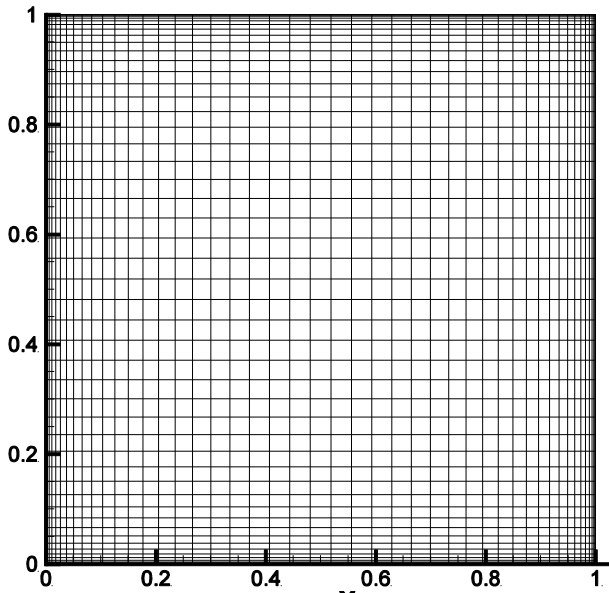
Re=50, Kn=0.00285



NS

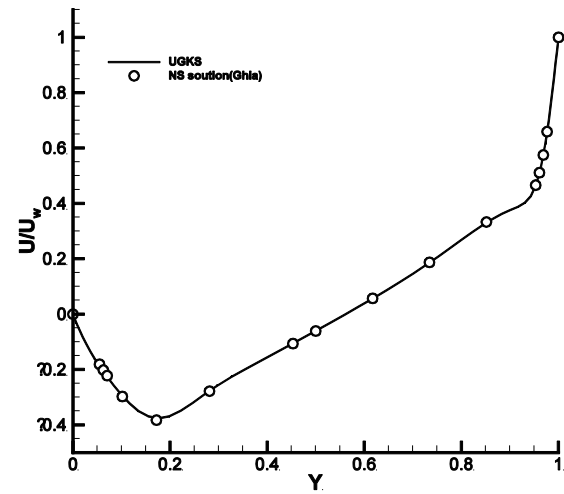
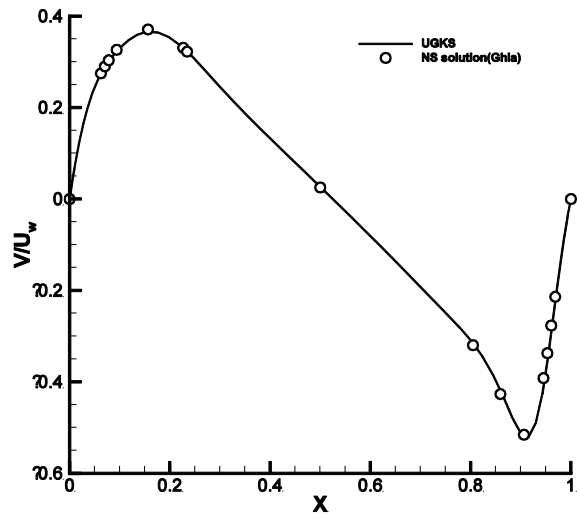
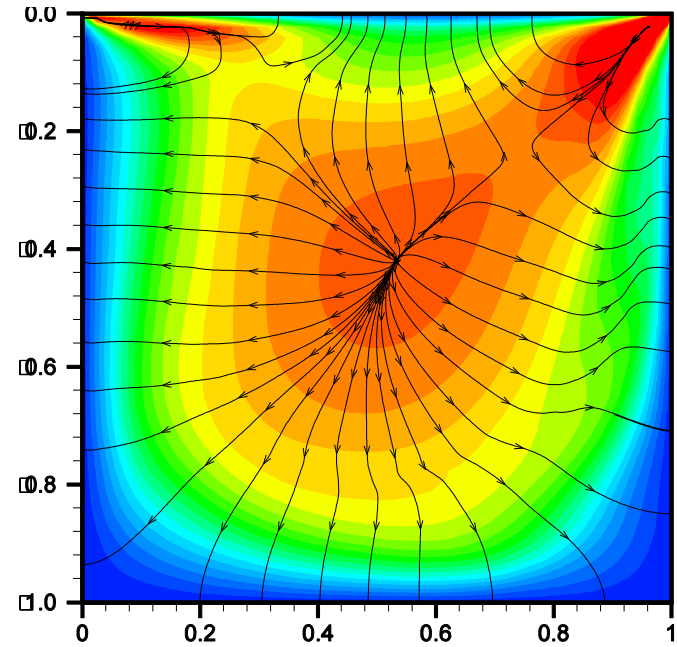
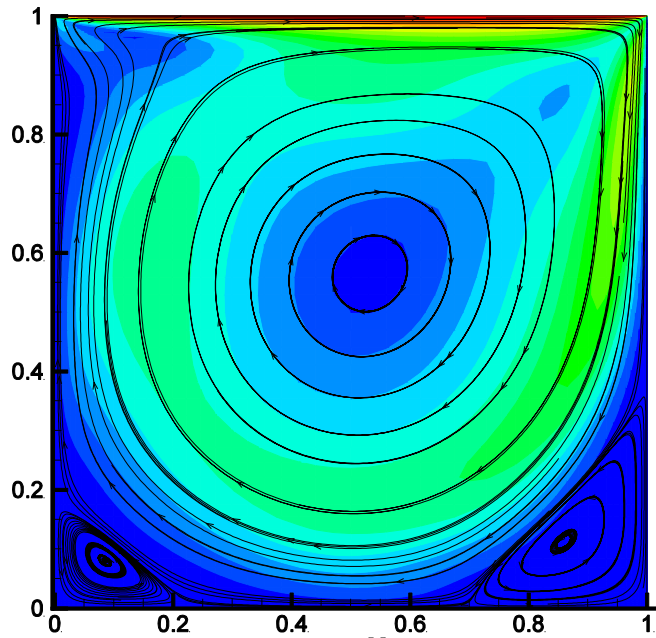


Re=100, Kn=0.00142





# UGKS solutions: $Re=1000, Kn=0.000142$

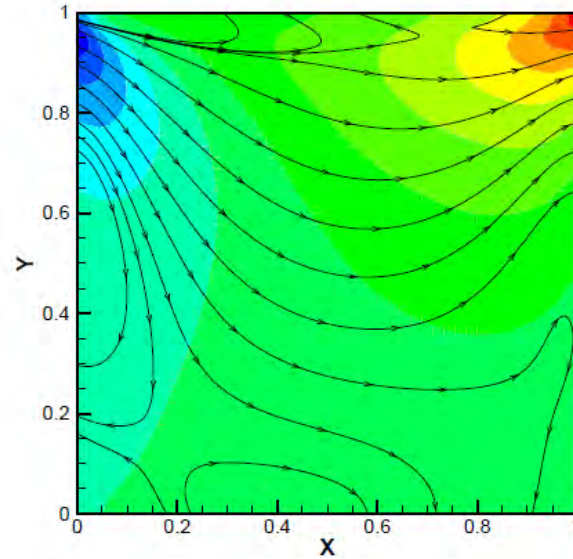
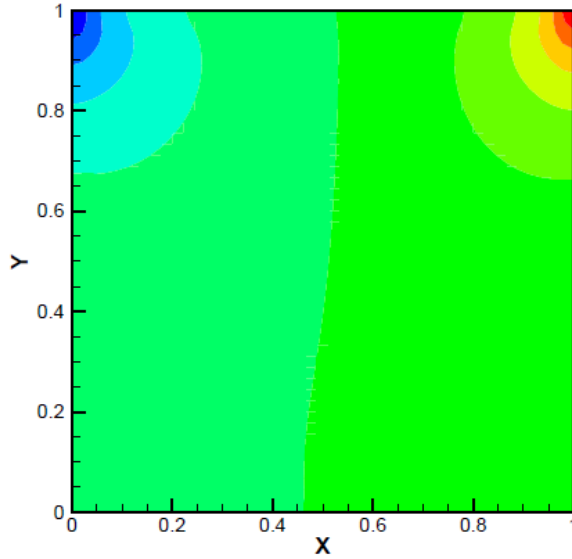




UGKS with gravity:

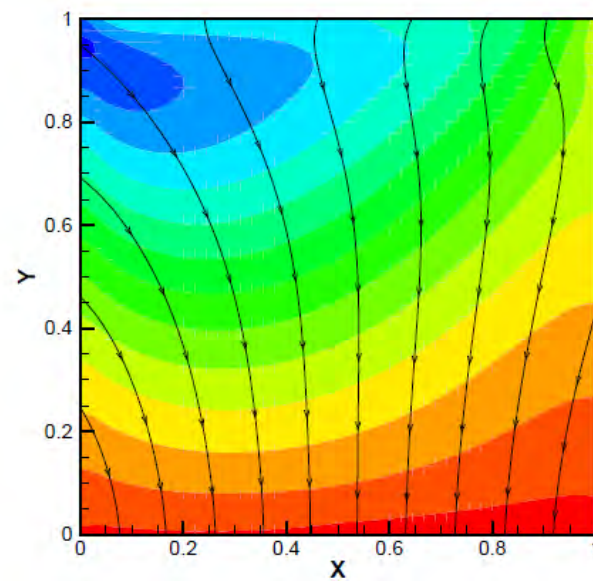
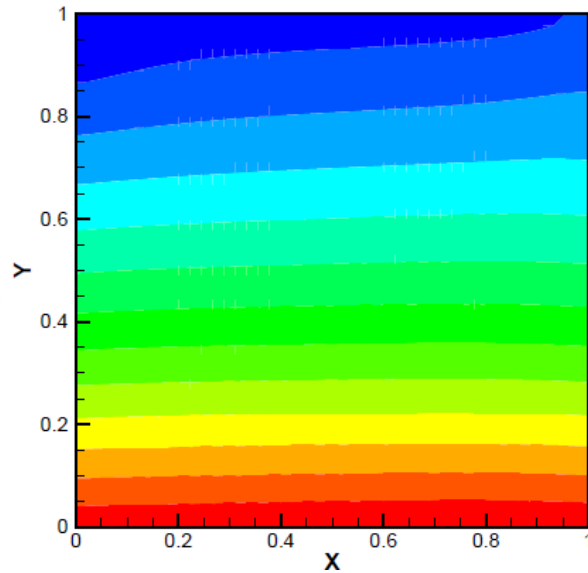
$$f_t + u_i f_{x_i} + \phi_i f_{u_i} = Q(f, f)$$

Without gravity



Gravity

$$\phi_y = -1.0$$



# UGKS vs DSMC

## UGKS

1. Time step determined by the CFL condition
2. No limitation on the mesh size
3. No statistical noise
4. Suitable for all Knudsen regimes
5. Unsteady flow simulation
6. High efficiency for low speed flow
7. Massive memory requirement for hypersonic flow
8. Implicit and multigrid can accelerate the computation greatly
9. Validated in the past 5 years and the validation and development will be continuously conducted

## DSMC

1. Time step should be less than the particle collision time
2. Cell size should be less than the particle mean free path
3. Significant statistical noise
4. Suitable in rarefied regime and high speed
5. Validating in the past 5 decades!



推向实战:



CARDC 博士学位论文

单位代码	90113
密 级	公开
学 号	

# 基于模型方程解析解的气体动力学 算法研究

博 士 生: 江定武

导 师: 邓小刚 院 士

副 导 师: 毛枚良 研究员

学科专业: 力学、流体力学

研究方向: 气体动力学方法

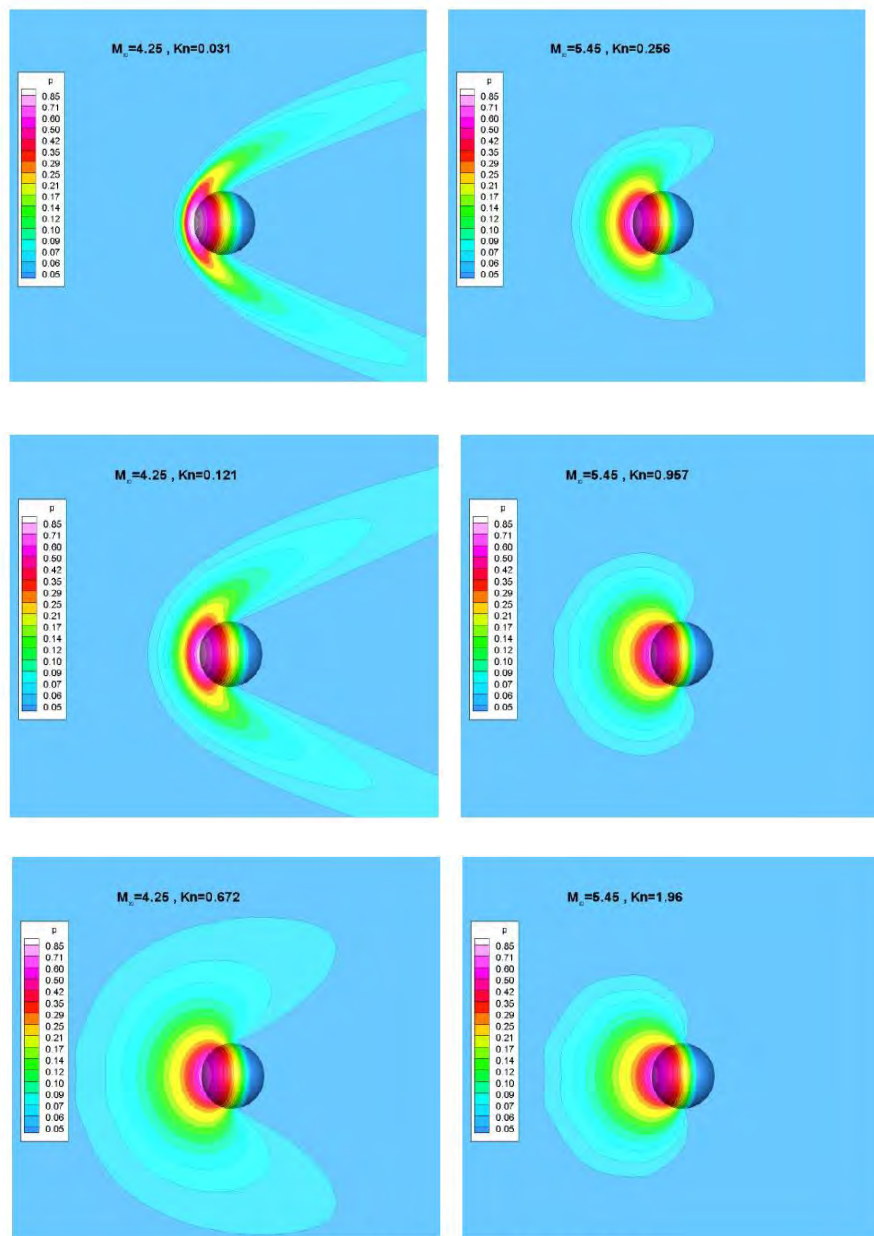


图 6.1 圆球算例，对称面及固壁压力分布

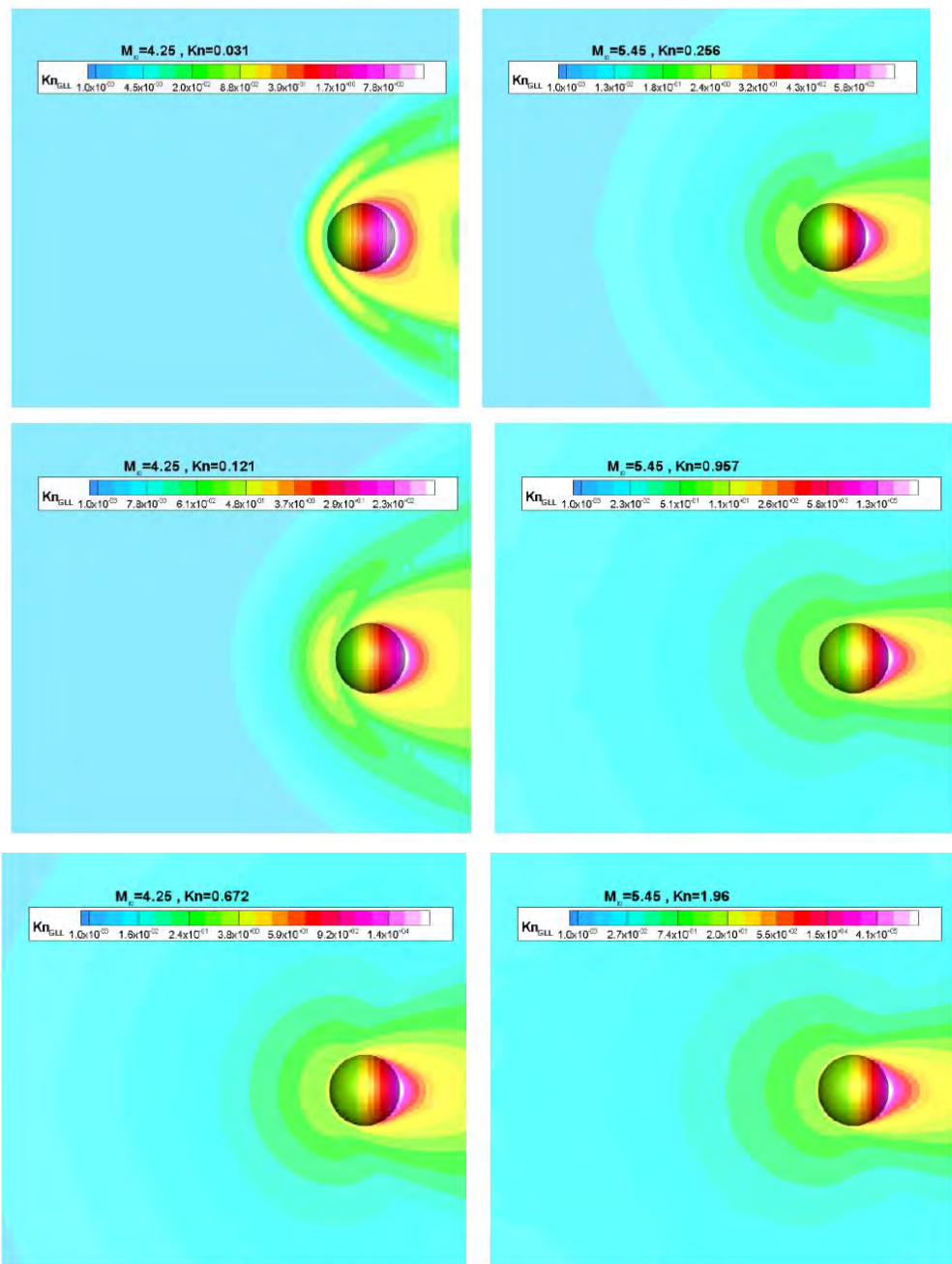


图 6.4 圆球算例，对称面及固壁局部努森数分布



表 6.1 圆球阻力系数比较 (UGKS.vs.EXP)

$M_\infty$	Re	$Kn_\infty$	UGKS(Nitrogen)	Exp (Air)	偏差 (%)
4.25	9.55	0.672	2.356	2.42	2.64%
4.25	19.0	0.338	2.101	2.12	0.87%
4.25	53.0	0.121	1.694	1.69	-0.27%
4.25	80.5	0.080	1.558	1.53	-1.80%
4.25	150.0	0.043	1.410	1.37	-2.91%
4.25	210.0	0.031	1.355	1.35	-0.39%
5.45	4.2	1.960	2.595	2.60	0.18%
5.45	8.6	0.957	2.449	2.44	-0.36%
5.45	16.8	0.490	2.248	2.28	1.41%
5.45	32.1	0.256	2.005	2.04	1.71%

表 6.2 圆球阻力系数比较 (NS.vs.EXP)

$M_\infty$	Re	$Kn_\infty$	NS+noslip		NS+slip	
			阻力值	偏差 (%)	阻力值	偏差 (%)
4.25	9.55	0.672	7.400	205.77%	4.774	97.26%
4.25	19.0	0.338	4.792	126.02%	3.177	49.87%
4.25	53.0	0.121	2.826	67.23%	2.015	19.20%
4.25	80.5	0.080	2.379	55.47%	1.775	16.00%
4.25	150.0	0.043	1.921	40.21%	1.543	12.63%
4.25	210.0	0.031	1.743	29.09%	1.455	7.78%

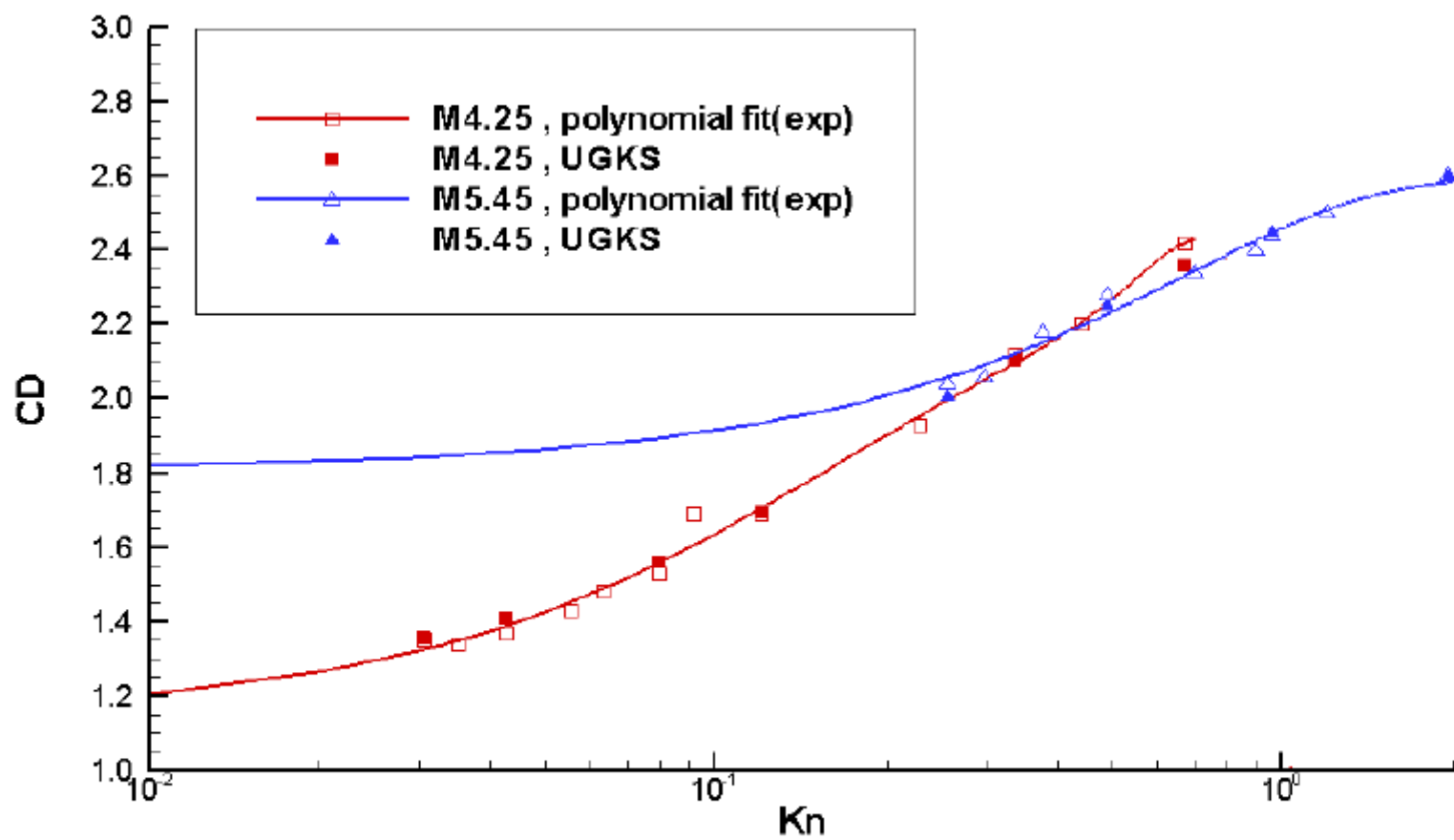


图 6.19 圆球阻力比较

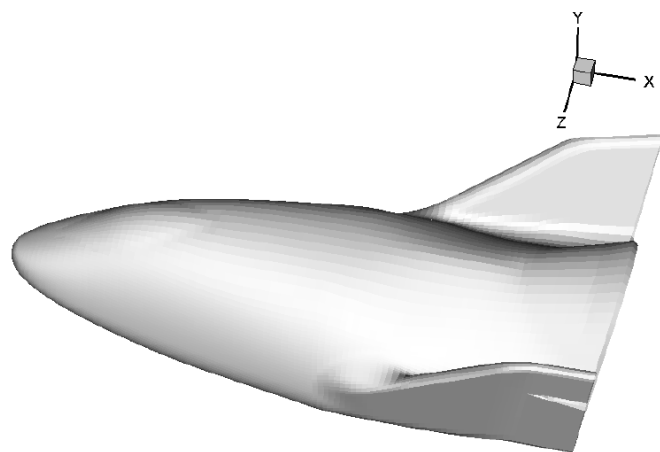
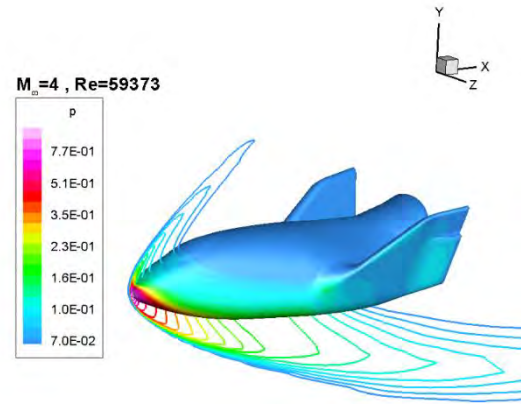
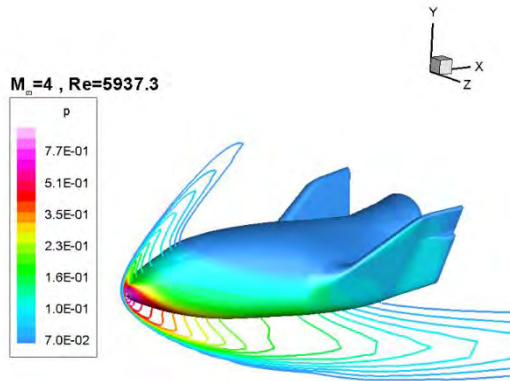
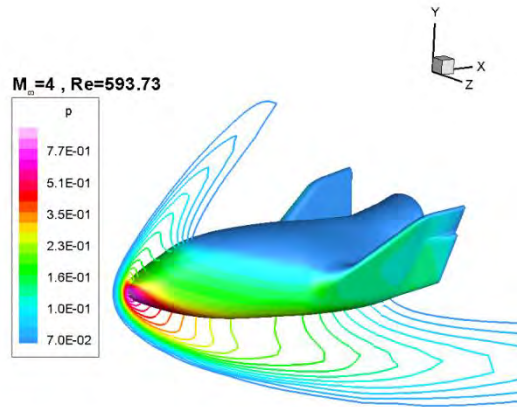
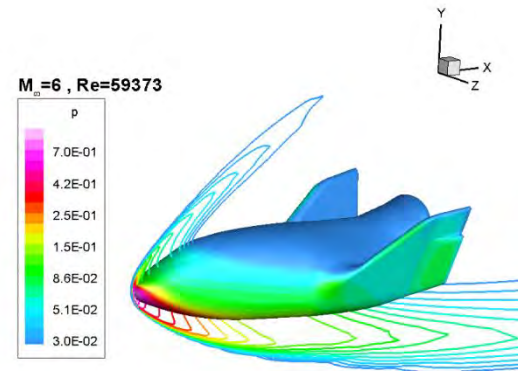
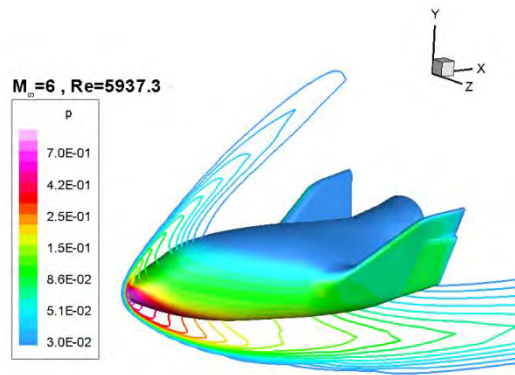
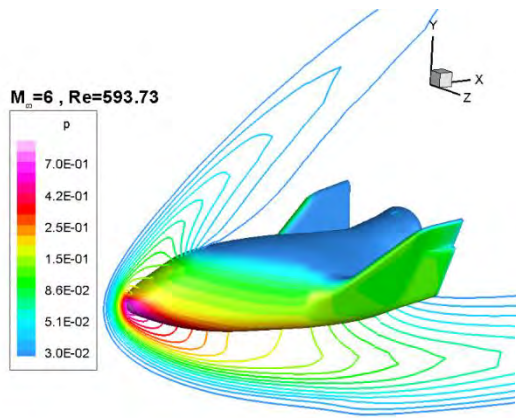


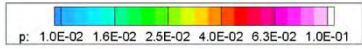
表 6.3 X38 力系数比较

$M_\infty$	Re	$Kn_\infty$	来流介质	轴向力	法向力	俯仰力矩	升力	阻力
4	593.73	8.41E-03	Argon	0.3991	0.3929	0.1664	0.2327	0.5094
4	5937.3	8.41E-04		0.1956	0.3146	0.1419	0.2288	0.2914
4	59373	8.41E-05		0.1150	0.2821	0.1293	0.2257	0.2045
6	593.73	1.26E-02		0.4179	0.3728	0.1536	0.2074	0.5202
6	5937.3	1.26E-03		0.1955	0.2887	0.1255	0.2045	0.2825
6	59373	1.26E-04		0.1103	0.2550	0.1126	0.2019	0.1908
4	593.73	8.24E-03	Nitrogen	0.4176	0.4015	0.1695	0.2345	0.5298
6	593.73	1.24E-02		0.4330	0.3765	0.1539	0.2057	0.5357

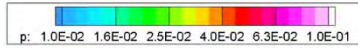
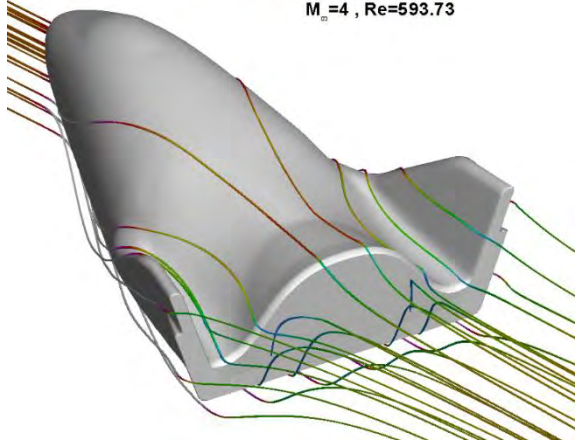




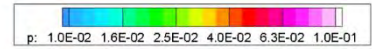
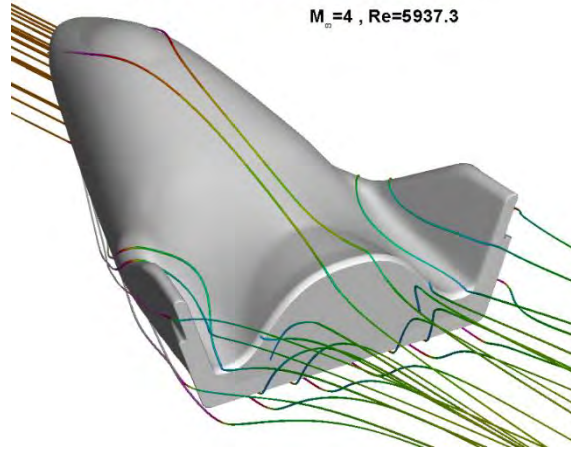




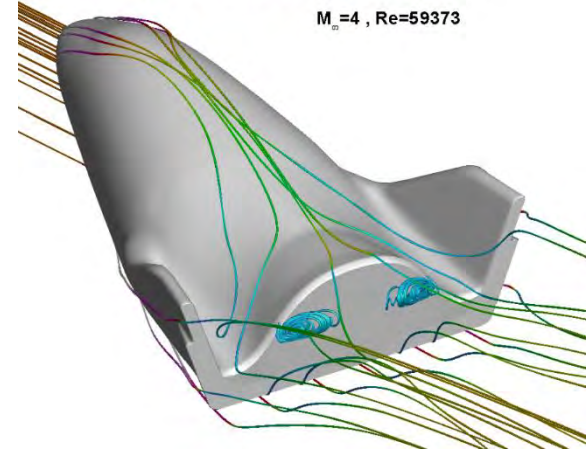
$M_\infty = 4$ ,  $Re = 593.73$

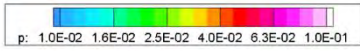


$M_\infty = 4$ ,  $Re = 5937.3$

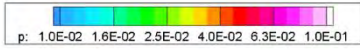
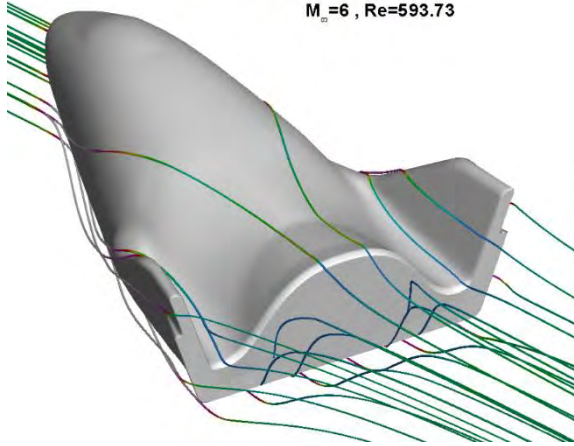


$M_\infty = 4$ ,  $Re = 59373$

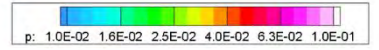
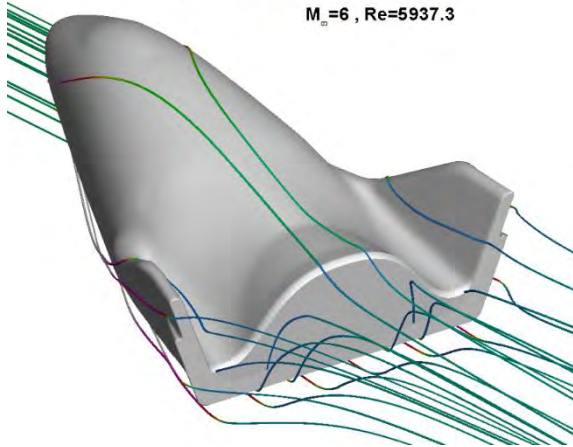




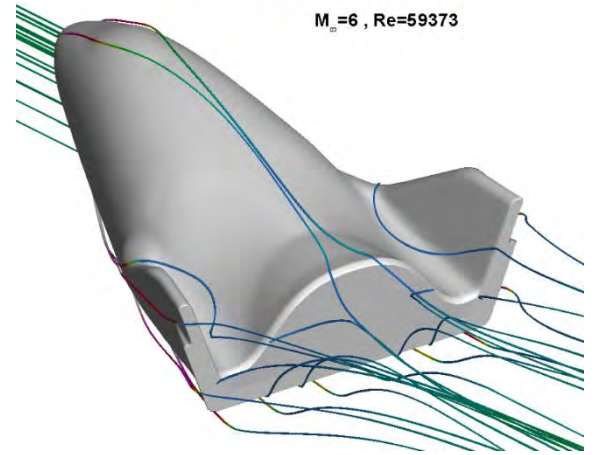
$M_\infty = 6$ ,  $Re = 593.73$



$M_\infty = 6$ ,  $Re = 5937.3$



$M_\infty = 6$ ,  $Re = 59373$



# **Modeling and Computation in Multiscale Transport Processes**

- **Rarefied Flow**
- **Radiative and Neutron Transport**
- **Plasma Physics**
- **Non-equilibrium Thermodynamics**

# Multiple frequency radiative transfer equations

$$\begin{cases} \frac{\epsilon^2}{c} \frac{\partial I}{\partial t} + \epsilon \vec{\Omega} \cdot \nabla I = \sigma(B(\nu, T) - I), \\ \epsilon^2 C_v \frac{\partial T}{\partial t} \equiv \epsilon^2 \frac{\partial U}{\partial t} = \int_{4\pi} \int_0^\infty \sigma (I - B(\nu, T)) d\nu d\vec{\Omega}. \end{cases}$$

$I(\vec{r}, \vec{\Omega}, t)$ : Radiation intensity,  $T(\vec{r}, t)$ : Material temperature,  
 $\sigma(\vec{r}, T)$ : Opacity,  $a$ : Radiation constant,  $c$ : Speed of light,  
 $\epsilon > 0$ : Knudsen number,  $C_v(\vec{r}, t)$ : Specific heat,  
 $\vec{r}$ : Spatial variable,  $\vec{\Omega}$ : Angular variable,  $t$ : Time variable.

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1}$$



## Macroscopic equations

$$\begin{cases} \frac{\epsilon^2}{\mathbf{c}} \frac{\partial \rho}{\partial t} + \epsilon \nabla \cdot \langle \vec{\Omega} I \rangle = \sigma(\phi - \rho), & \langle \vec{\Omega} I \rangle := \int \vec{\Omega} I d\vec{\Omega}, \\ \epsilon^2 \frac{\partial \phi}{\partial t} = \beta \sigma(\rho - \phi). \end{cases}$$

Evaluate macroscopic variables first

$$\begin{aligned} \rho_{i,j}^{n+1} &= \rho_{i,j}^n + \frac{\Delta t}{\Delta x} (\Phi_{i-1/2,j} - \Phi_{i+1/2,j}) \\ &\quad + \frac{\Delta t}{\Delta y} (\Psi_{i,j-1/2} - \Psi_{i,j+1/2}) + \frac{\sigma \mathbf{c} \Delta t}{\epsilon^2} (\phi_{i,j}^{n+1} - \rho_{i,j}^{n+1}), \\ \phi_{i,j}^{n+1} &= \phi_{i,j}^n + \frac{\beta \sigma \Delta t}{\epsilon^2} (\rho_{i,j}^{n+1} - \phi_{i,j}^{n+1}), \end{aligned}$$

Interface radiation intensity

$$\begin{aligned} I_m(t, x_{i-1/2}, y_j, \mu_m, \xi_m) &= e^{-\nu_{i-1/2,j}(t-t^n)} I_{m,0}(x_{i-1/2} - \frac{c\mu_m}{\epsilon}(t-t^n)) \\ &\quad + \int_{t^n}^t e^{-\nu_{i-1/2,j}(t-s)} \frac{c\sigma_{i-1/2,j}}{2\pi\epsilon^2} \phi(s, x_{i-1/2} - \frac{c\mu_m}{\epsilon}(t-s)) ds, \end{aligned}$$



## Microscopic equation for the update of radiation intensity

$$I_{i,j,m,g}^{n+1} = I_{i,j,m,g}^n + \frac{\Delta t}{\Delta x} (F_{i-1/2,j,m,g} - F_{i+1/2,j,m,g}) + \frac{\Delta t}{\Delta y} (H_{i,j-1/2,m,g} - H_{i,j+1/2,m,g}) + \frac{c\Delta t}{\epsilon^2} ((\sigma_g^e)_{i,j}^{n+1} \phi_{g,i,j}^{n+1} - (\sigma_g^a)_{i,j}^{n+1} I_{i,j,m,g}^{n+1}),$$

# Homogeneous problems

$$\sigma(x, \nu, T) = \frac{\sigma_0(x)}{(h\nu)^3 \sqrt{kT}}$$

$$\sigma_0 = 10 \text{ keV}^{7/2}/\text{cm},$$

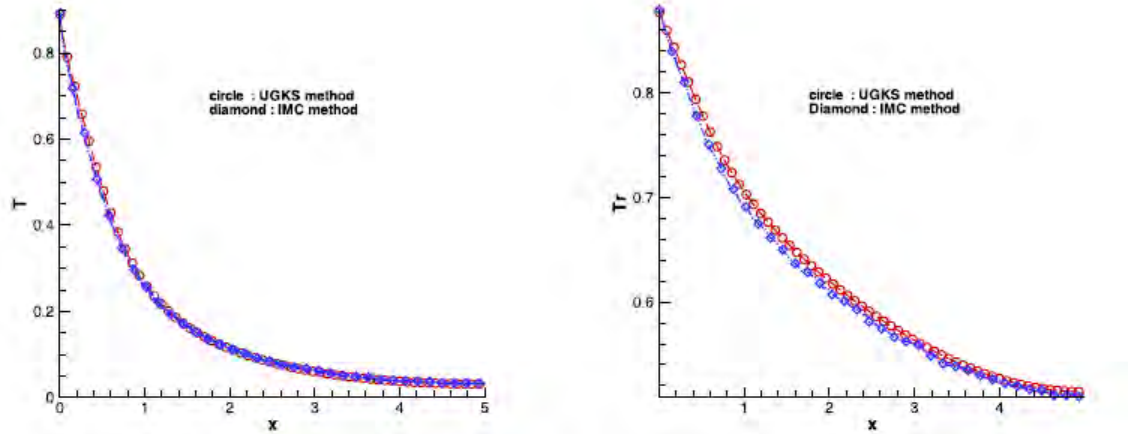


Fig. 2. Results at 1 ns for Case 1 of Example 1 with homogeneous opacity  $\sigma_0 = 10 \text{ keV}^{7/2}/\text{cm}$ .

$$\sigma_0 = 100 \text{ keV}^{7/2}/\text{cm}$$

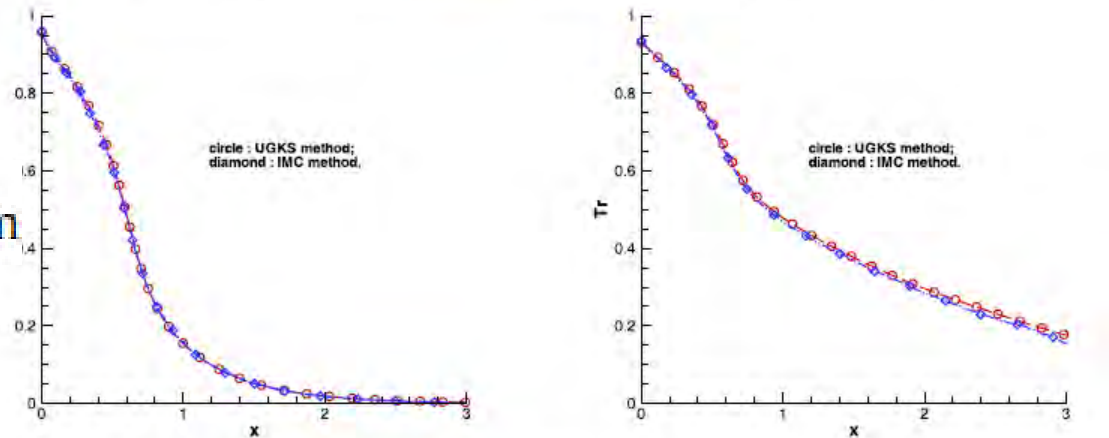


Fig. 3. Results at 1 ns for Case 1 of Example 1 with homogeneous opacity  $\sigma_0 = 100 \text{ keV}^{7/2}/\text{cm}$ .

$$\sigma_0 = 1000 \text{ keV}^{7/2}/\text{cm}$$

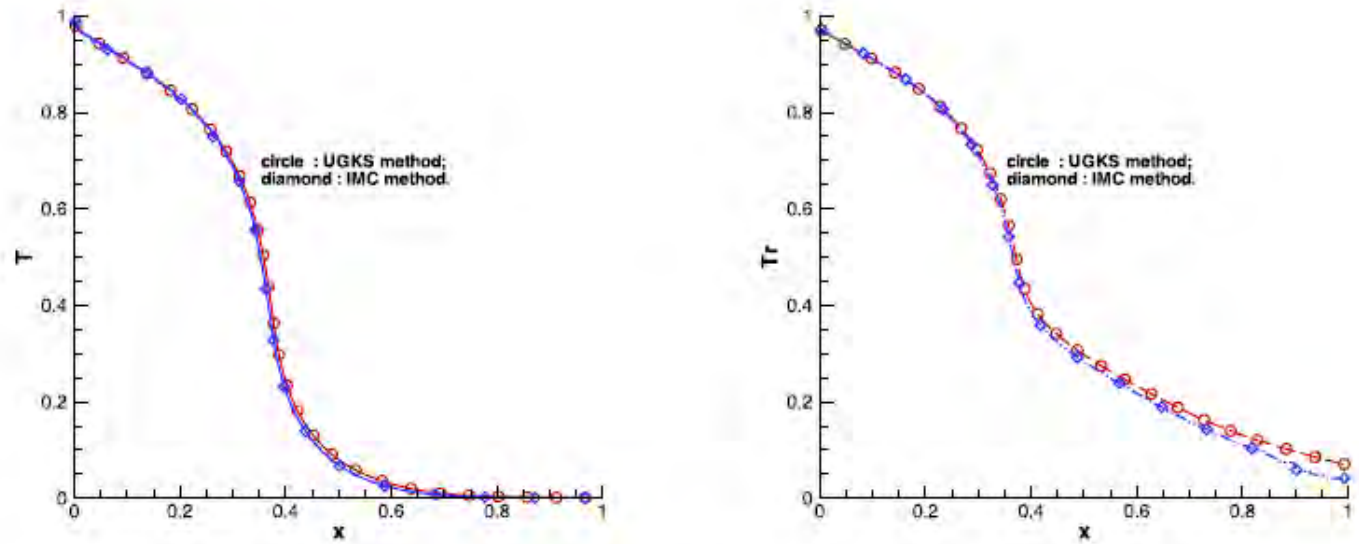
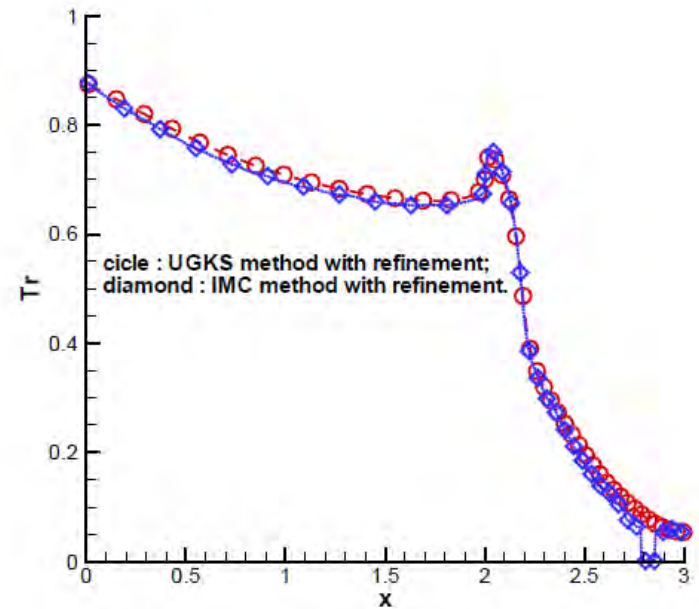
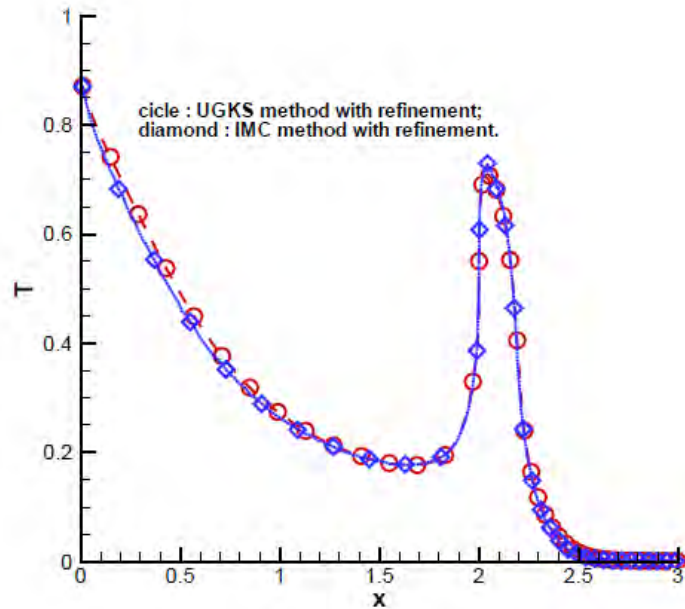
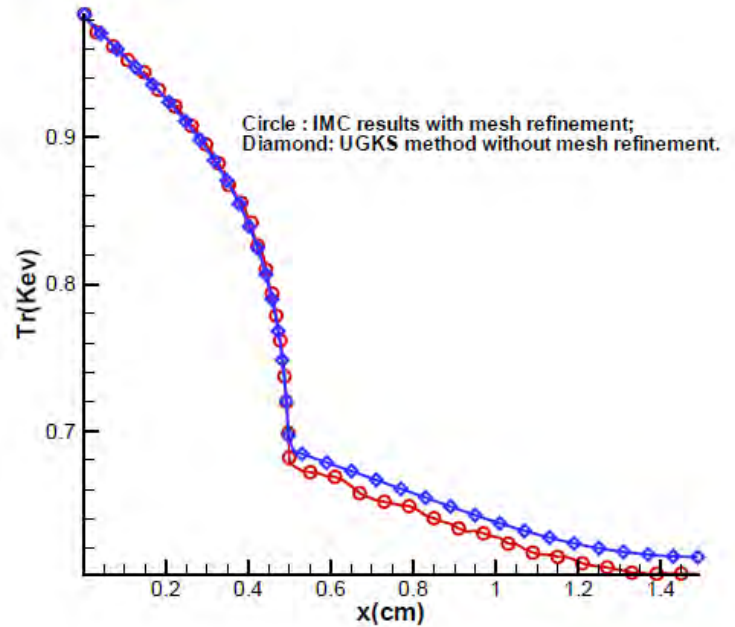
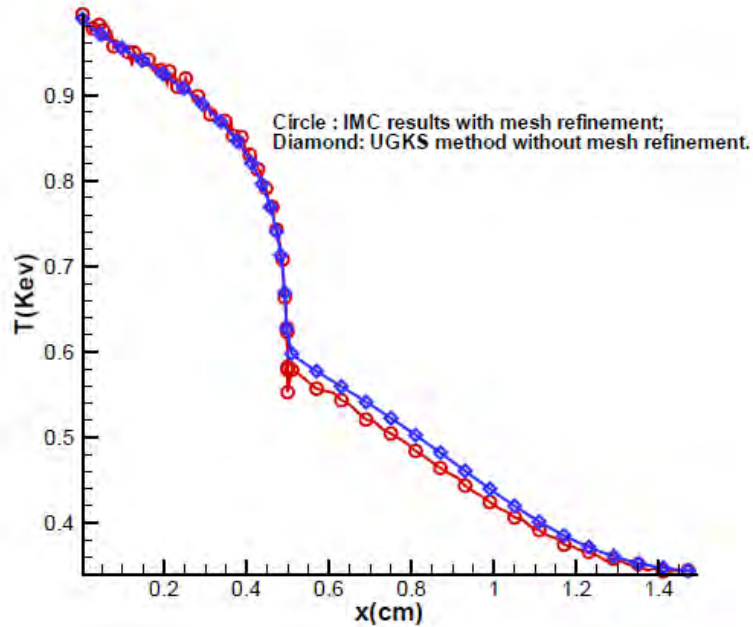


Fig. 4. Results at 1 ns for Case 1 of Example 1 with homogeneous opacity  $\sigma_0 = 1000 \text{ keV}^{7/2}/\text{cm}$ .

$$\sigma_0(x) = \begin{cases} 10 \text{ keV}^{7/2} / \text{cm}, & 0 \text{ cm} < x < 2 \text{ cm}, \\ 1000 \text{ keV}^{7/2} / \text{cm}, & 2 \text{ cm} < x < 3 \text{ cm}. \end{cases}$$



$$\sigma_0(x) = \begin{cases} 1000 \text{ keV}^{7/2} / \text{cm}, & 0 \text{ cm} < x < 0.5 \text{ cm}, \\ 10 \text{ keV}^{7/2} / \text{cm}, & 0.5 \text{ cm} < x < 1.5 \text{ cm}. \end{cases}$$



**Table 1**

The computation time of UGKS and IMC for Example 1.

Example 1		UGKS	IMC
Case 1	$\sigma_0 = 10$	21 minutes	96 minutes
	$\sigma_0 = 100$	22 minutes	173 minutes
	$\sigma_0 = 1000$	40 minutes	1344 minutes
Case 2	1st heterogeneous problem	8 minutes	363 minutes
Case 3	2nd heterogeneous problem	34 minutes	5184 minutes

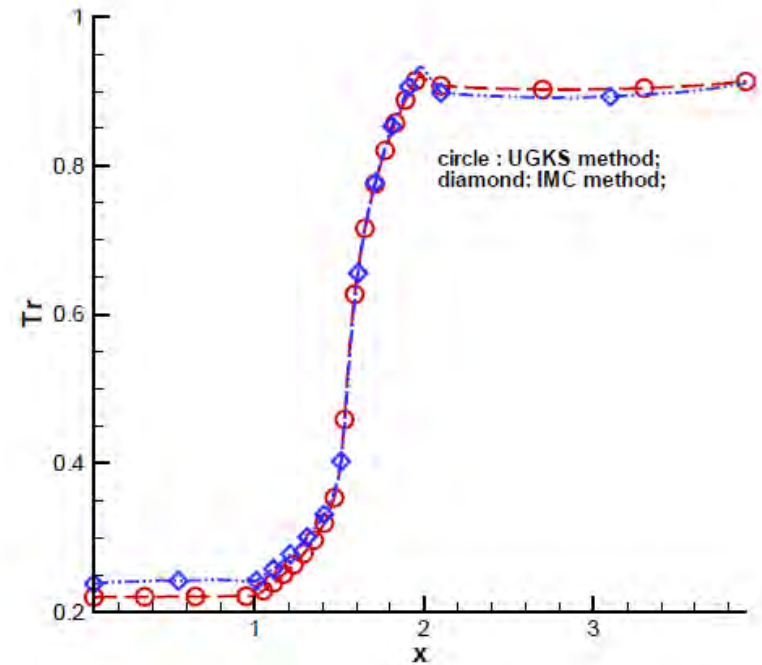
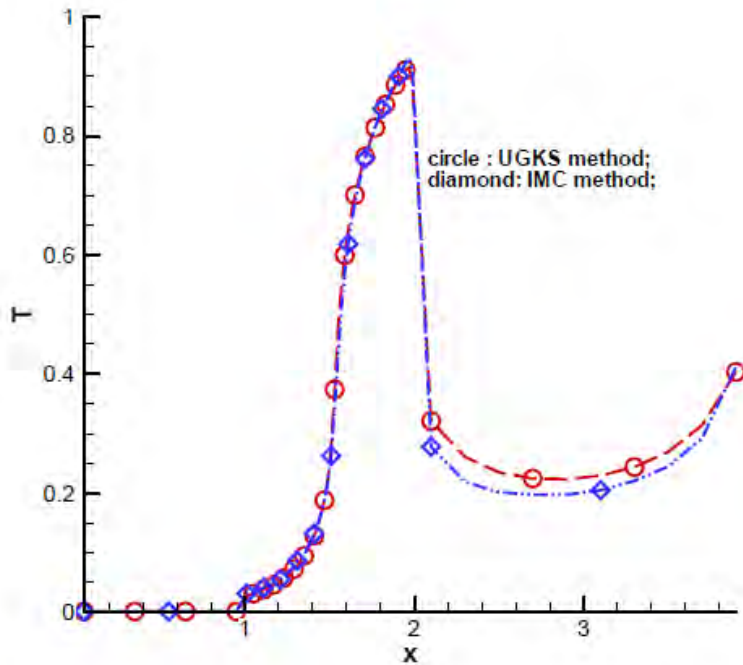
$$\sigma(\nu, T, x) = \gamma(x) \frac{1 - e^{-h\nu/kT}}{(h\nu)^3},$$

$$\gamma(x) = \begin{cases} 1 \text{ keV}^3/cm, & 0cm < x < 1cm, \\ 1000 \text{ keV}^3/cm, & 1cm < x < 2cm, \\ 1 \text{ keV}^3/cm, & 2cm < x < 4cm. \end{cases}$$

**Table 2**

The computation time of UGKS and IMC for Example 2.

UGKS	IMC
2 minutes	63 minutes





# Plasma Simulation

Vlasov-BGK system for ion and electron:

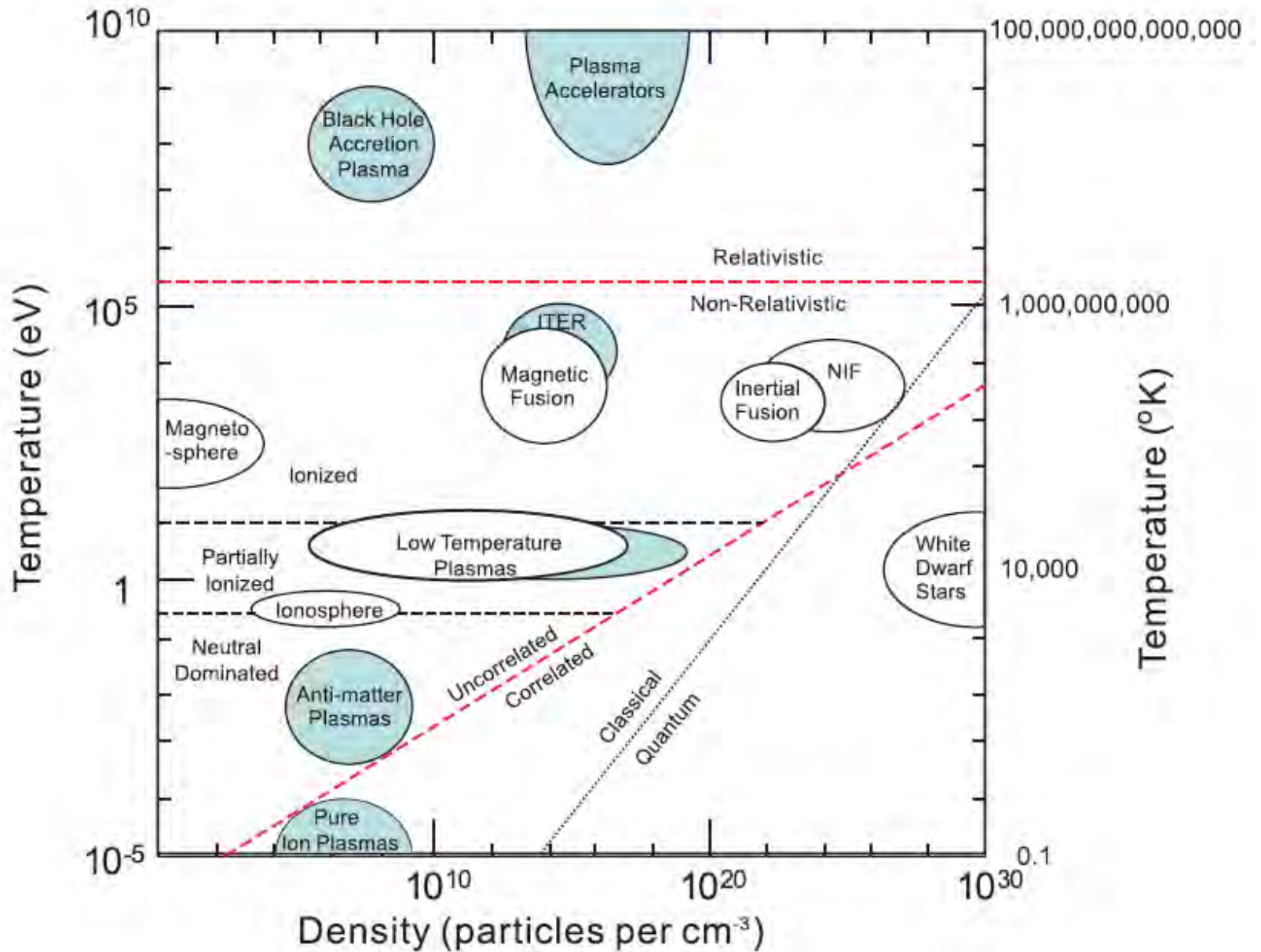
$$\frac{\partial f_\alpha}{\partial t} + v \cdot \nabla_x f_\alpha + \frac{q_\alpha}{m_\alpha} (E + v_\alpha \times B) \cdot \nabla_v f_\alpha = \sum_\beta Q_{\alpha,\beta}(f_\alpha, f_\beta)$$

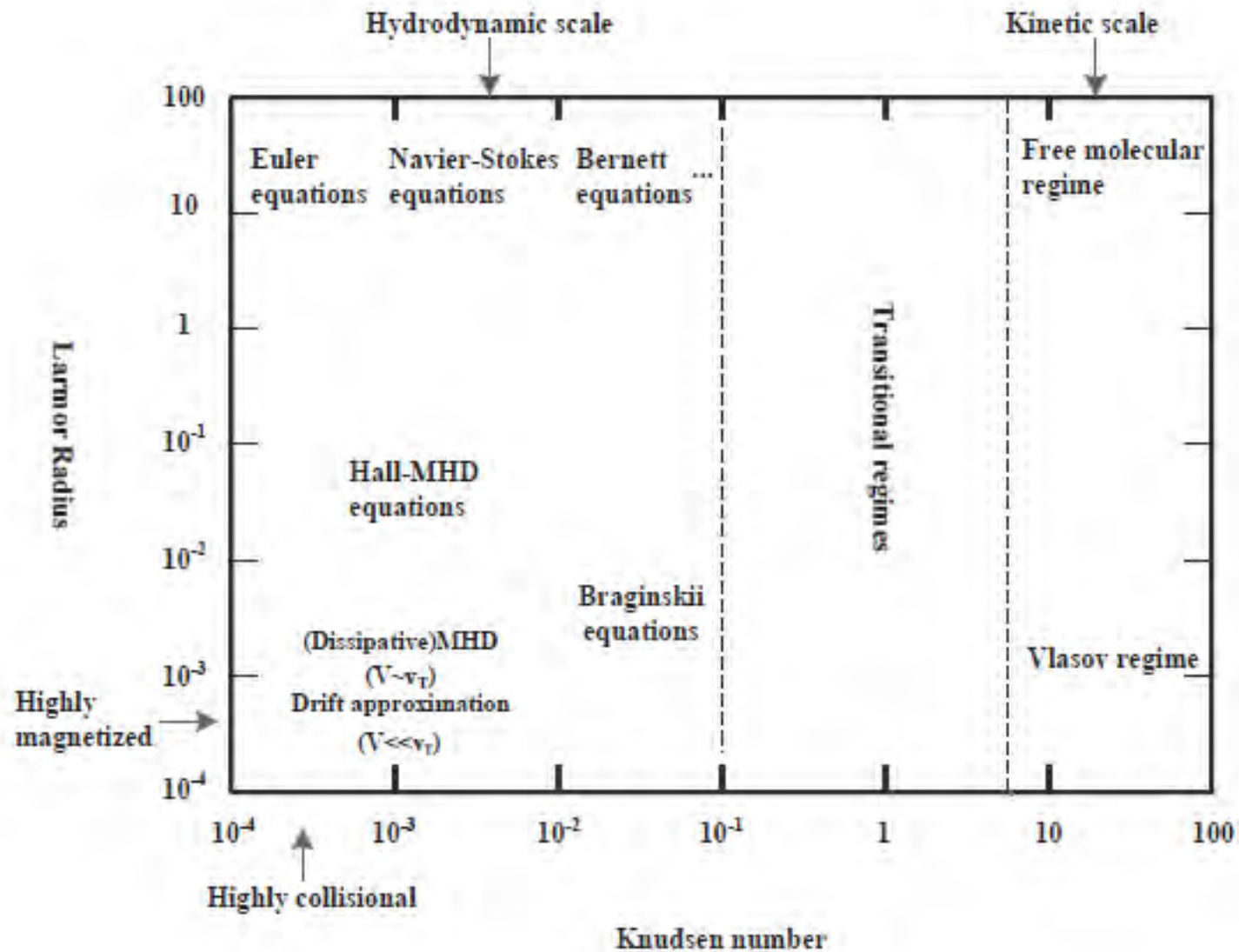
Maxwell equations for electro-magnetic fields

$$\frac{\partial B}{\partial t} = -\nabla \times E, \quad \frac{\partial E}{\partial t} = c^2 \nabla \times B - \frac{1}{\mu_0} J$$

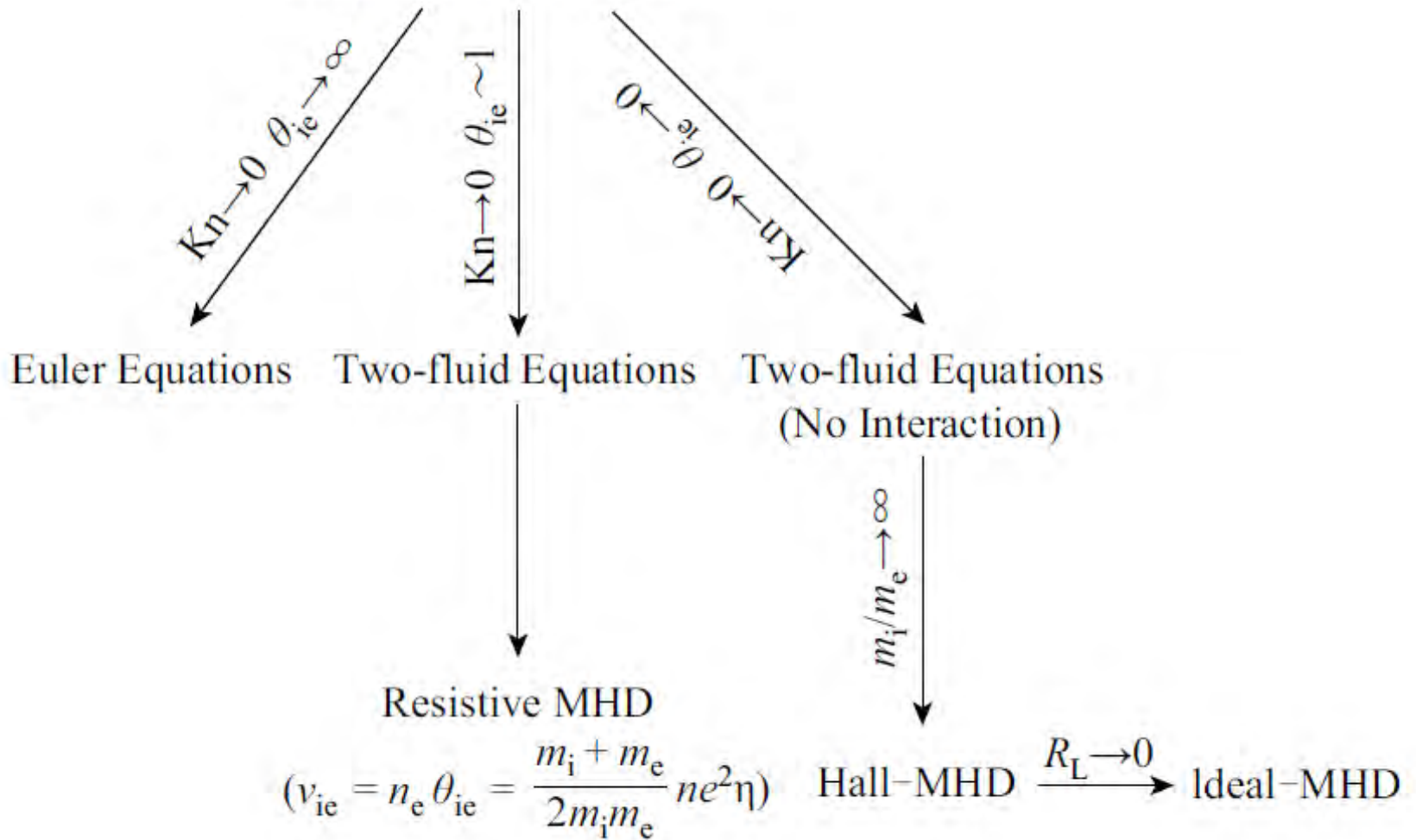
$$\nabla \cdot E = \frac{1}{\epsilon_0} (\rho_e - \rho_i), \quad \nabla \cdot B = 0$$

C. Liu





BGK–Maxwell Equations

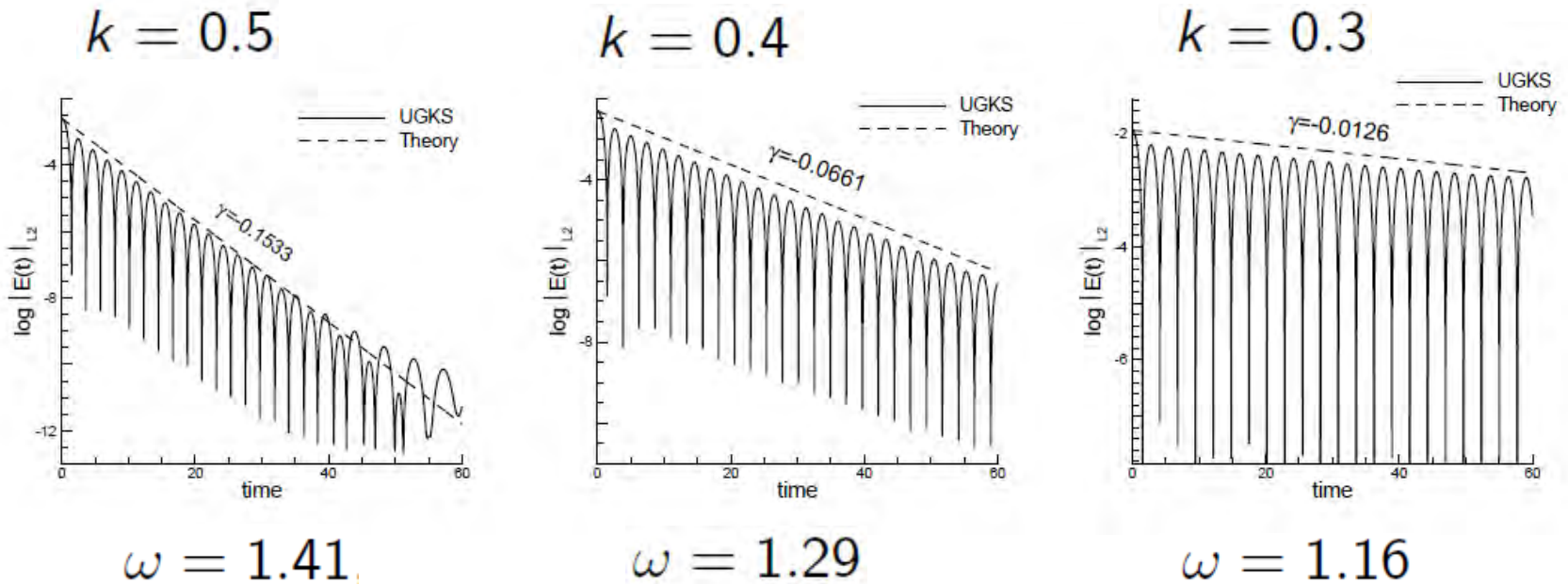


# Linear Landau damping

Consider Landau damping for the Vlasov Poisson system with initial condition:

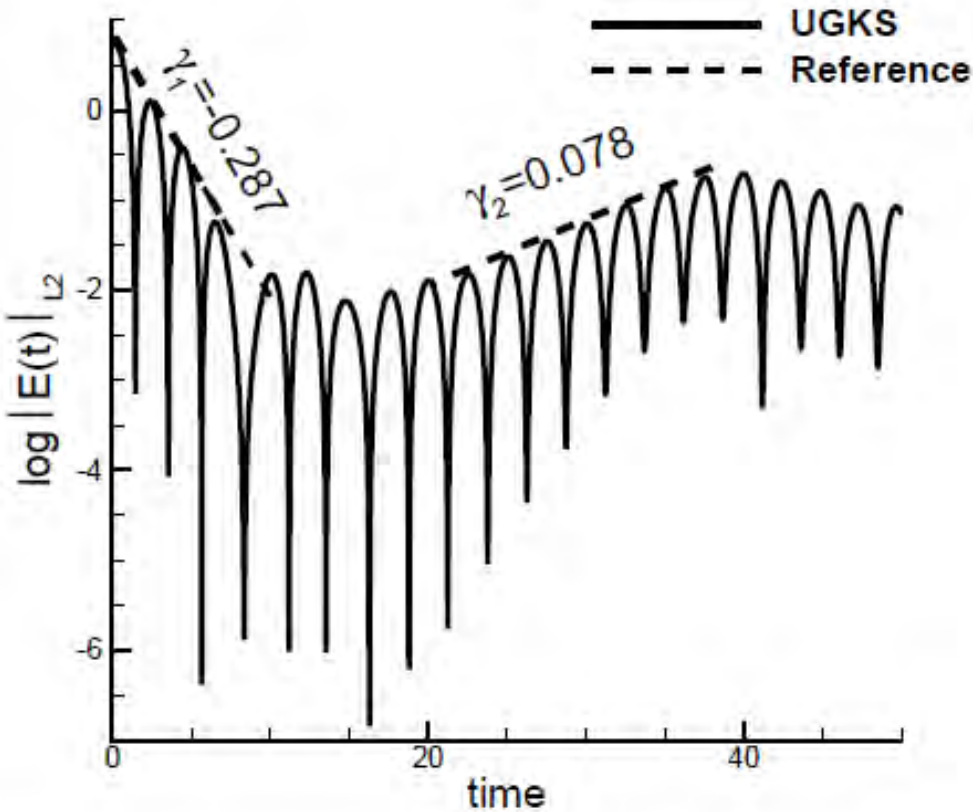
$$f_0(x, v) = \frac{1}{\sqrt{2\pi}} (1 + \alpha \cos(kx)) e^{-\frac{v^2}{2}}$$

with  $\alpha = 0.01$  for linear case. The length of the domain in the  $x$  direction is  $L = \frac{2\pi}{k}$

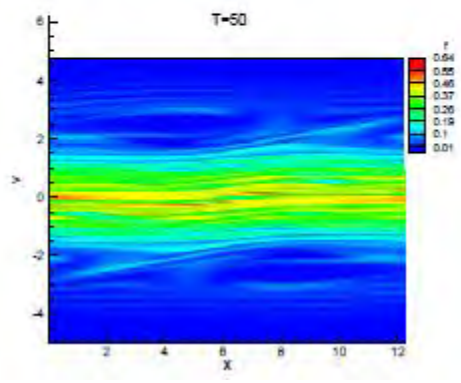
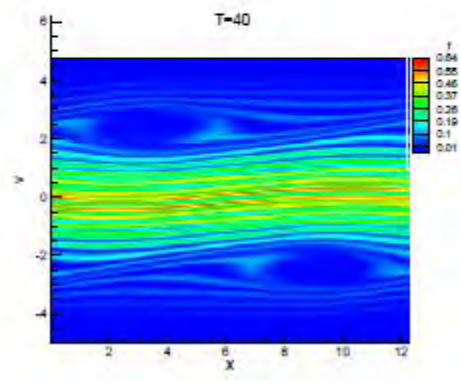
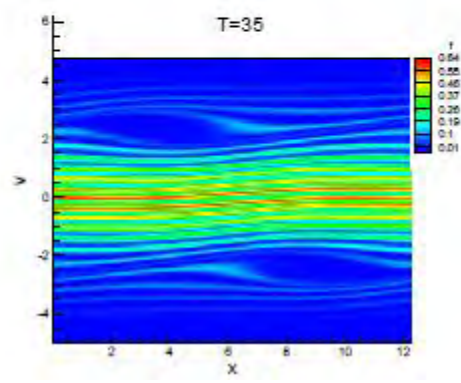
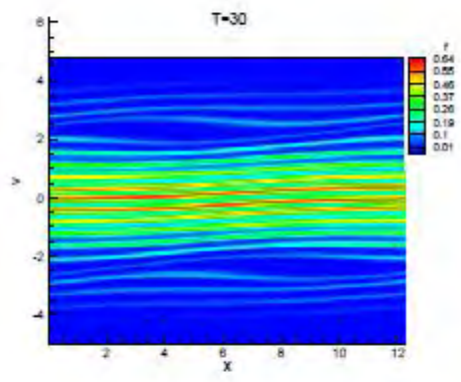
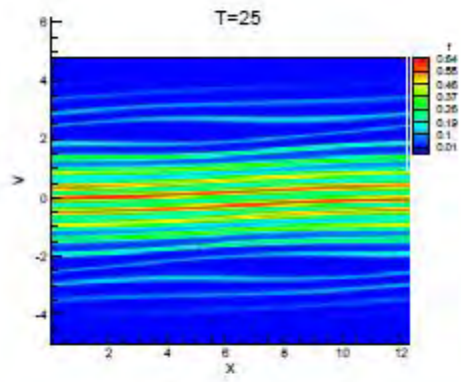
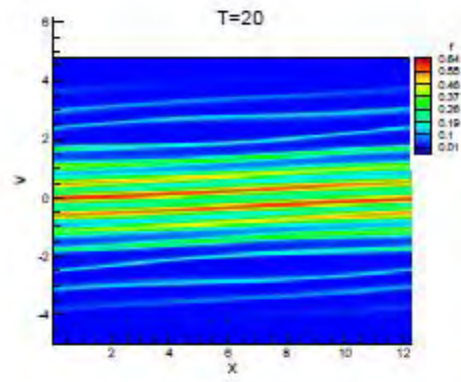
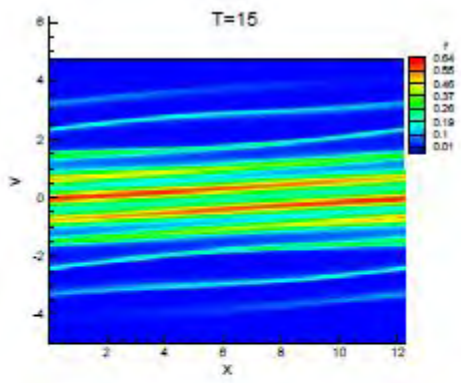
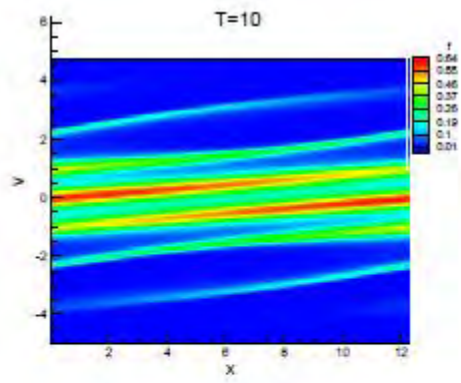
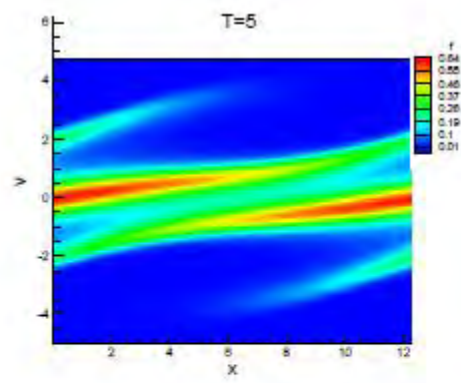


Nonlinear Landau Damping

$$\alpha = 0.5 \text{ and } k = 0.5$$



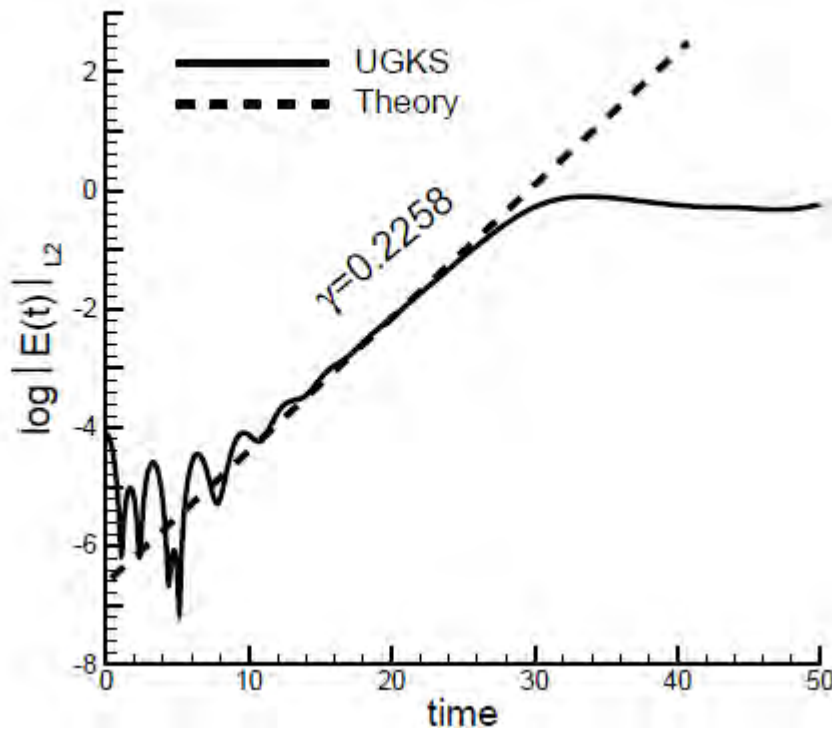






## Linear two stream instability

$$f_0(x, v) = \frac{2}{7\sqrt{2\pi}}(1 + 5v^2)(1 + \alpha((\cos(2kx) + \cos(3kx))/1.2 + \cos(kx)))e^{-\frac{v^2}{2}}$$



$$\alpha = 0.001, k = 0.2$$

## Velocity distribution contours at $t=70$

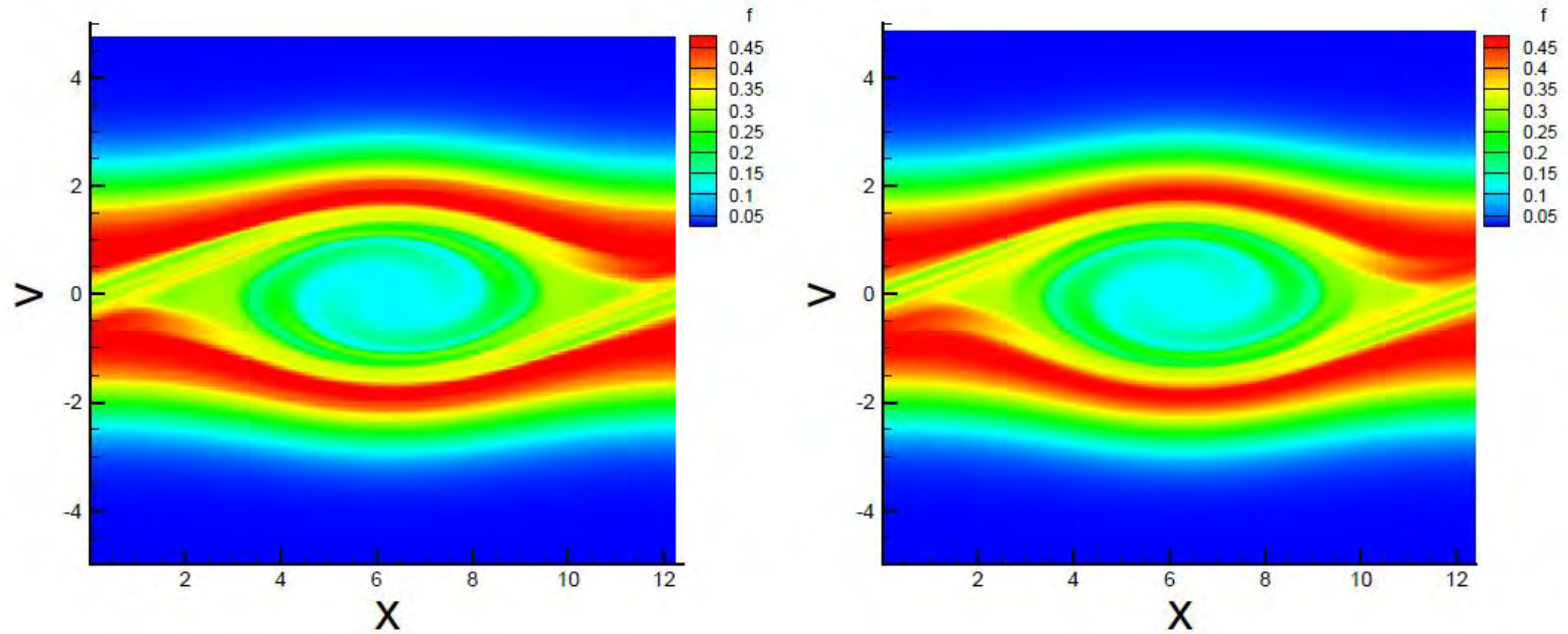


Figure: Linear two stream instability. Velocity distribution contours at  $t = 70$ .  $N_x \times N_v = 256 \times 256$  (left);  $N_x \times N_v = 512 \times 512$  (right).

## Nonlinear two stream instability

$$f(x, u, t = 0) = \frac{1}{2v_{th}\sqrt{2\pi}} \left[ \exp\left(-\frac{(u-U)^2}{2u_t^2}\right) + \exp\left(-\frac{(u+U)^2}{2u_t^2}\right) \right] (1 + \alpha \cos(kx))$$

$$\alpha = 0.05, U = 0.99, u_t = 0.3, k = \frac{2}{13}$$

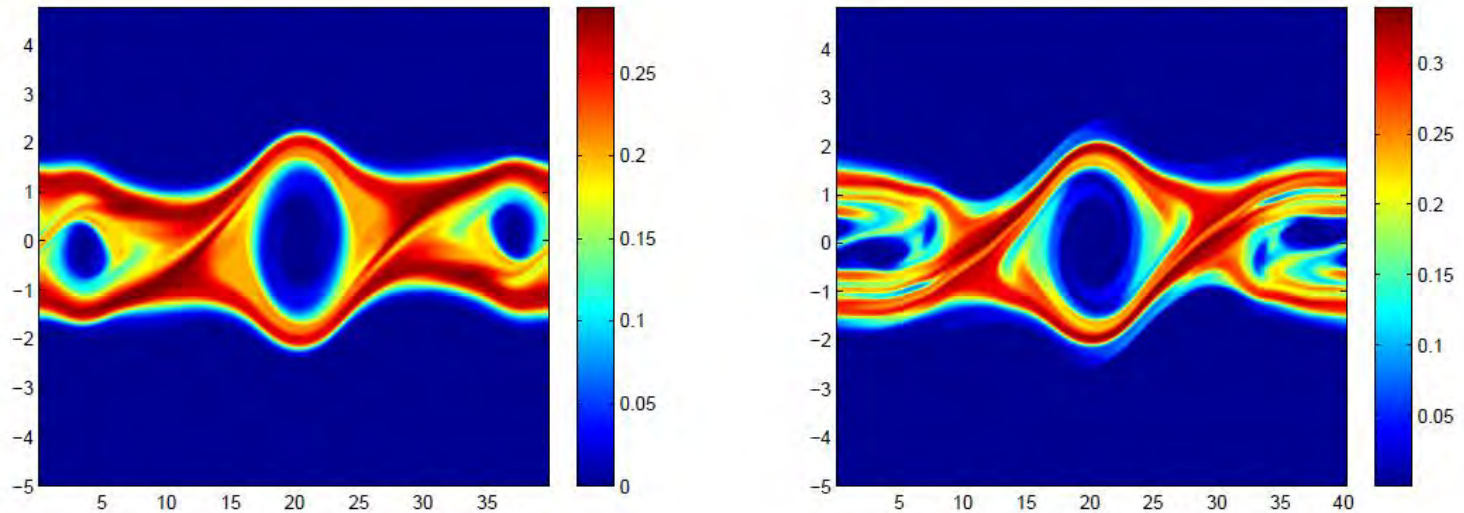


Figure 12: Two stream instability (nonlinear). Velocity distribution contours at  $t = 70$ .  $N_x \times N_u = 256 \times 256$  (left);  $N_x \times N_u = 512 \times 512$  (right)

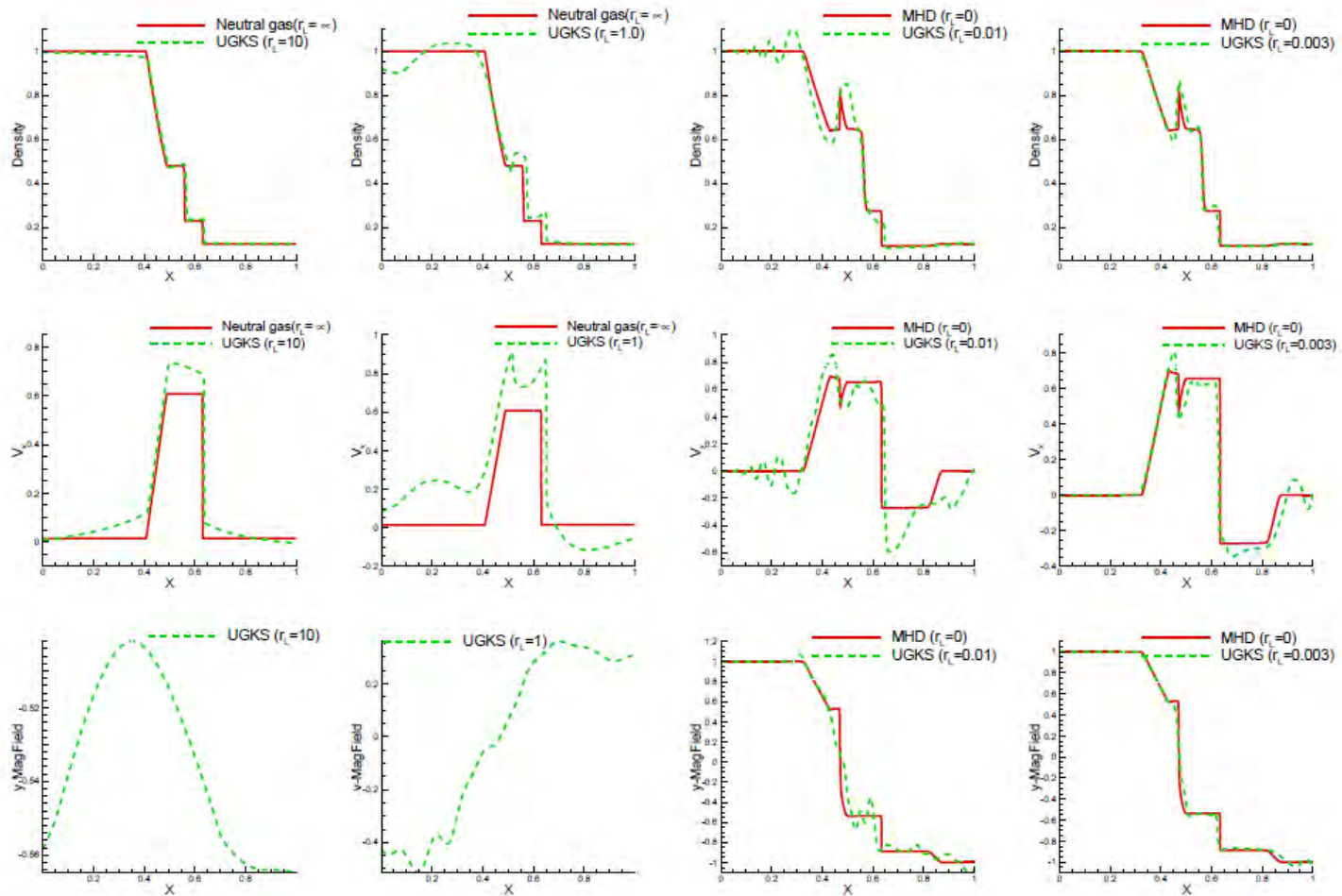
The Brio-Wu shock tube is a standard test case for MHD solvers in continuum regime with initial condition shown in following figure.

The ion to electron mass ration is set to 1836 ( $\infty$  in MHD). The normalized Debye length is set to 0.01. The normalized speed of light is set to 100. The ion Larmor radius is varied as  $r_L = 10, 1, 0.01, 0.003$ . The Knudsen number is set to  $10^{-4}$ . The grid points in physical space are 1000. The grid points in velocity spaces are 32 in each direction.

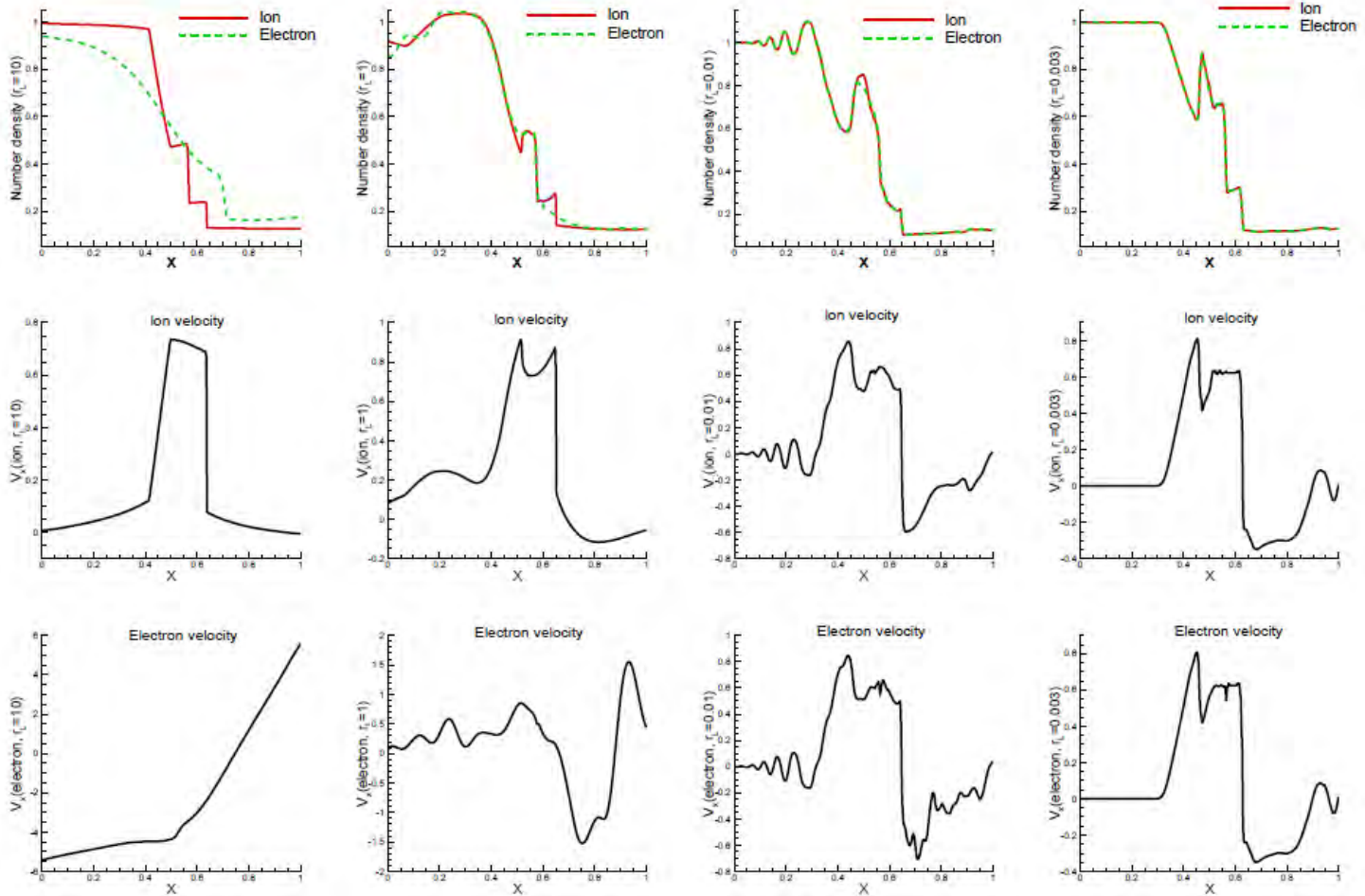
$\rho_i = 1.0, P_i = 5.0 \times 10^{-5}, \vec{V}_i = \mathbf{0};$	$\rho_i = 0.125, P_i = 5.0 \times 10^{-6}, \vec{V}_i = \mathbf{0};$
$\rho_e = 1.0 \frac{m_e}{m_i}, P_e = 5.0 \times 10^{-5}, \vec{V}_e = \mathbf{0};$	$\rho_e = 0.125 \frac{m_e}{m_i}, P_e = 5.0 \times 10^{-6}, \vec{V}_e = \mathbf{0};$
$\vec{B} = (0.75, 1.0, 0);$	$\vec{B} = (0.75, -1.0, 0);$
$\vec{E} = \mathbf{0}.$	$\vec{E} = \mathbf{0}.$

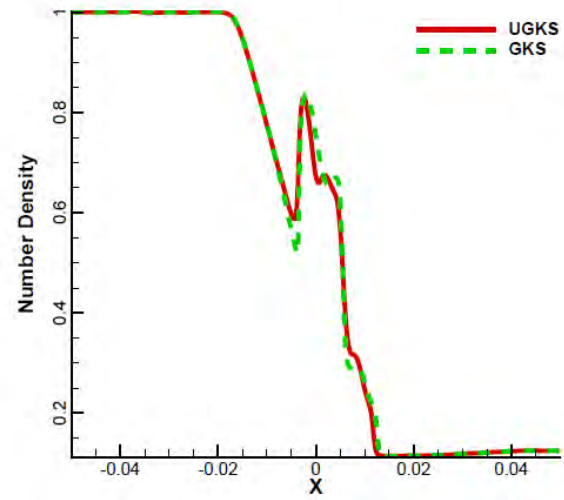
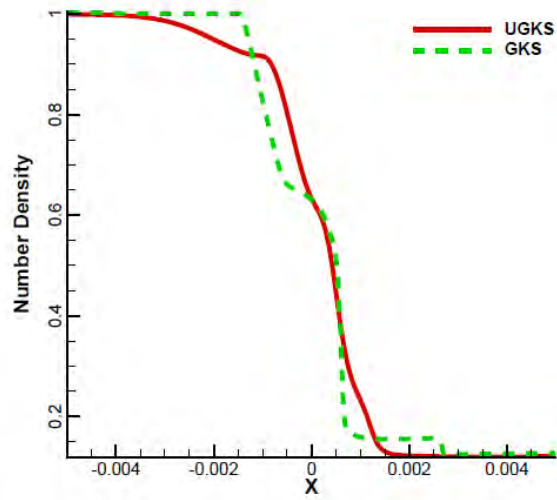
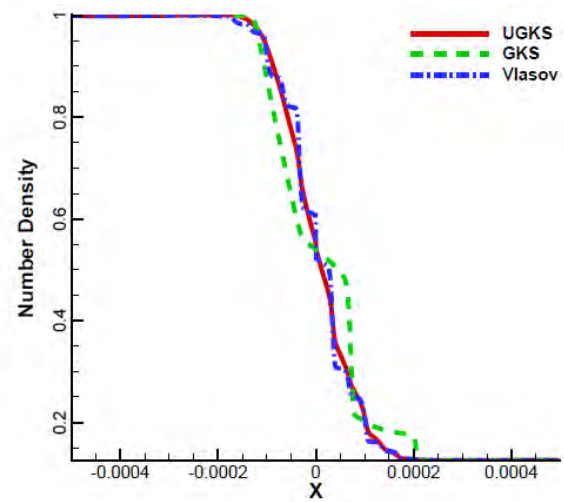
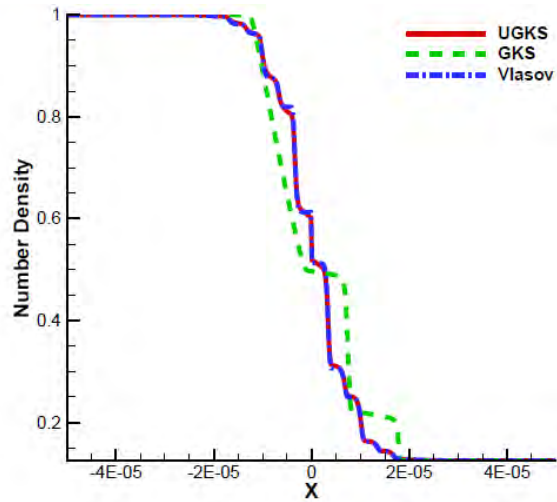


Results of the density (top), velocity (middle) and magnetic field (bottom) profiles are shown in the following figure with  $r_L = 10, 1, 0.01, 0.003$  from left to right.



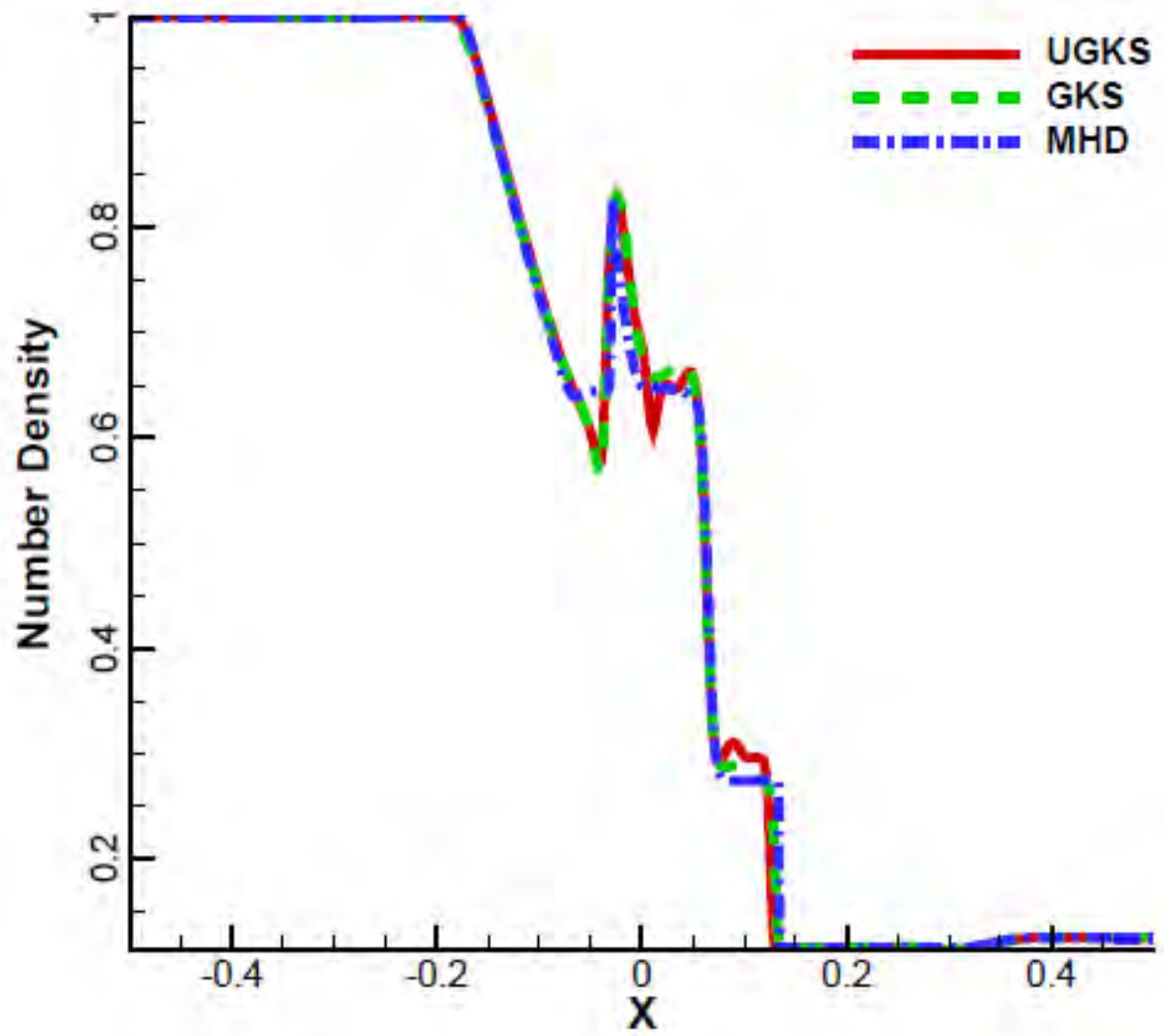
The following figures show the density and velocity profiles for ions and electrons with  $r_L = 10, 1, 0.01, 0.003$  from left to right.



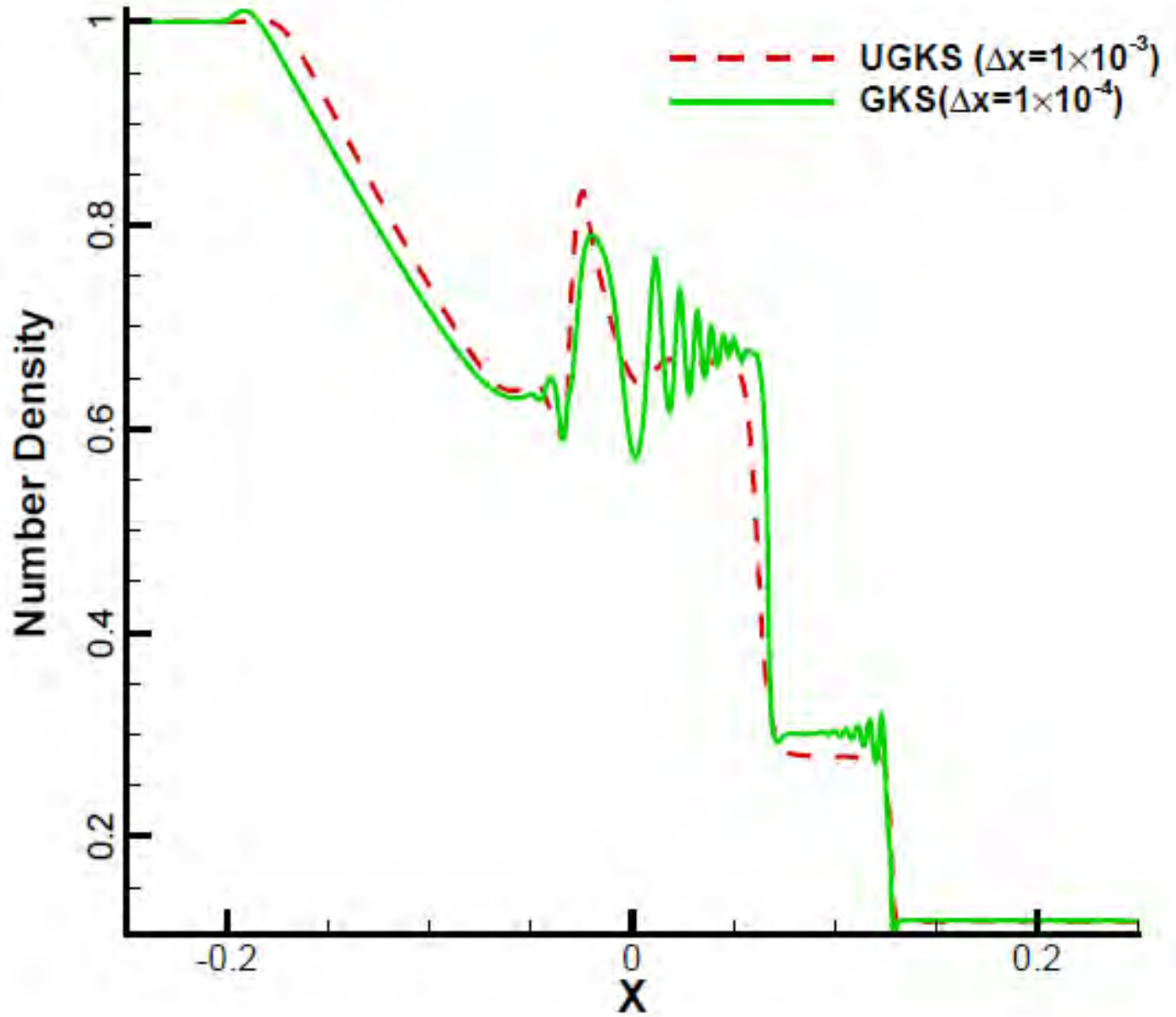


$$t = 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2},$$

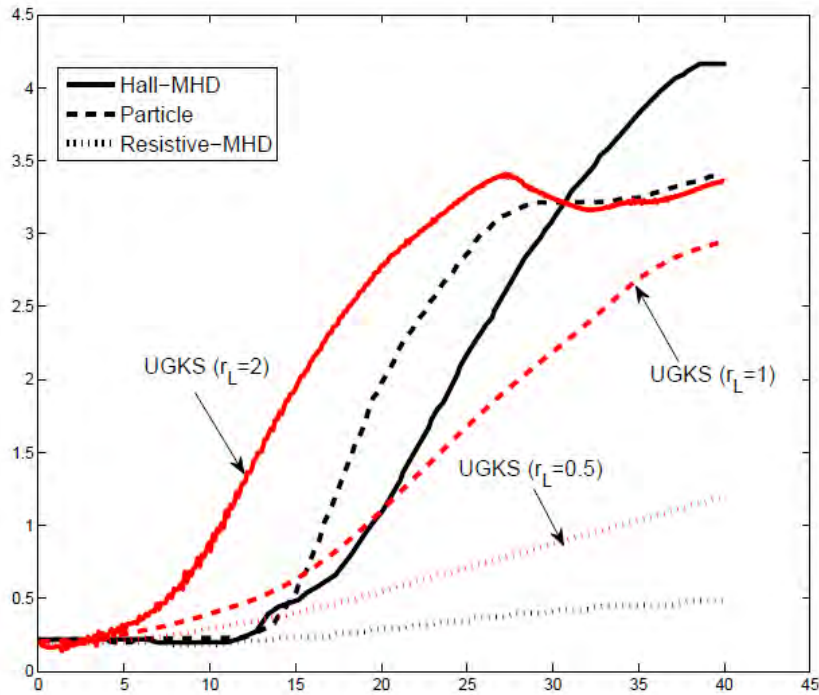




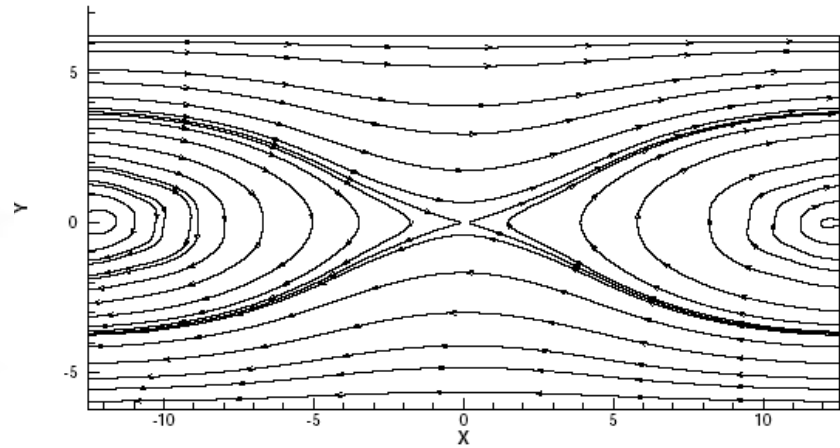
t=0.1



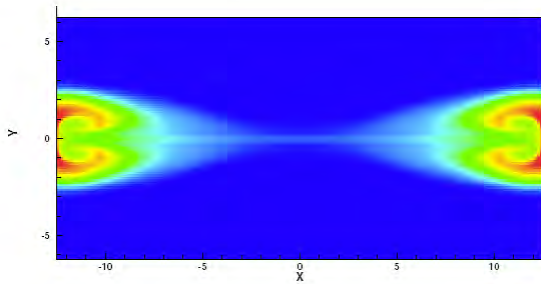
# Magnetic Reconnection



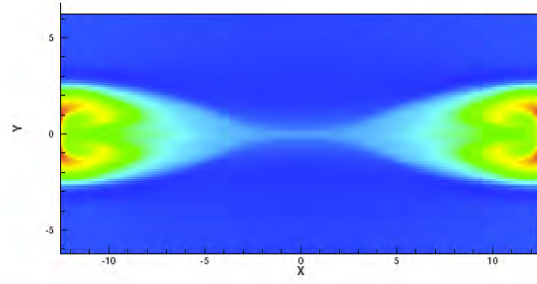
y-component absolute magnetic field



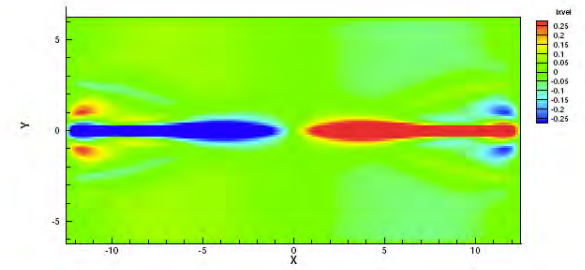
magnetic field distribution



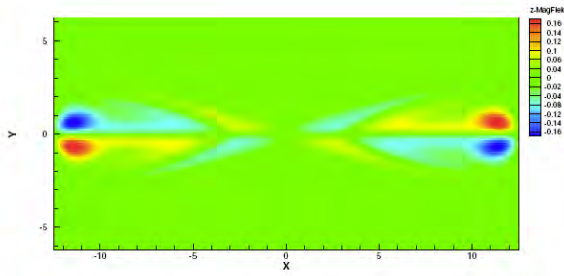
ion density



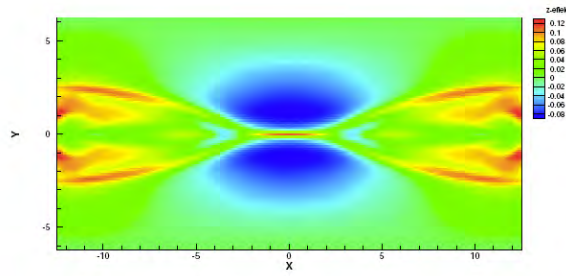
electron density



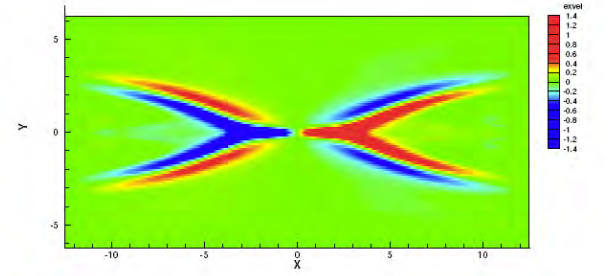
x-momentum of ion



z-direction magnetic field

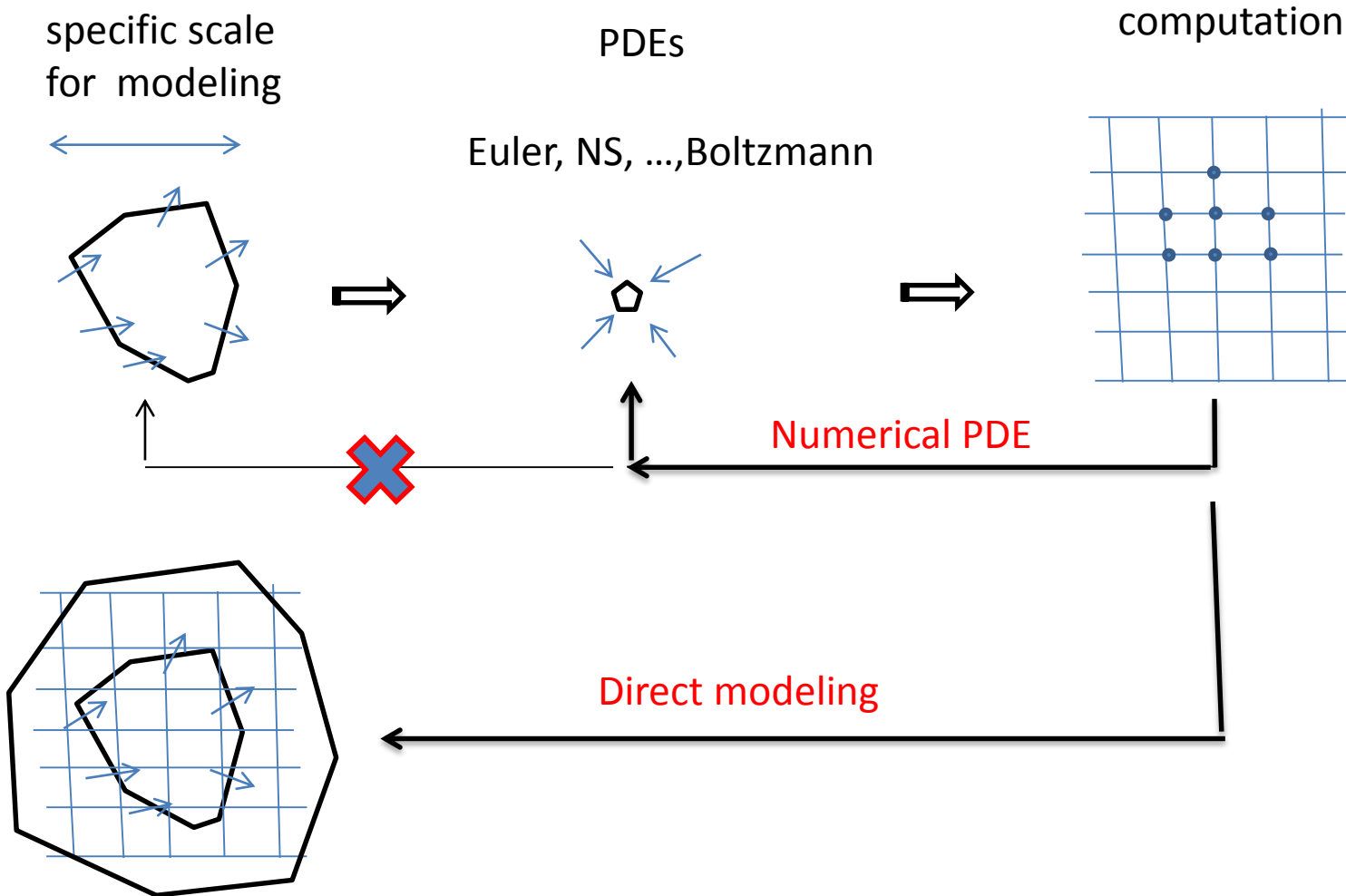


z-direction electric field

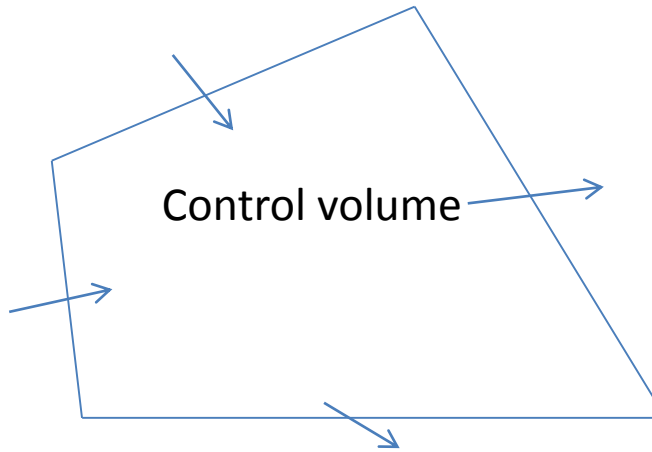


x-momentum of electron

# DIRECTION OF COMPUTATIONAL FLUID DYNAMICS



# Direct Modeling for CFD



$$\Delta x \xrightarrow{\times} 0, \quad \Delta t \xrightarrow{\times} 0$$

Consistency ?

Convergence ?

Order of accuracy (numerical, physical) ?

...



# Direct Modeling for Computations

Direct description of transport process in a discretized space; Construction of the evolution model;

Development of the algorithm

**Recover a Multiple Scale Transporting Process**

UGKS { **Non-equilibrium Gas Dynamics:** Boltzmann  $\leftrightarrow$  Navier-Stokes equations  
**Radiative transfer:** ray transport  $\leftrightarrow$  diffusion equations  
**Plasma:** Vlasov equation  $\leftrightarrow$  Magneto-hydrodynamics  
**turbulence ?**