Direct Modeling for Computational Fluid Dynamics

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International Conference on Progress in Fluid Dynamics and Simulation (Oct 25-27, 2014)

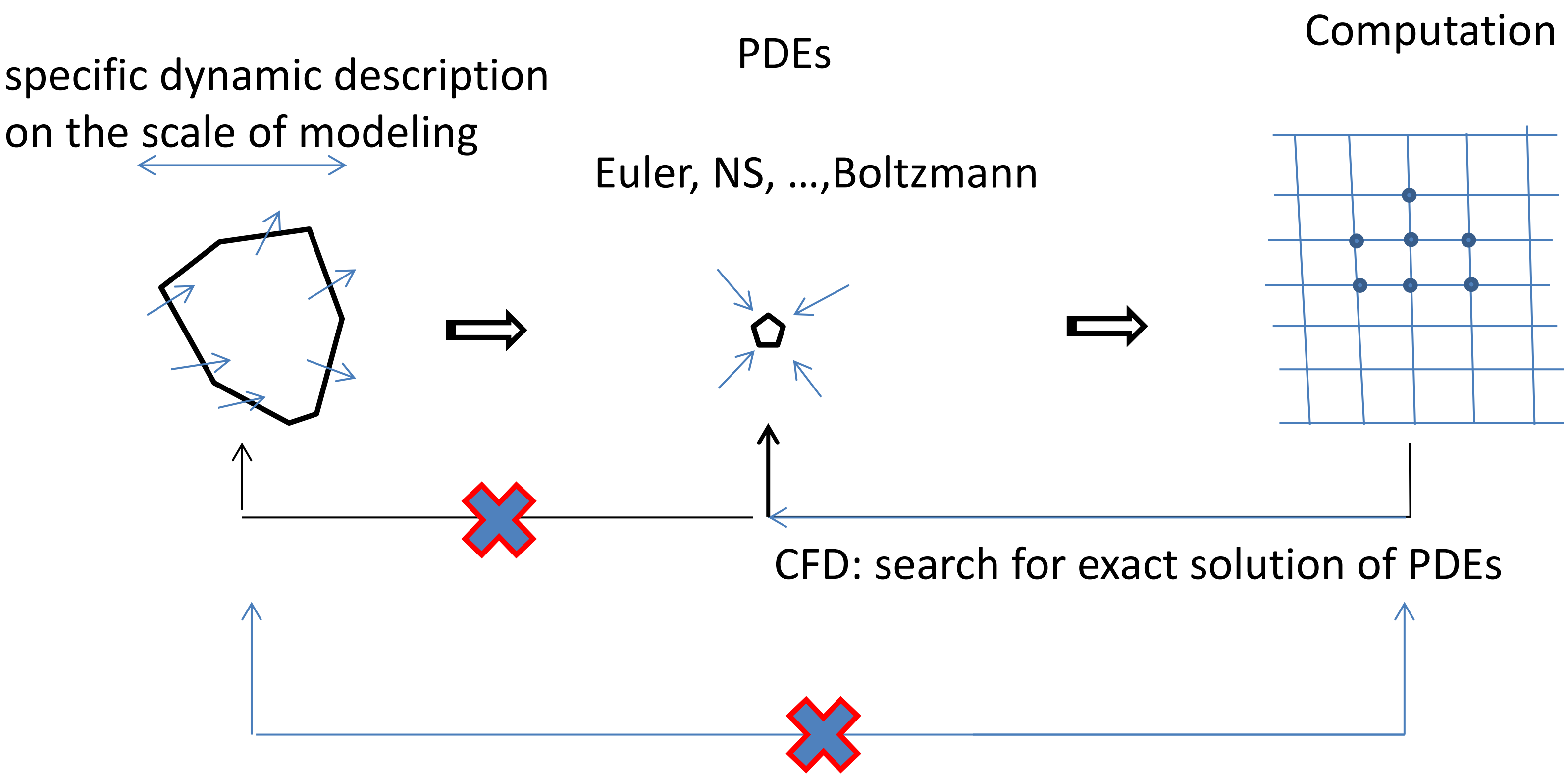
Contents

- Connection among modeling, PDEs, and CFD
- Direct modeling method for CFD

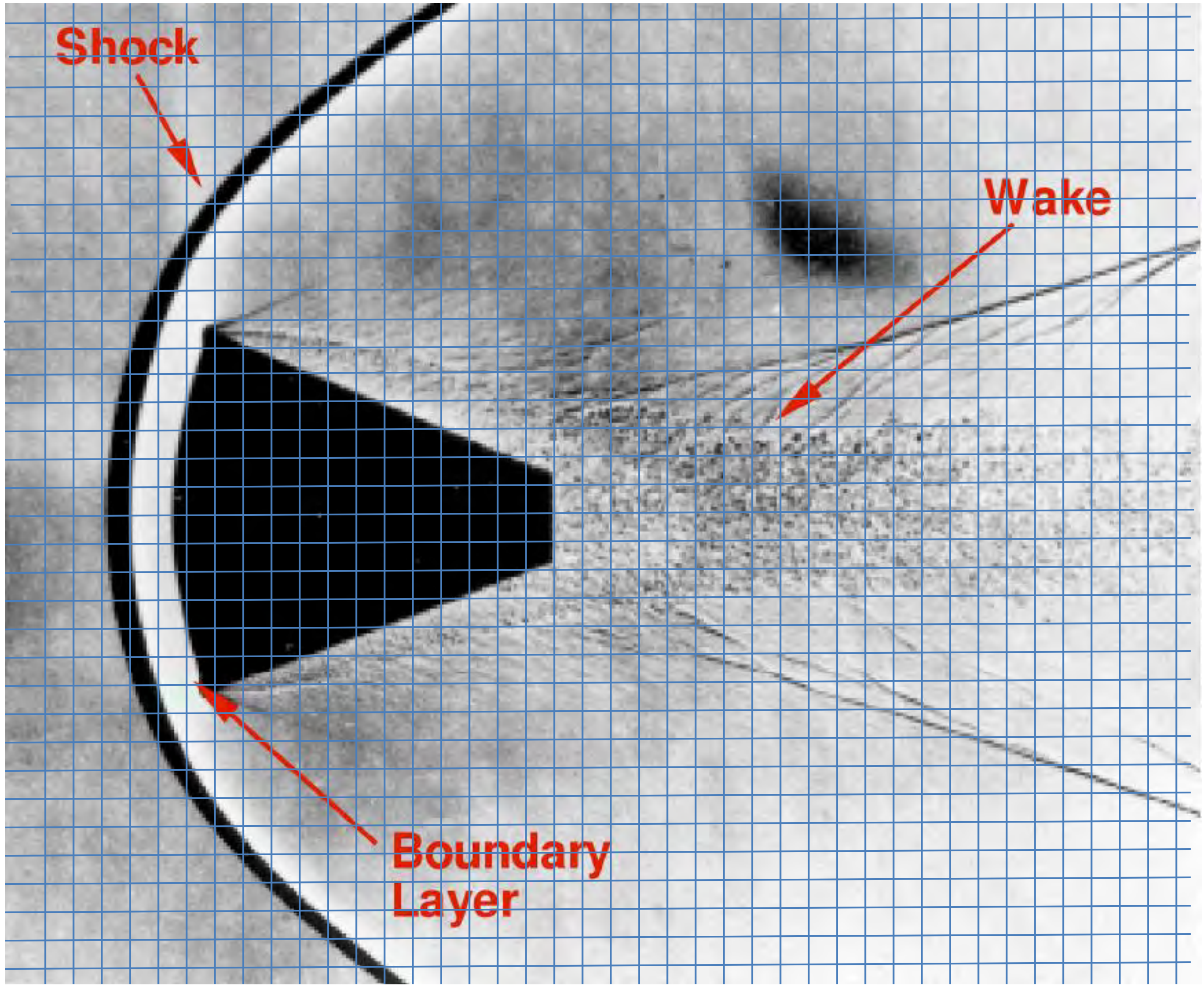
  Unified Gas-kinetic Scheme (UGKS, all flow regimes)

  Gas-kinetic Scheme (GKS, continuum flow regime)
- Conclusion

Current CFD Methodology



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


Shock
Wake
Boundary
Layer

Near Space flow modeling

free molecular

100km

(Boltzmann or DSMC)

Transitional

Near space
No valid governing equations

60km

slip

20km

(Navier-Stokes)

continuum

Under a reasonable number of mesh points

Current Computational Fluid Dynamics -> Numerical PDEs

Physical problem

Navier–Stokes equations *(general)*

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla p + \nabla\cdot\mathbf{T} + \mathbf{f},$$

Governing equation

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

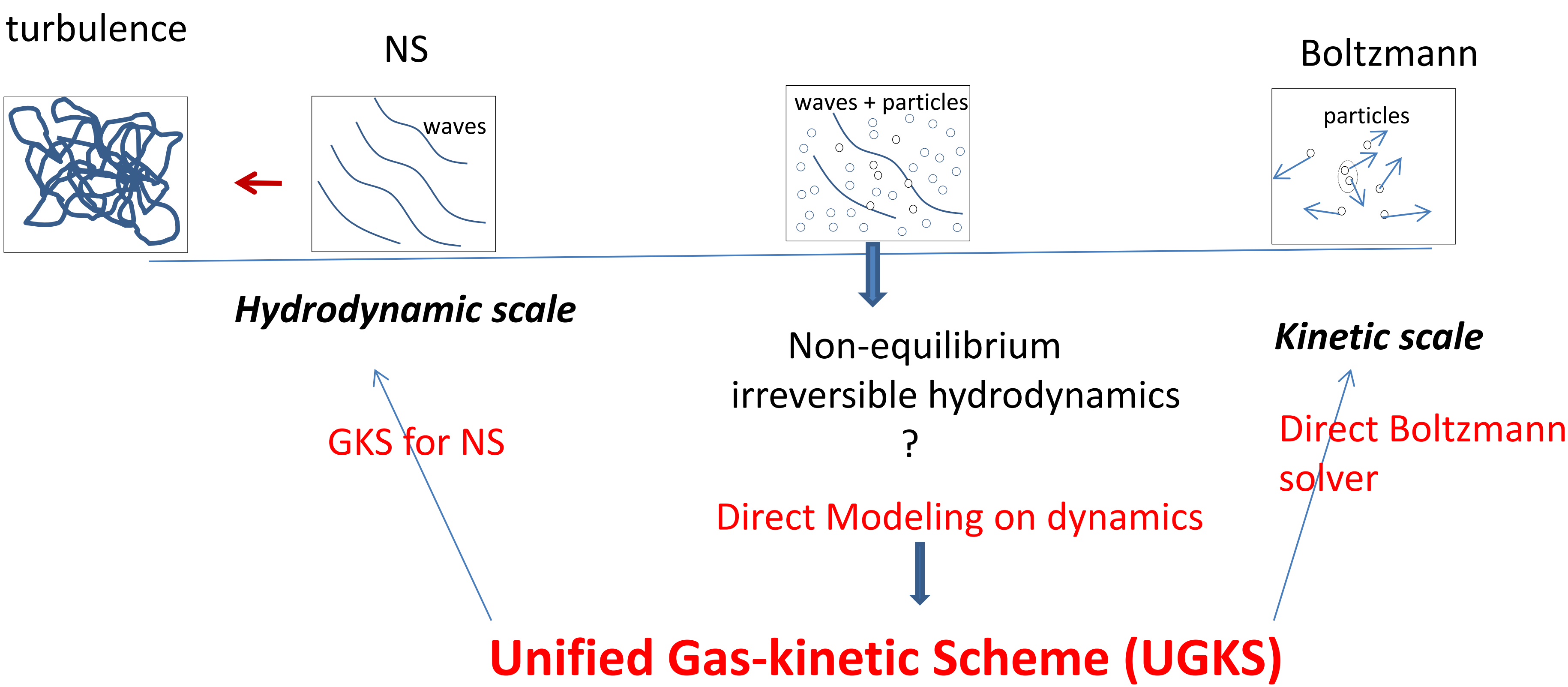
(FDM,FEM,FVM, etc.**)**

Numerical scheme

Limitations：

1. All PDEs are valid in their modeling scales.
2. Due to limited cell size and time step, never know the exact numerical governing eqns.
3. Numerical cell size and time step are not dynamic quantities,
   don't participate flow evolution (underlying assumption), but introduce errors ONLY.
4. mesh size scale and modeling scale of PDE may be different significantly.
   Is $\vec{q} = -\kappa\nabla T$ still valid in scales of 1m, 10m, 1km mesh size?
5. Where is the principle of CFD?

Principle of CFD: direct modeling the flow physics in mesh size and time step scale



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

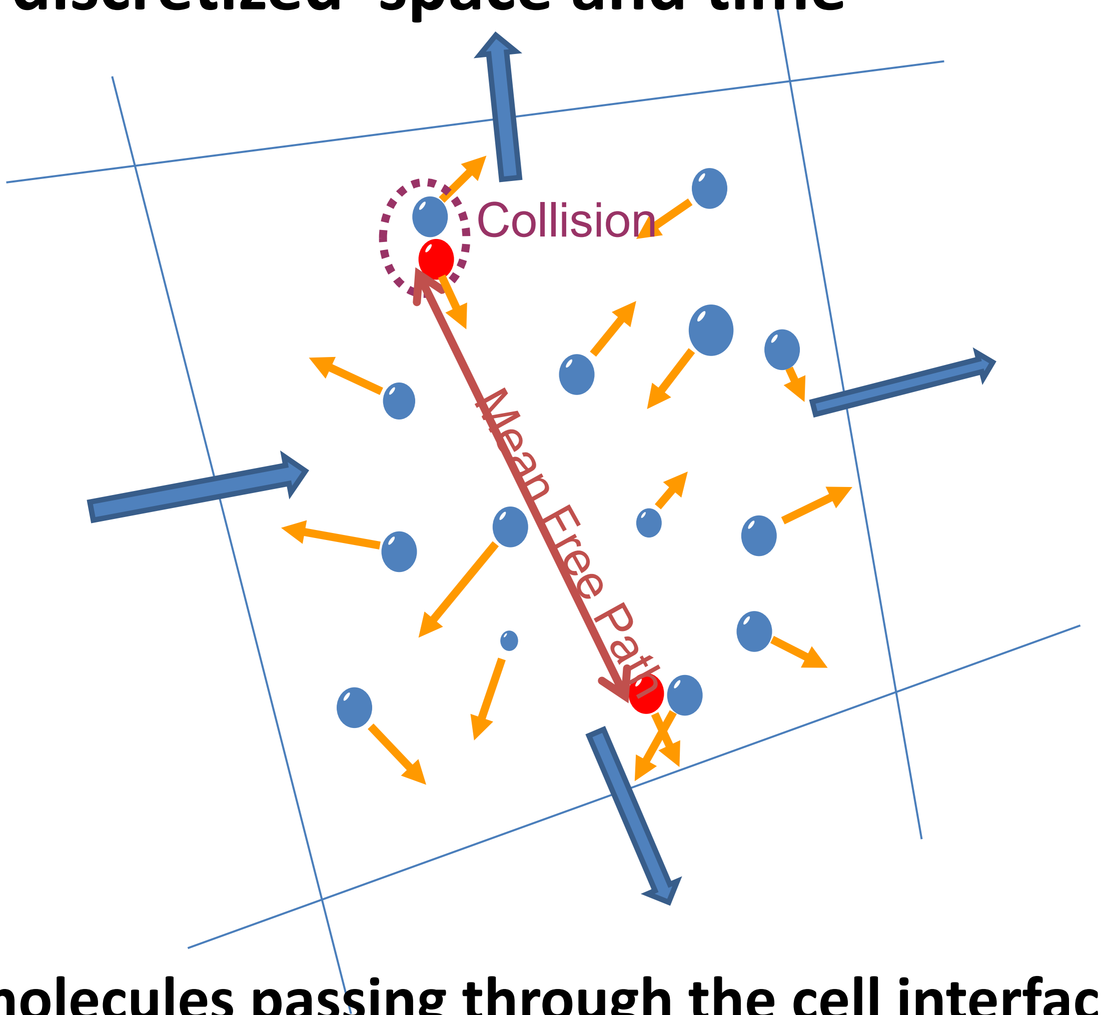
hydrodynamic dissipative layer | (????) | kinetic mean free path | molecular diameter

Different physical modeling scales

we need a continuum 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:

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

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

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

Remarks:

1. The above equation doesn't require f to be a continuous function of space and time.
2. The scales of Δx and Δt are independent of the particle mean free path and collision time.
3. If the above equation is considered as an integral solution of the Boltzmann equation, **a common mistake** is to use upwind to model the interface flux, i.e., free transport mechanism.

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):

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

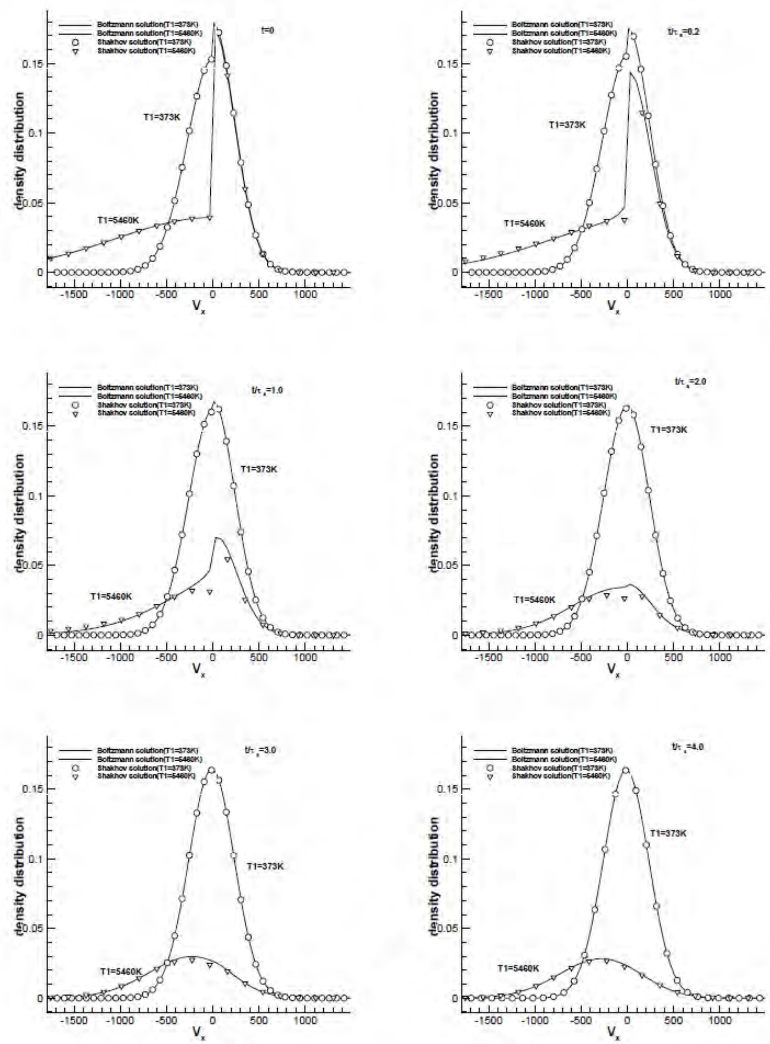
Update of conservative variables (marco):

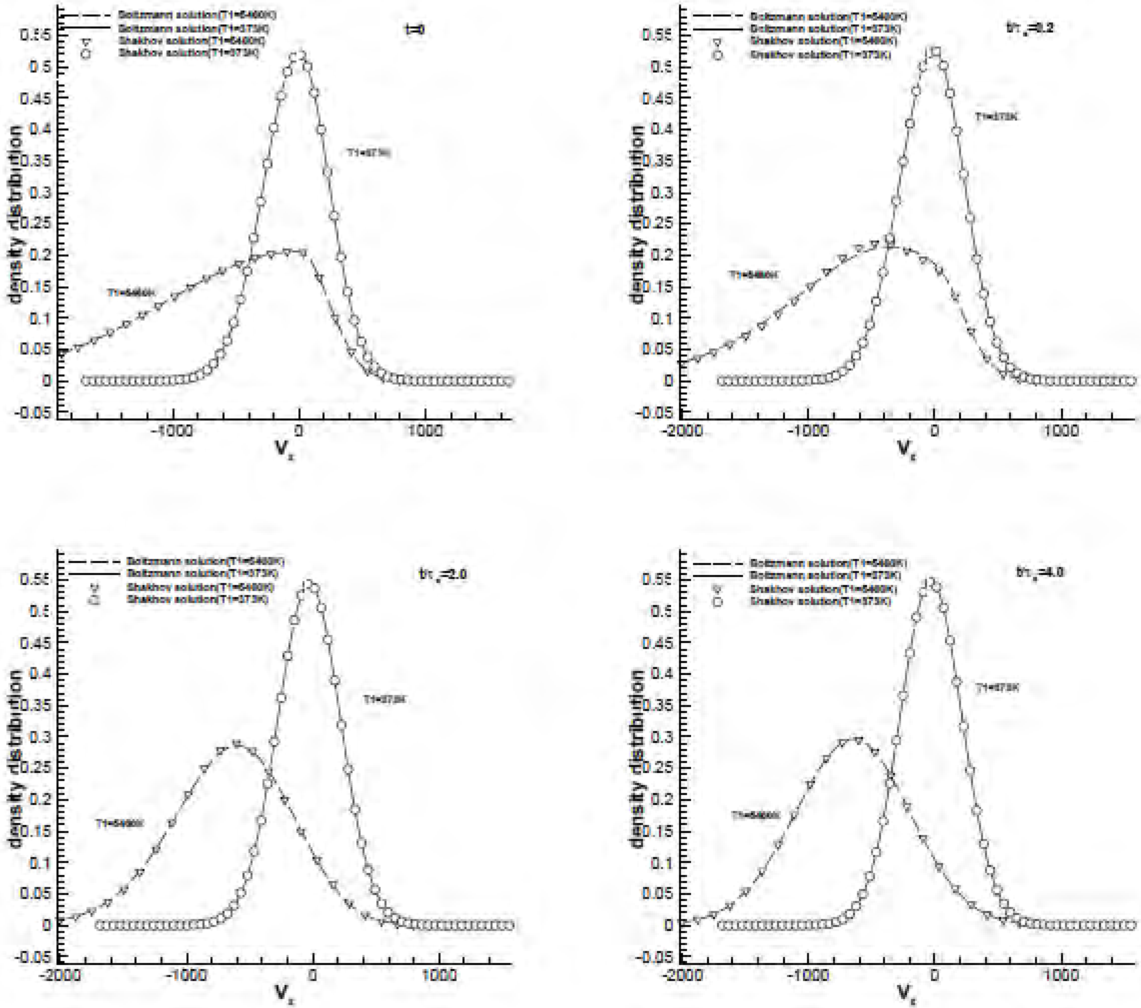
$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int u_k \psi (f_{j-1/2,k} - f_{j+1/2,k}) du_k d\xi dt$$

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

Modeling of collision term in different scale $(\Delta t/\tau)$

Experiments: full Boltzmann collision term vs Shakhov model





t=0
density distribution
V

Inner cell collision term modeling:

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

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.

$$Q(f,f) = \begin{cases} Q(Boltzmann), & \Delta t < 0.5\tau \\ Q(Boltzmann + Shakhov), & 0.5\tau \le \Delta t \le 3\tau \\ Q(Shakhov), & 3\tau < \Delta t \end{cases}$$

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)

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

Scale up

taking conservative moments:

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

Scale down

g^{n+1}

mass, momentum and energy

(macro-scale)

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

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

The update of gas distribution function becomes

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

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

$$+ \frac{\Delta t}{2}\left(\frac{g_{j,k}^{n+1} - f_{j,k}^{n+1}}{\tau^{n+1}} + \frac{g_{j,k}^{n} - f_{j,k}^{n}}{\tau^{n}}\right)$$

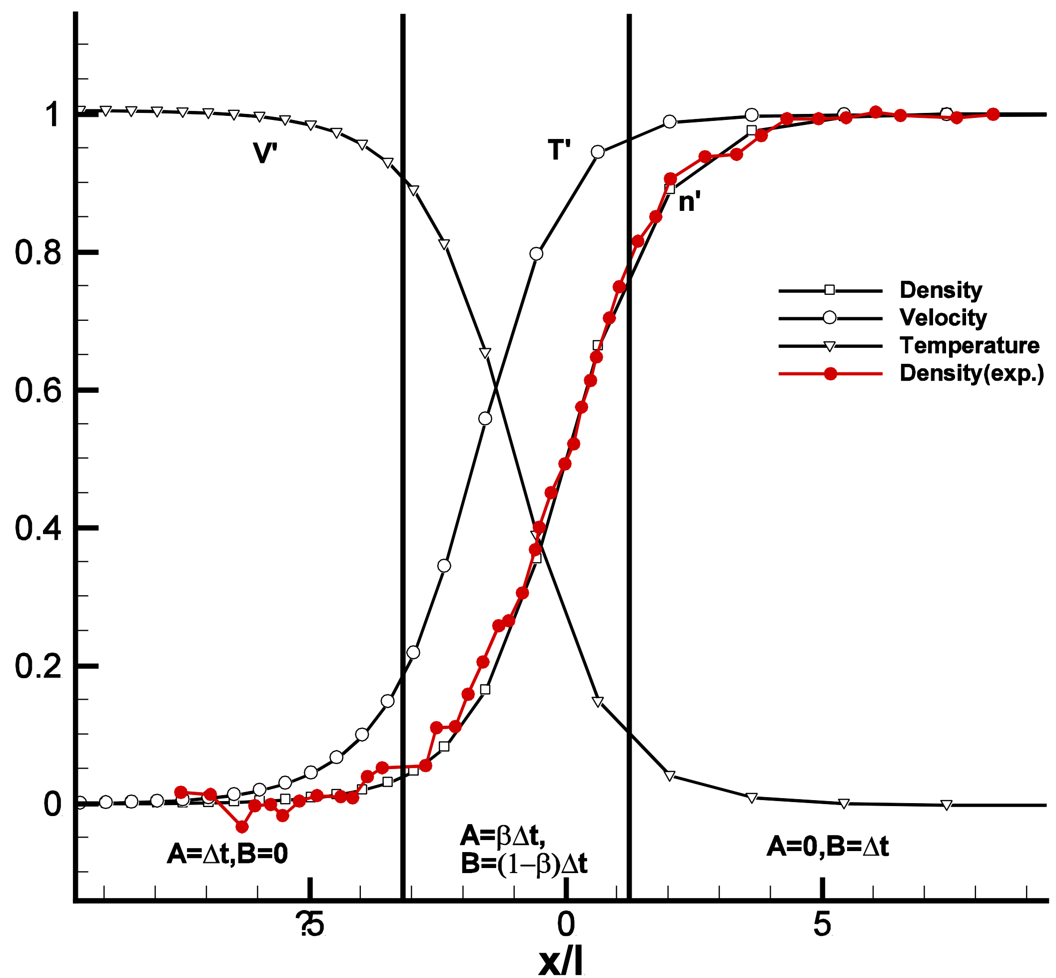
with the solution:

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

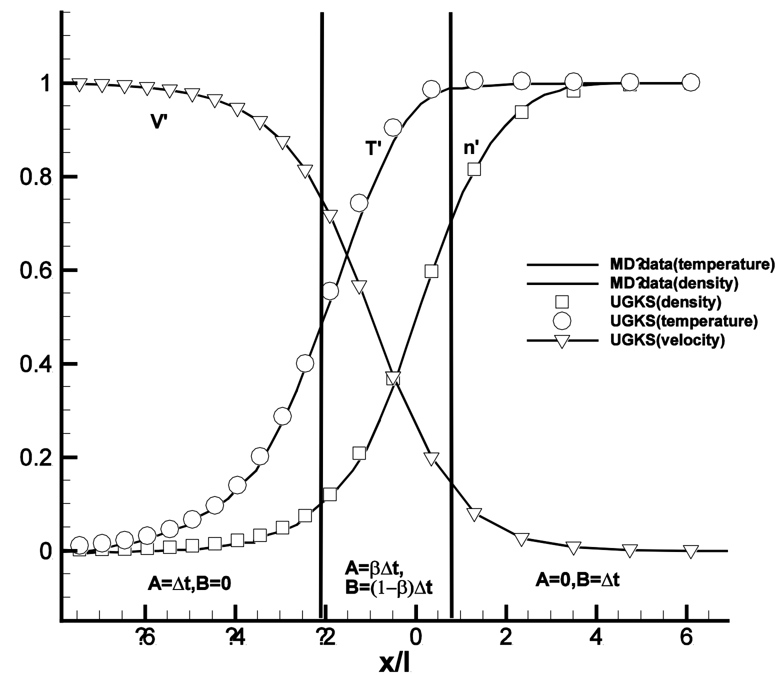
$$+ \frac{\Delta t}{2}\left(\frac{g_{j,k}^{n+1}}{\tau_j^{n+1}} + \frac{g_{j,k}^{n} - f_{j,k}^{n}}{\tau_j^{n}}\right)$$

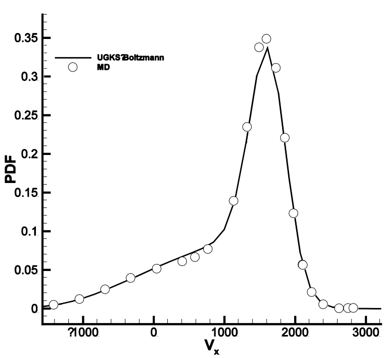
Shock Structure Calculations

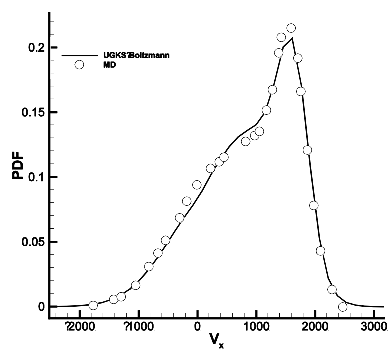
M=2.8 shock structure
(UGKS vs Experiments)

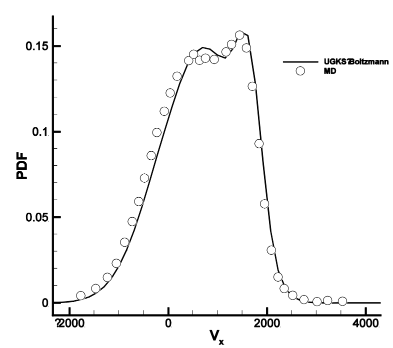


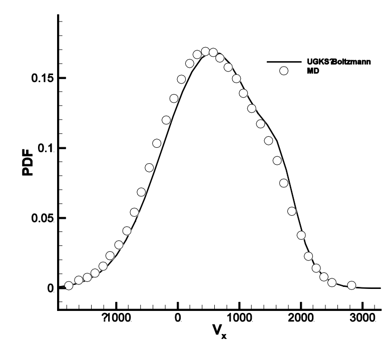
M=5 shock structure: UGKS vs MD



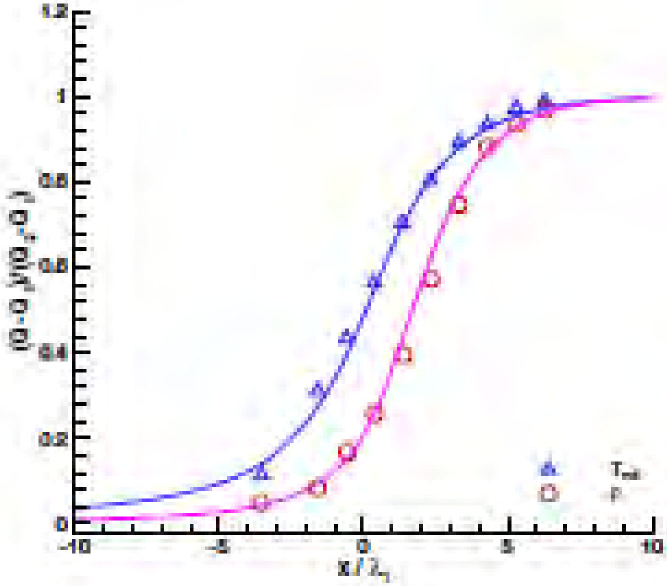




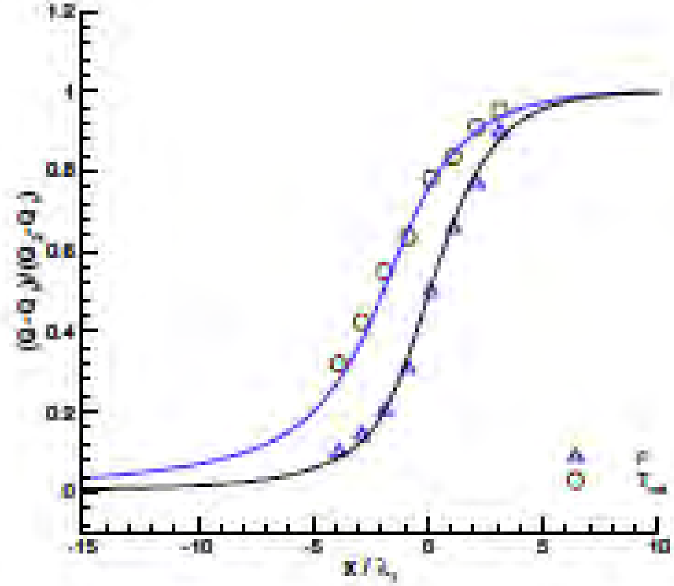




Nitrogen shock structures



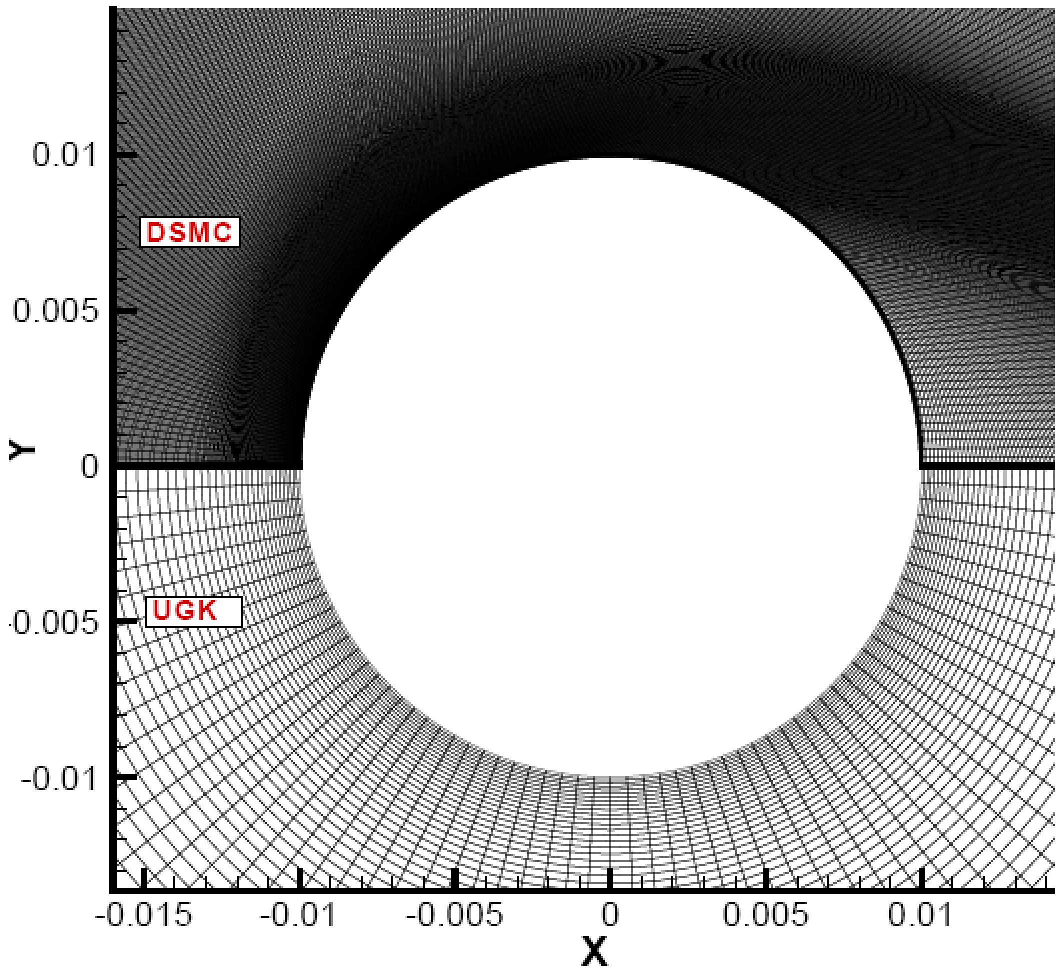
(a) Ma=7

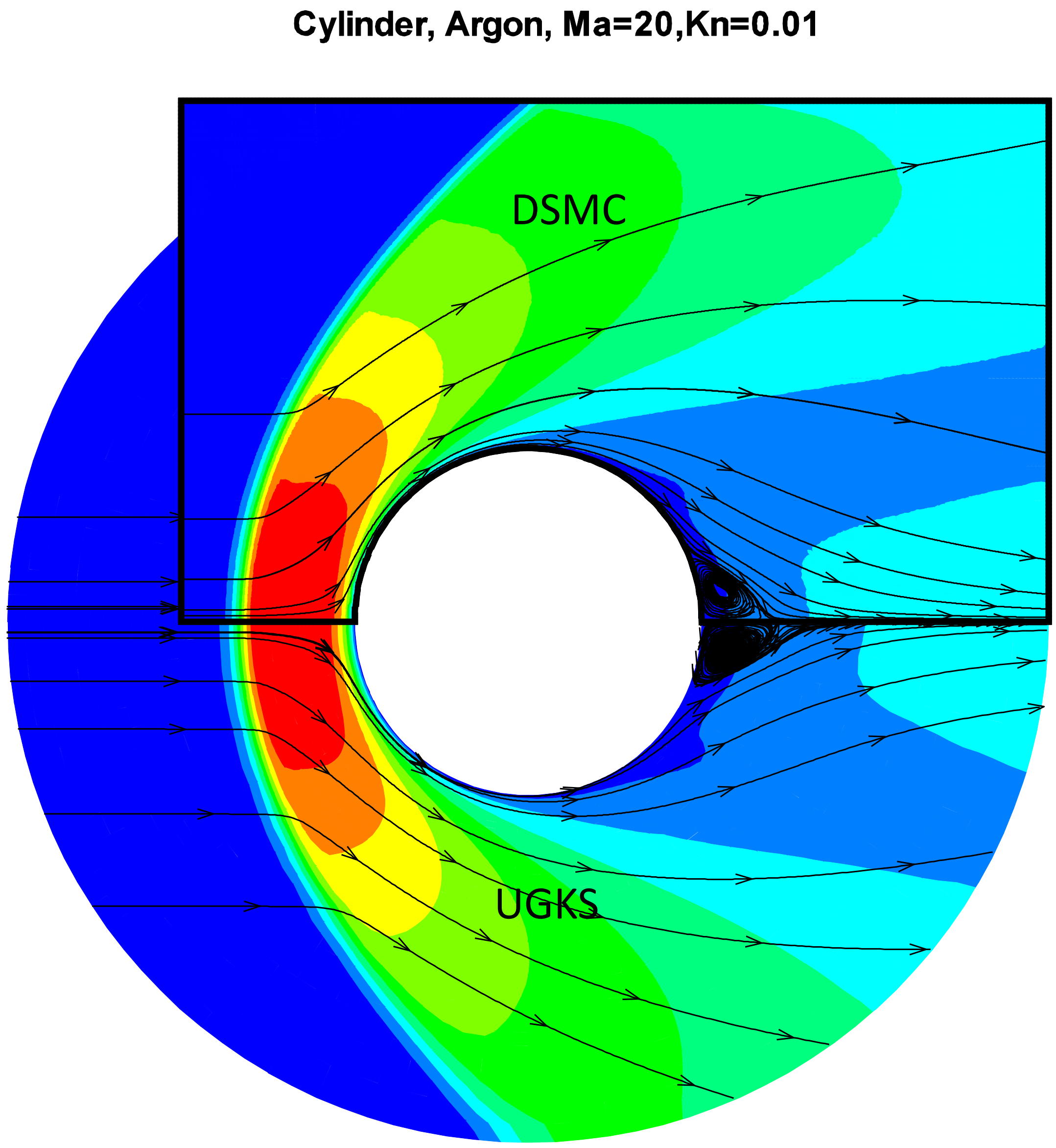


(b) Ma=12.9

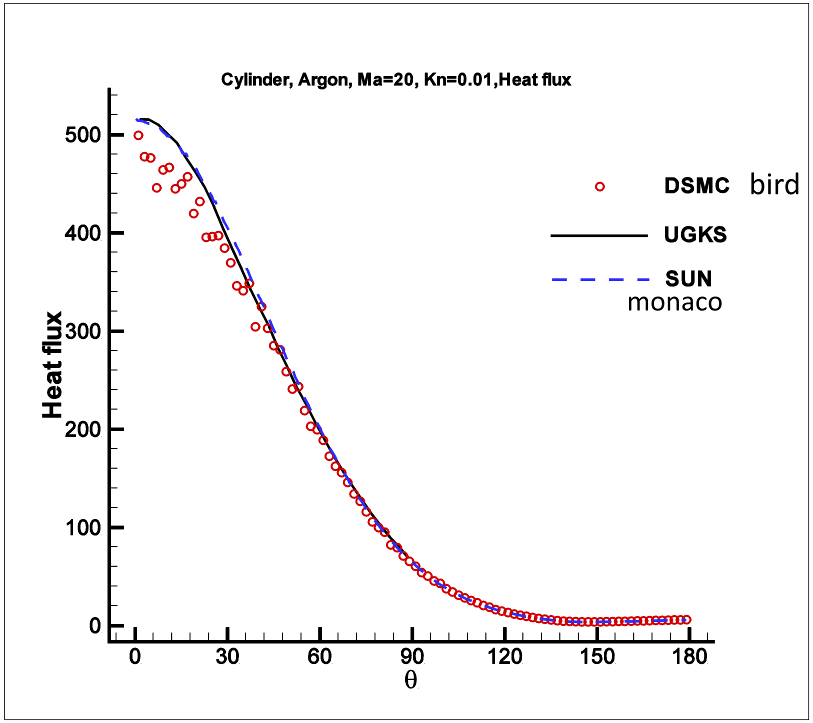
Flow passing through a cylinder

M=20, Kn=0.01

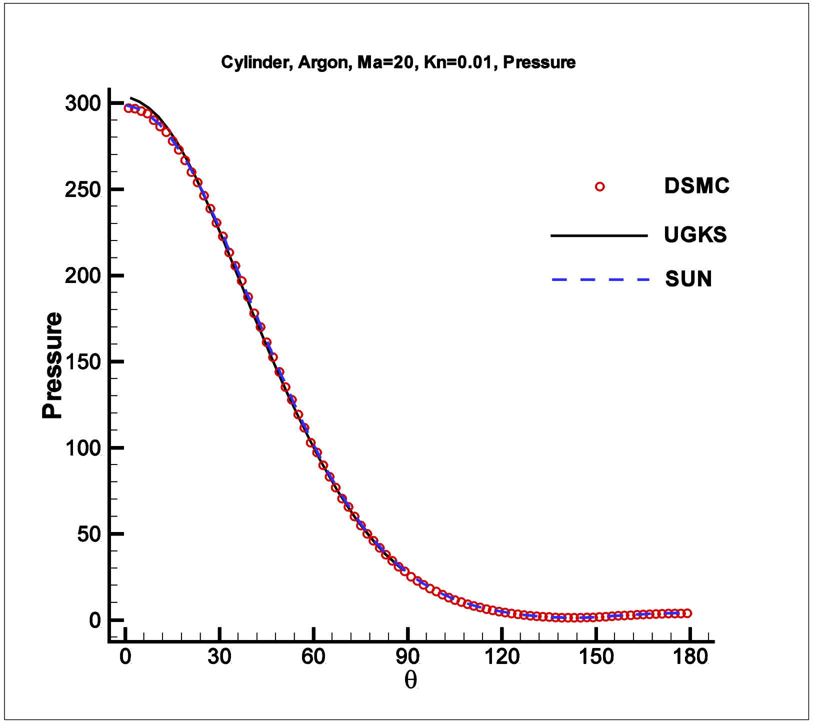



Cylinder, Argon, Ma=20,Kn=0.01
DSMC
UGKS

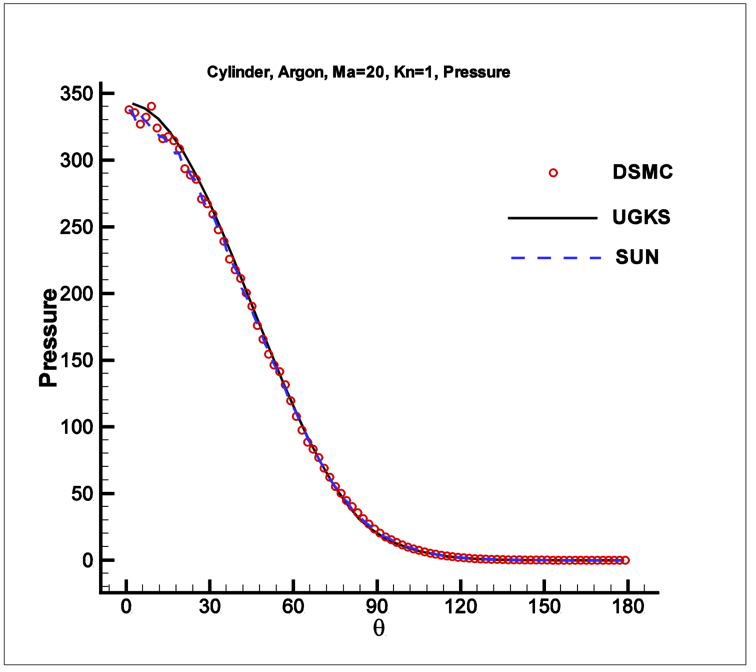
M=20, Kn=0.01



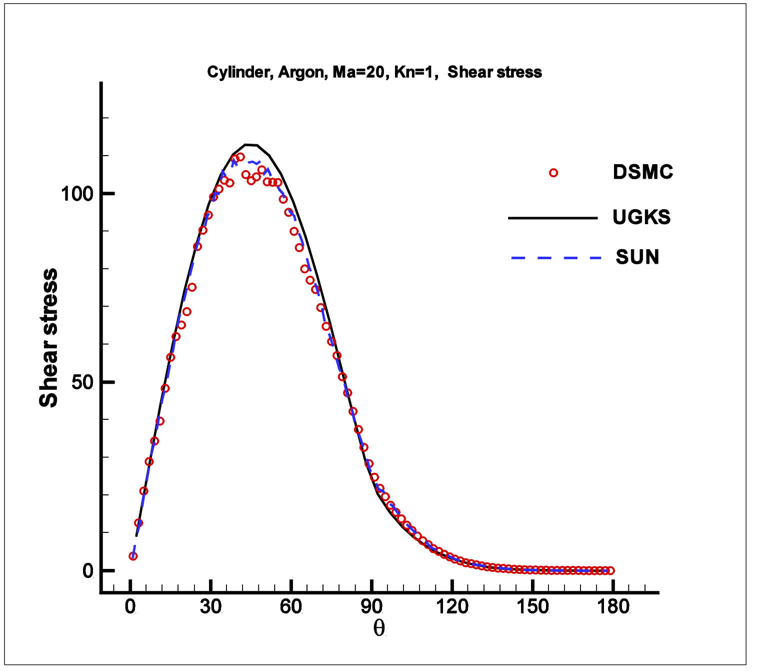
Cylinder, Argon, Ma=20, Kn=0.01,Heat flux
Heat flux
θ
DSMC bird
UGKS
SUN
monaco



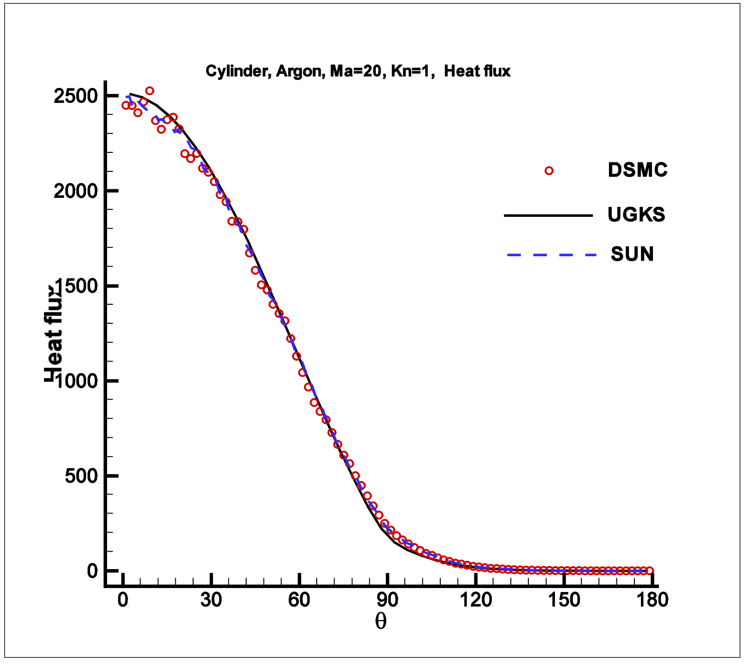
Cylinder, Argon, Ma=20, Kn=0.01, Pressure
Pressure
θ
DSMC
UGKS
SUN



Cylinder, Argon, Ma=20, Kn=1, Pressure
Pressure
θ
DSMC
UGKS
SUN



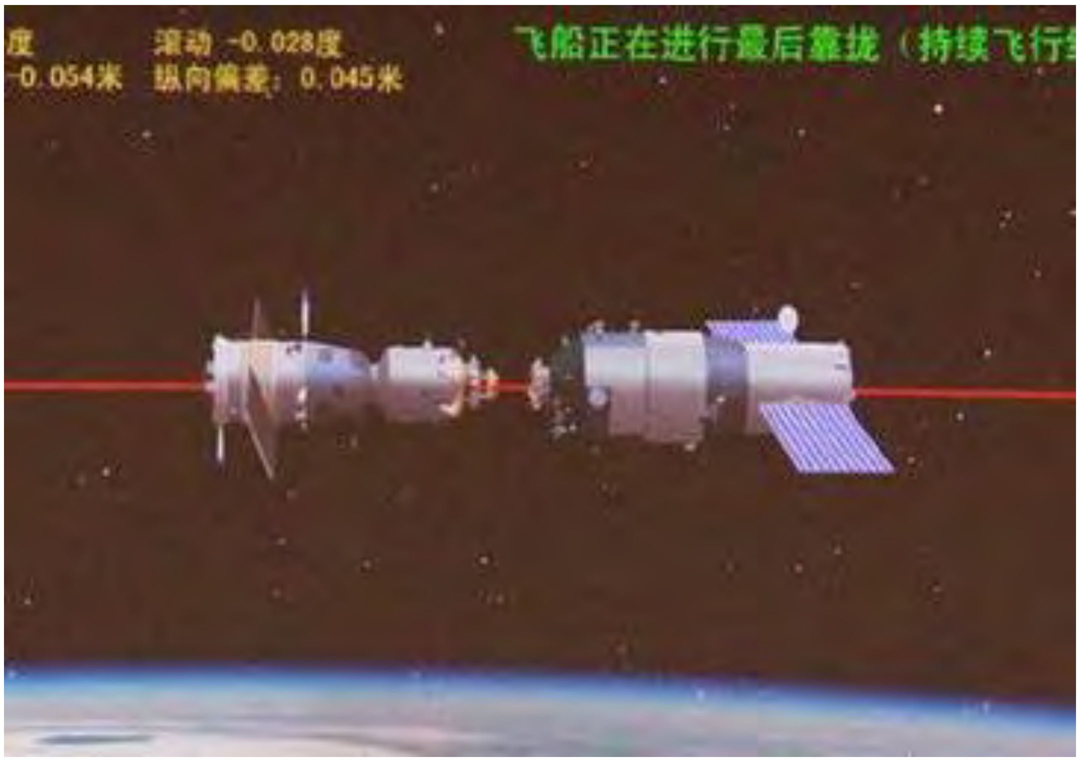
Cylinder, Argon, Ma=20, Kn=1, Shear stress
Shear stress
θ
DSMC
UGKS
SUN



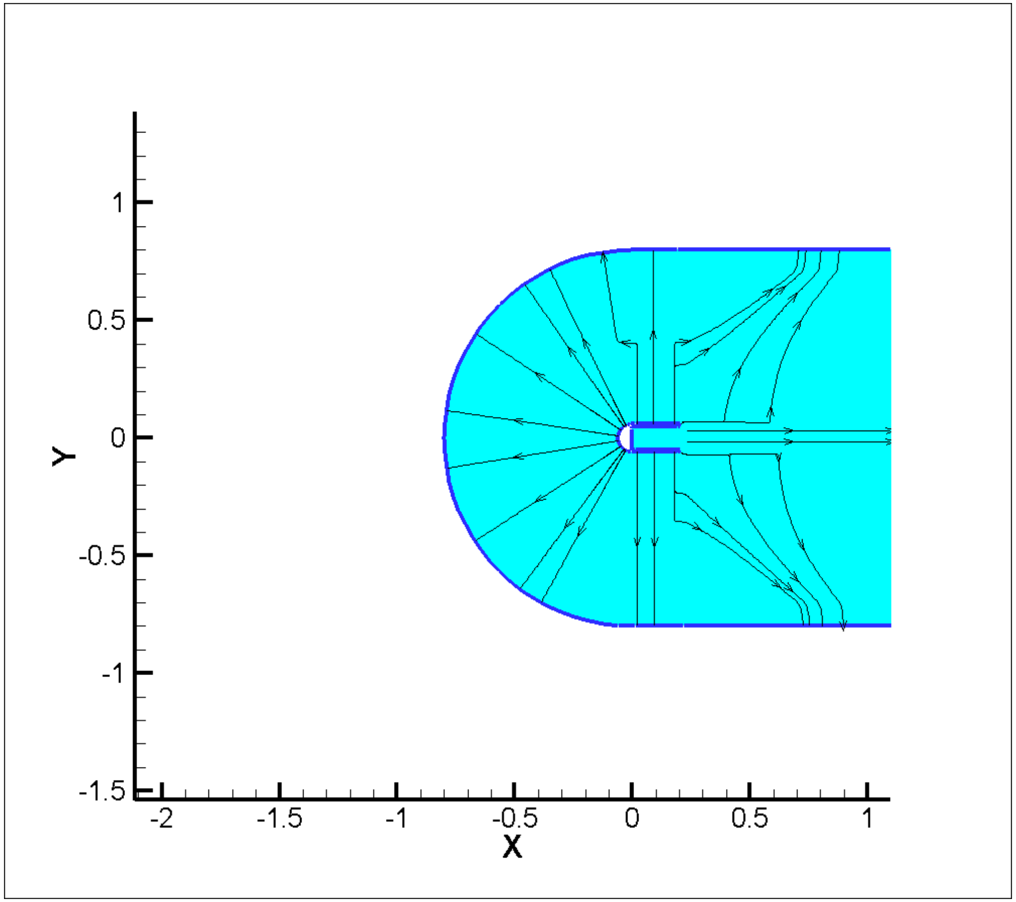
Cylinder, Argon, Ma=20, Kn=1, Heat flux
Heat flux
θ
DSMC
UGKS
SUN

M=20, Kn=1

Expansion flow from a nozzle



Expansion flow from a nozzle

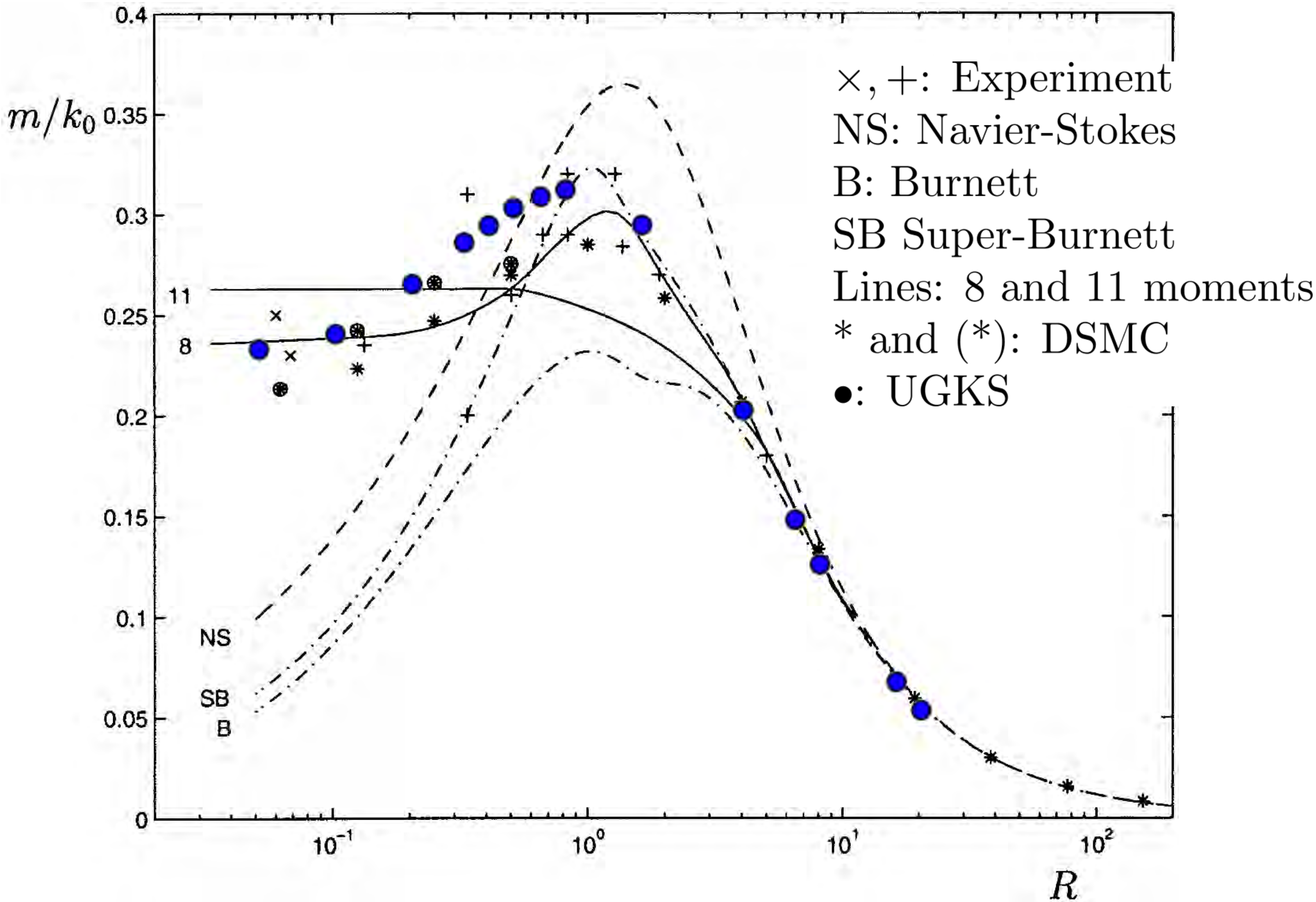


Density ratio

10000

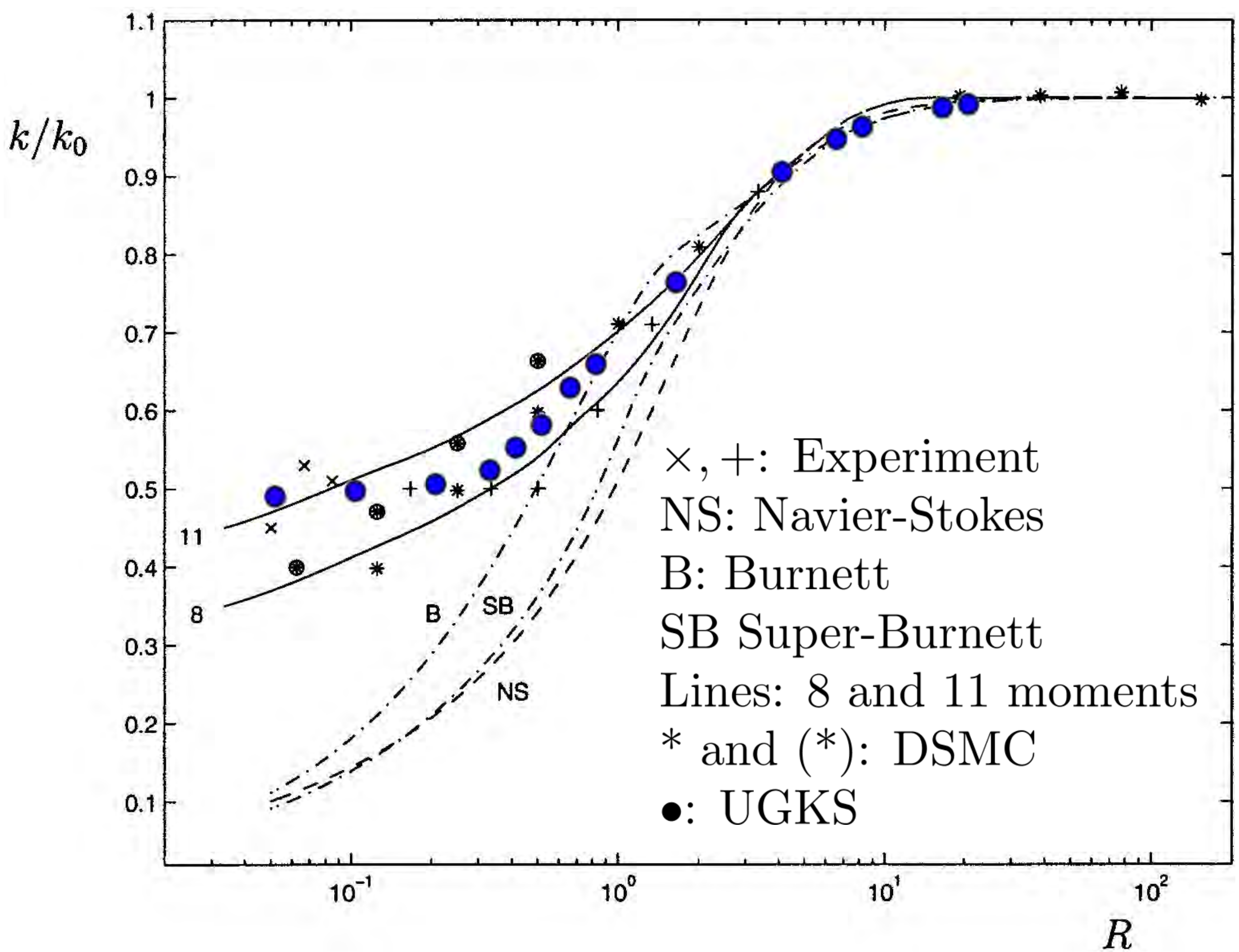
Sound wave propagation in simple gases

Absorption



m/k_0
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
11
8
NS
SB
B
10^{-1}
10^{0}
10^{1}
10^{2}
R
×, +: Experiment
NS: Navier-Stokes
B: Burnett
SB Super-Burnett
Lines: 8 and 11 moments
* and (*): DSMC
●: UGKS

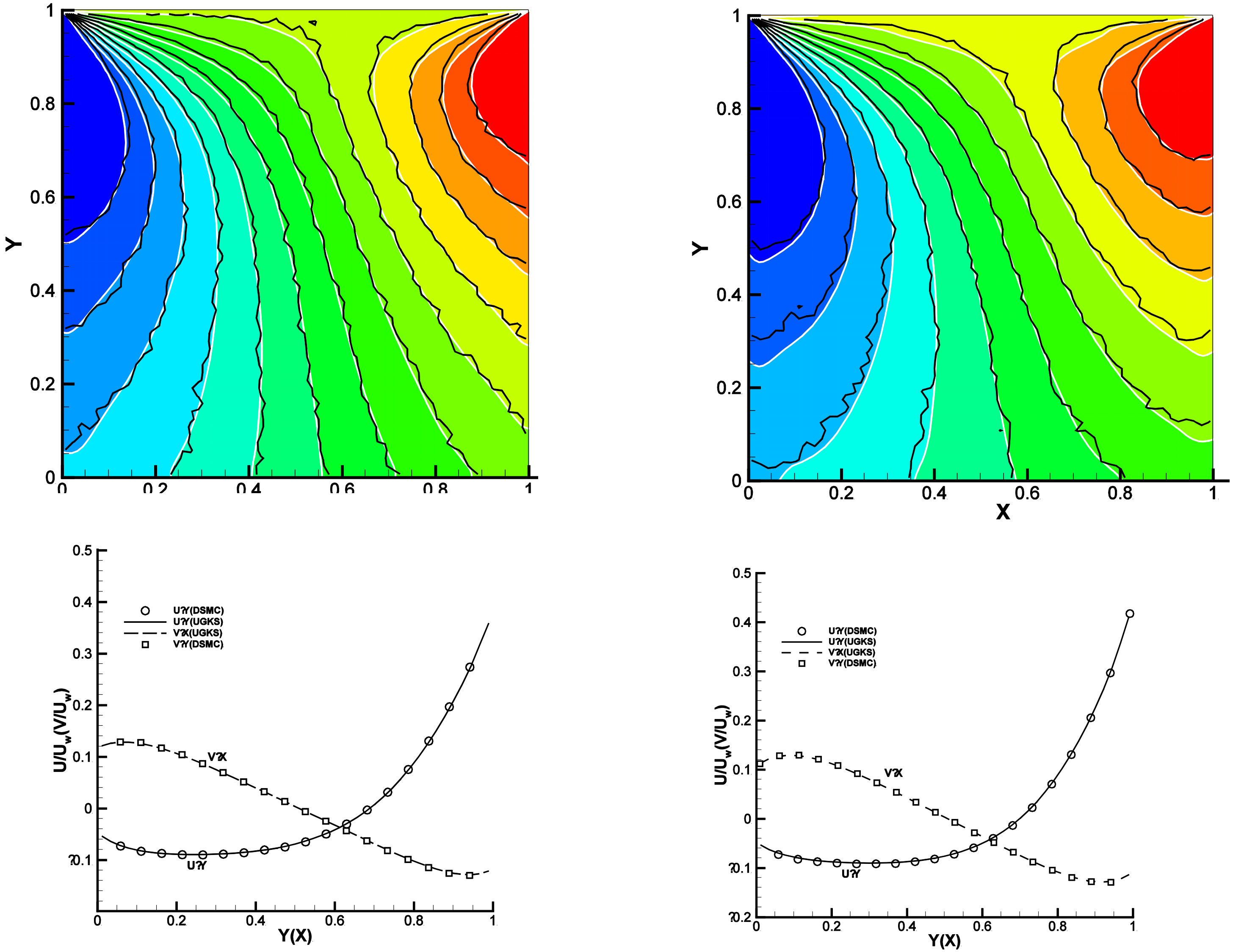
Speed



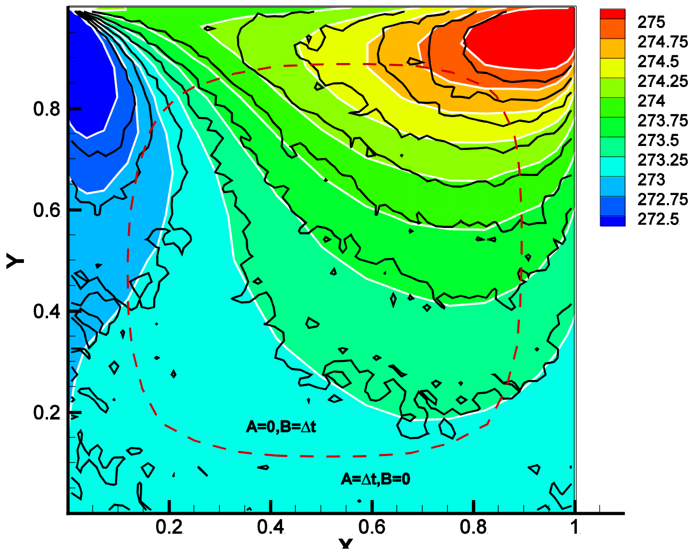
k/k_0
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10^{-1}
10^{0}
10^{1}
10^{2}
R
11
8
B
SB
NS
×, +: Experiment
NS: Navier-Stokes
B: Burnett
SB Super-Burnett
Lines: 8 and 11 moments
* and (*): DSMC
●: UGKS

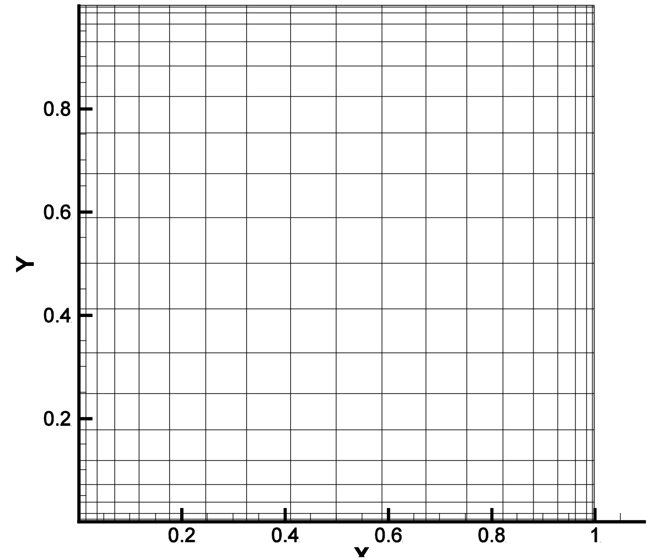
UGKS vs DSMC

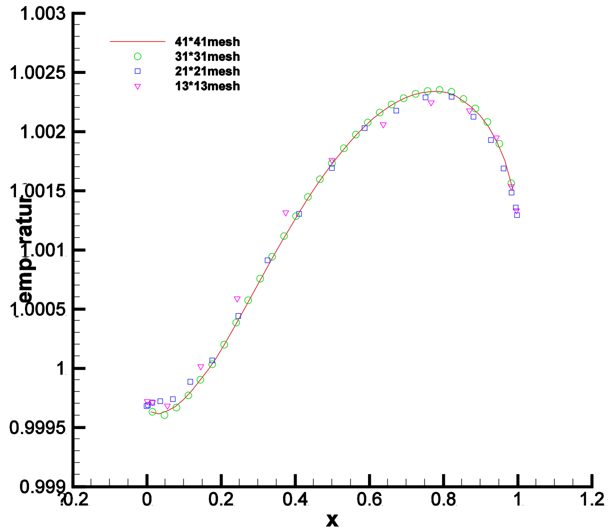
Kn=10 | Kn=1

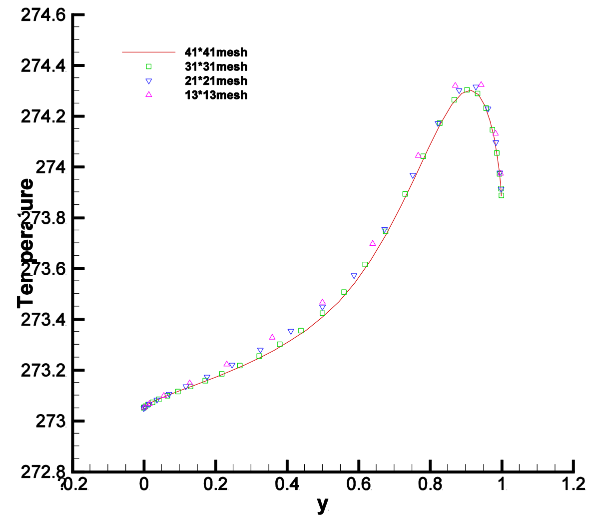


Kn=0.075 cavity case



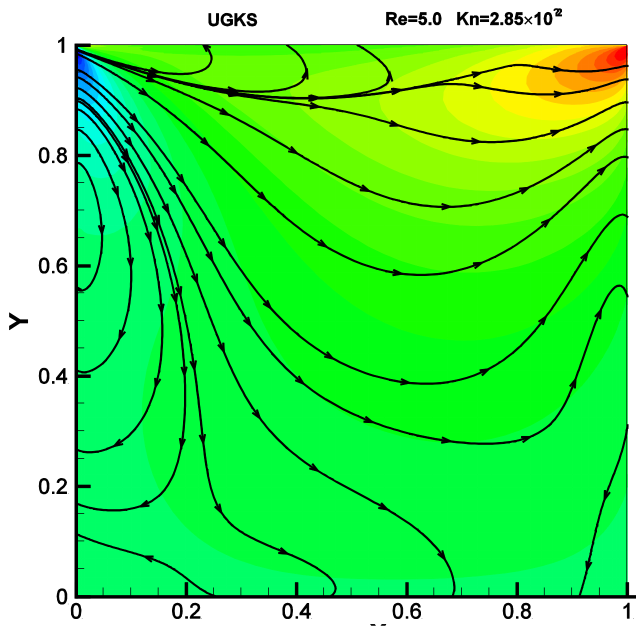


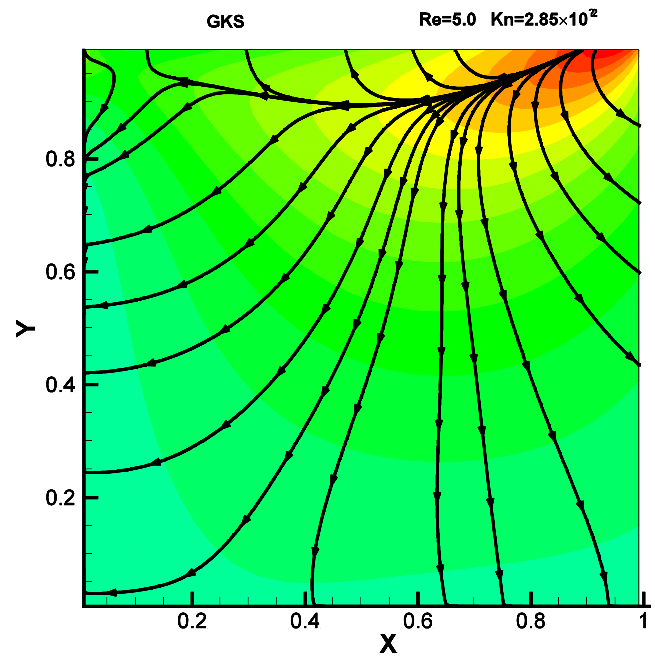




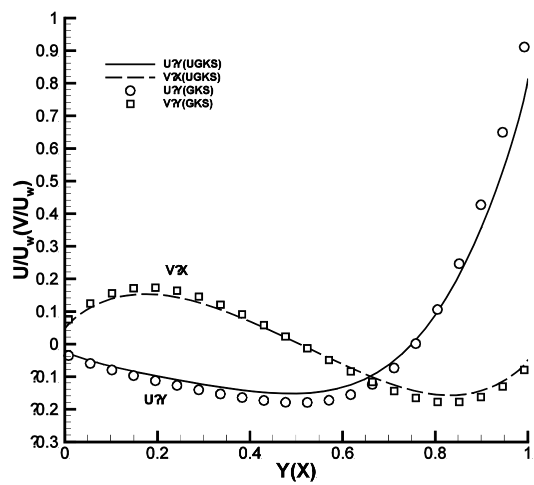
Re=5, Kn=0.0285

UGKS



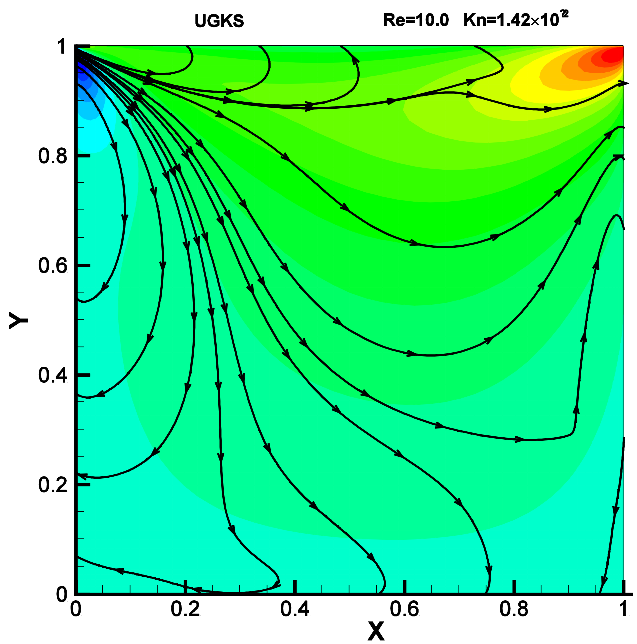


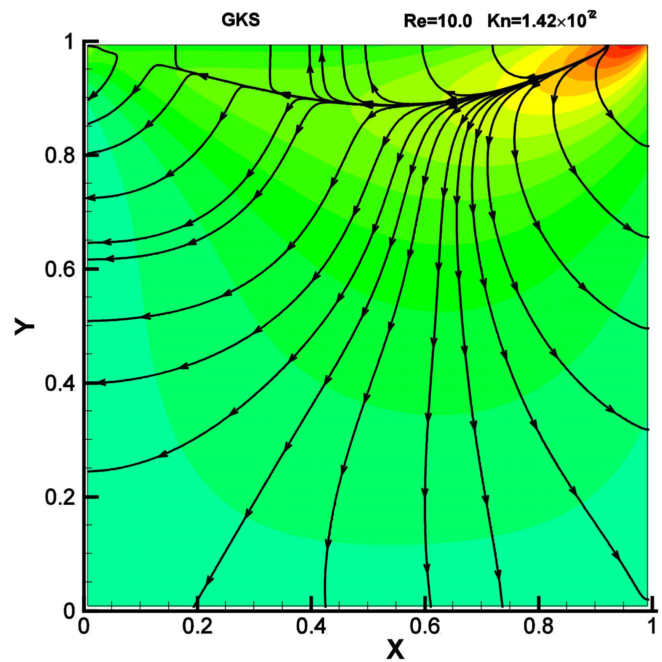
NS



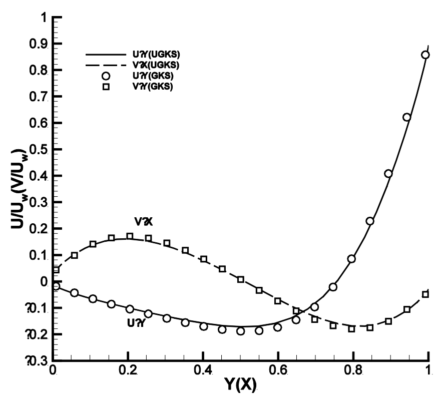
Re=10, Kn=0.0142

UGKS

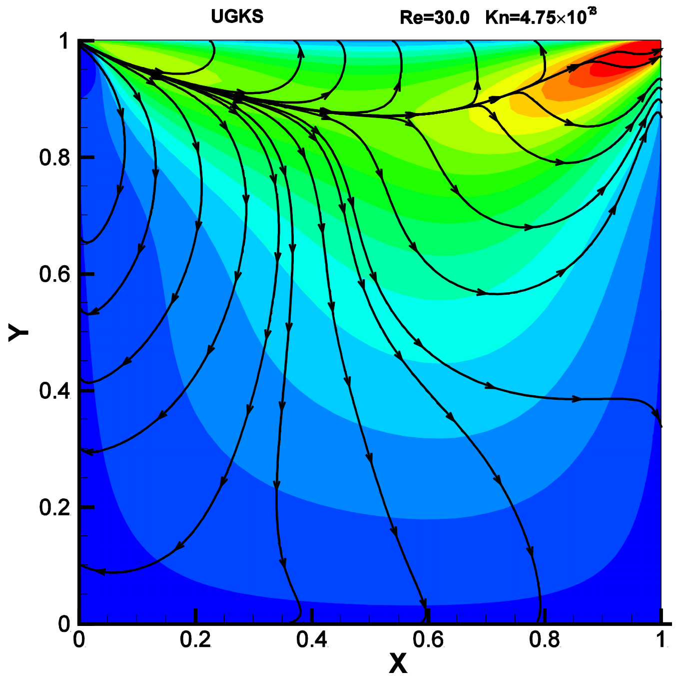


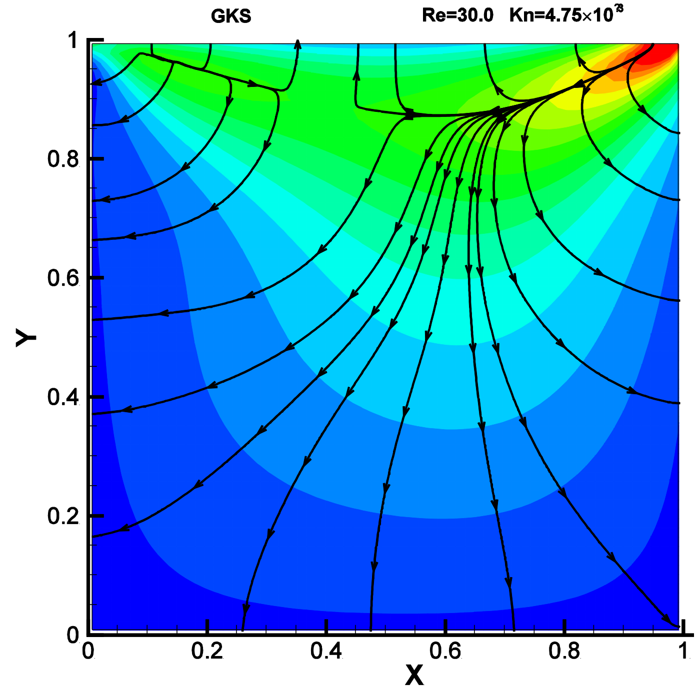


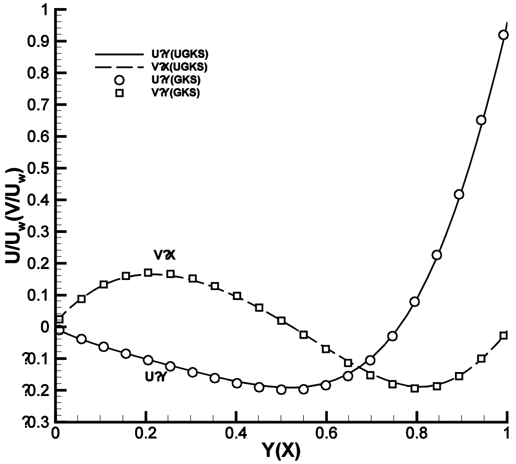
NS



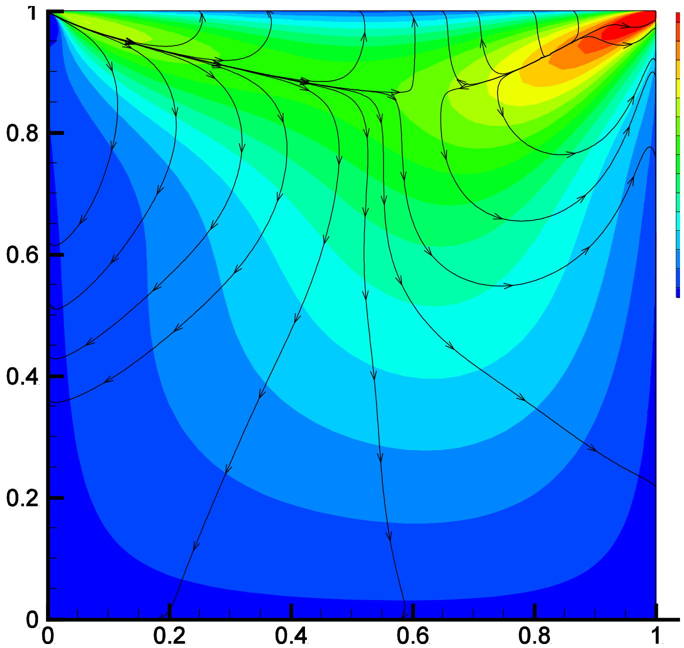
Re=30, Kn=0.00475

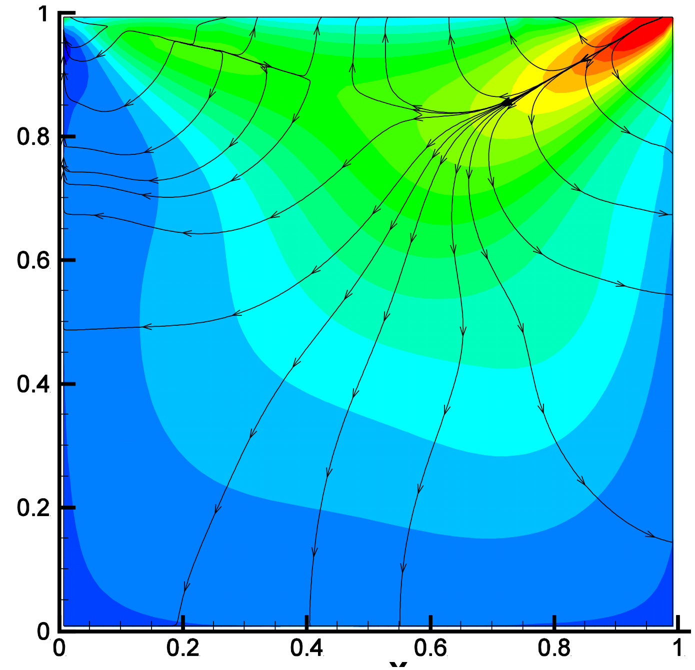


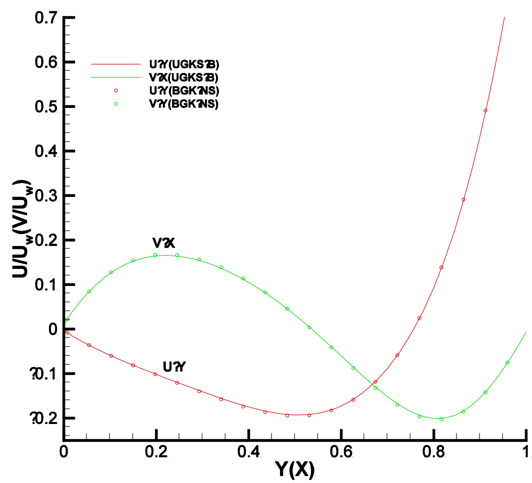




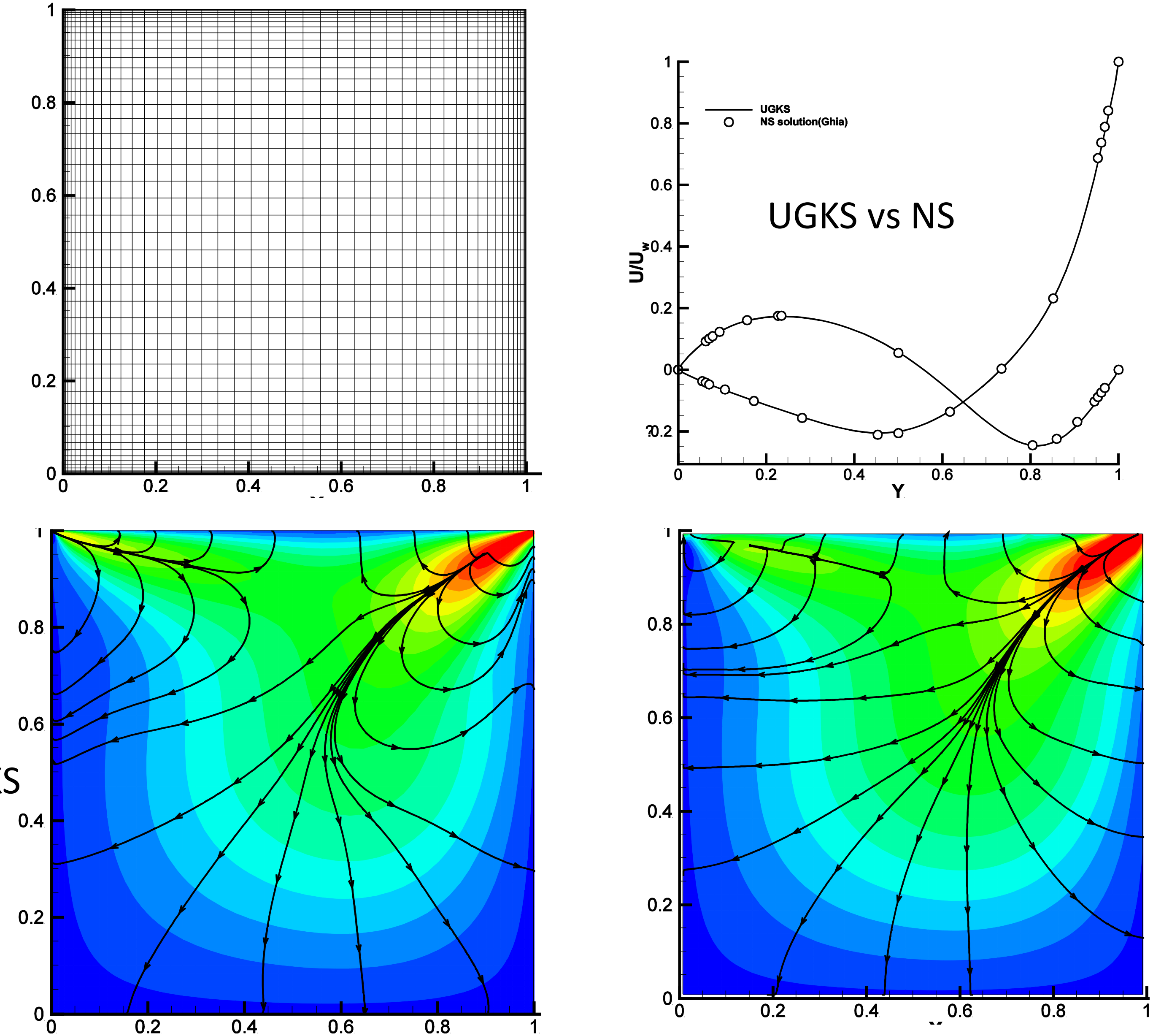
Re=50, Kn=0.00285







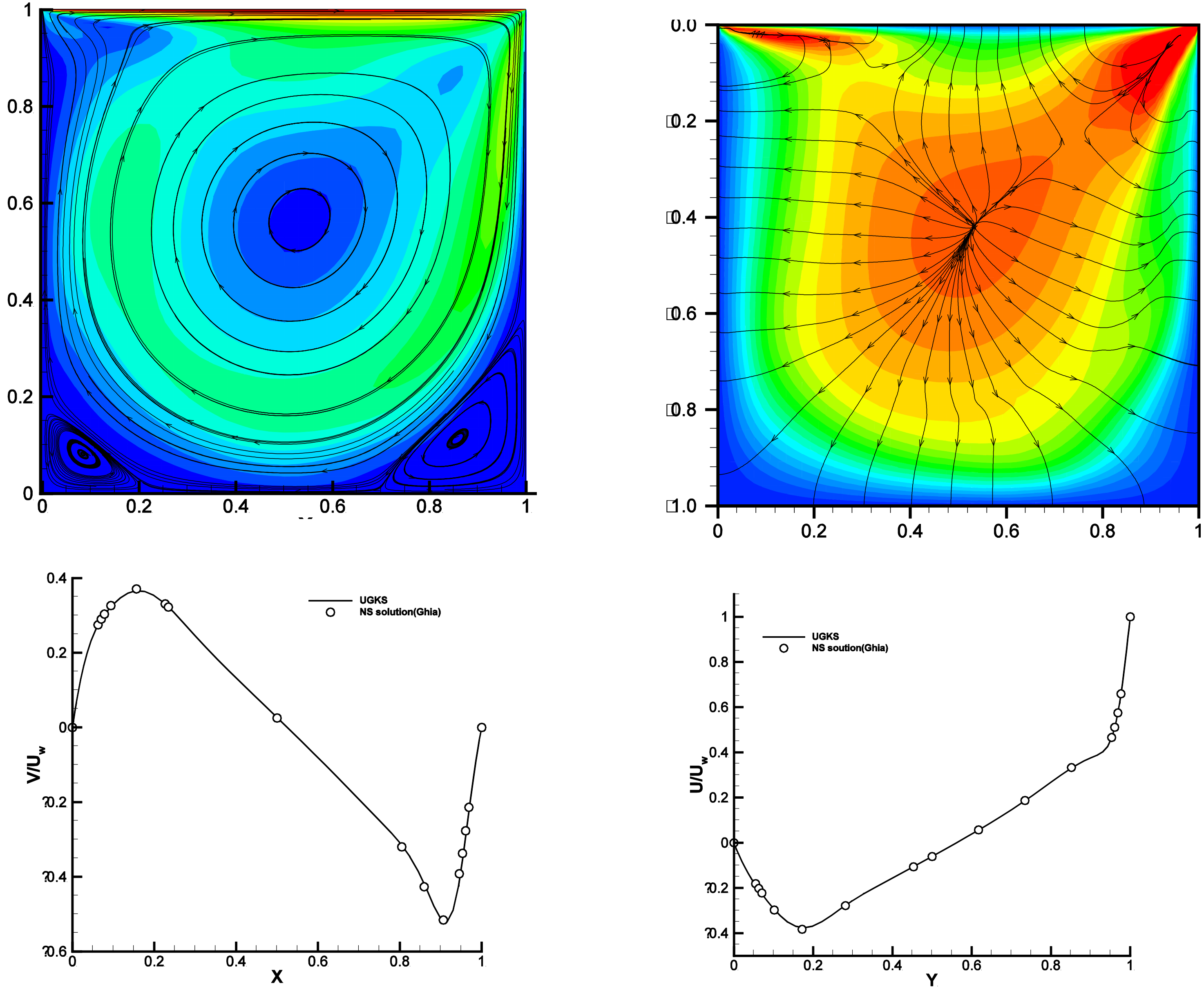
Re=100, Kn=0.00142



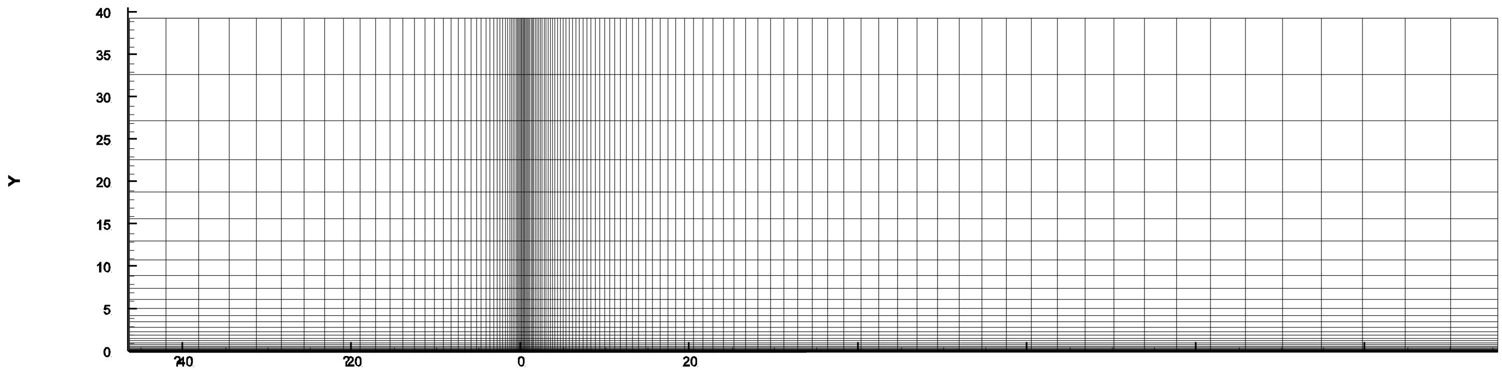
UGKS

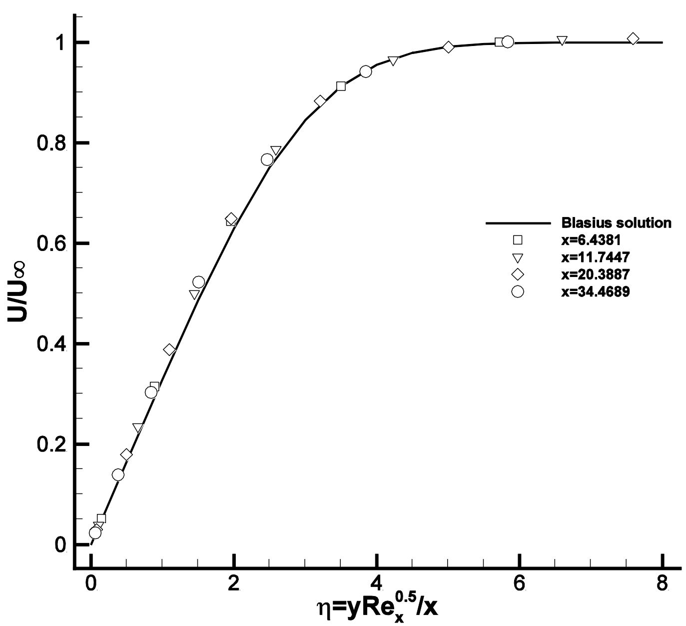
NS

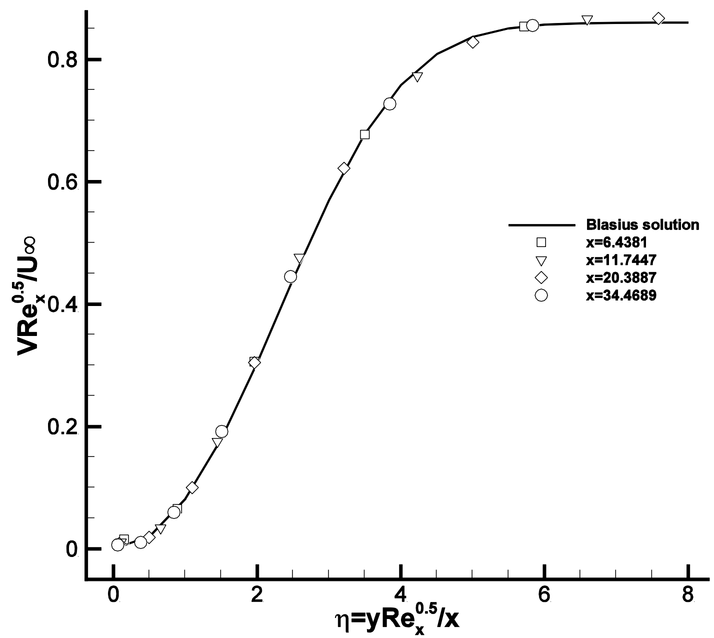
UGKS solutions: Re=1000,Kn=0.000142



UGKS solution for laminar boundary layer at $Re = 10^5$ and $M = 0.3$

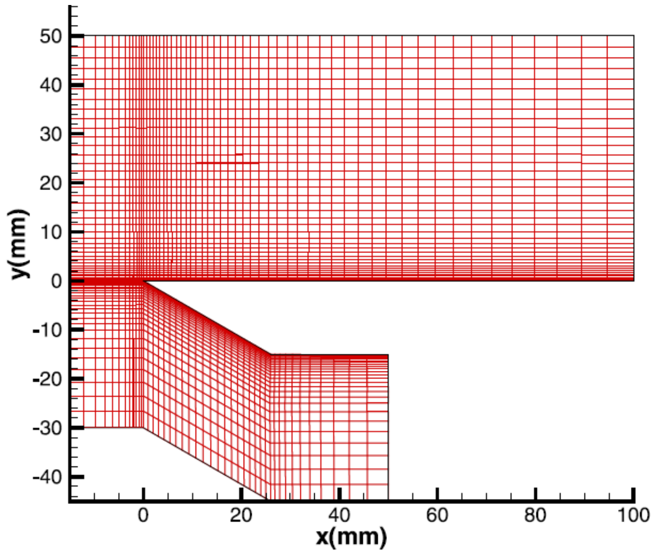


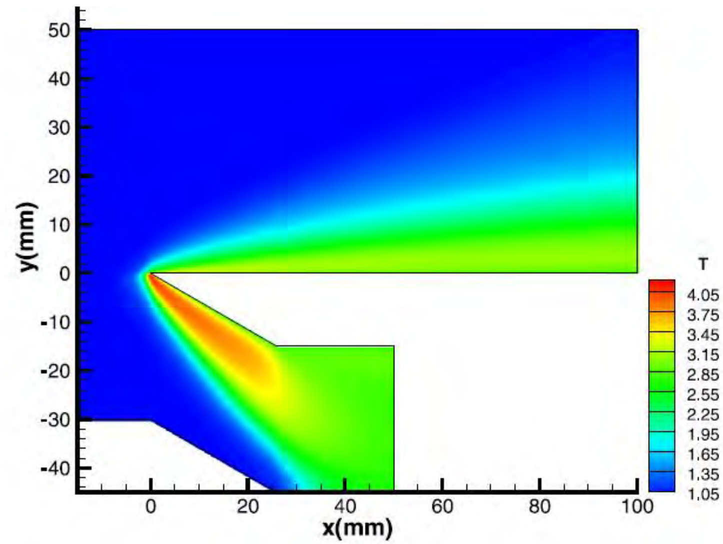


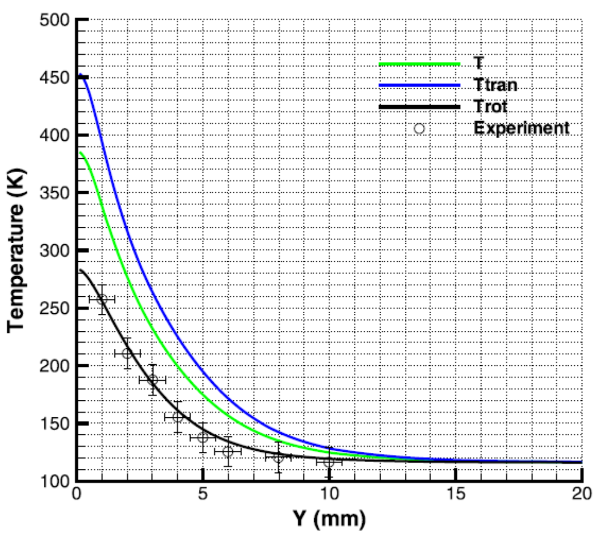


Diatomic Gases

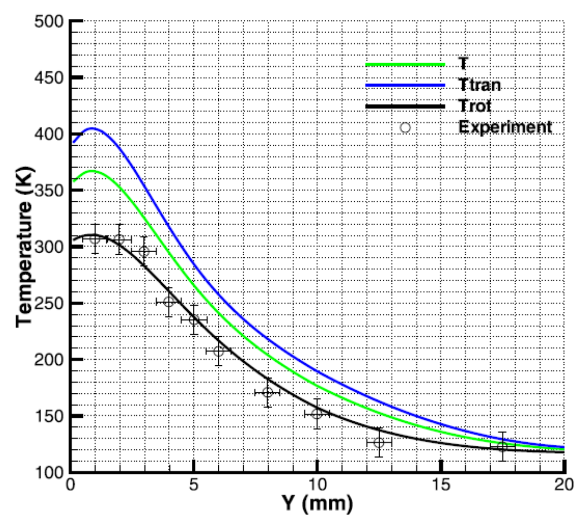
Flow passing a flat plate







(a) *temperature plot at* $x = 5mm$



(b) *temperature plot at* $x = 20mm$

Unified Gas-kinetic Scheme → GKS (NS solution)

~~Update of distribution function (micro):~~

~~$$f_{j,k}^{n+1} = f_{j,k}^{n} + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} [uf_{j-1/2,k}(t) - uf_{j+1/2,k}(t)]dt + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{x_{j-1/2}}^{x_{j+1/2}} \frac{g-f}{\tau} dxdt$$~~

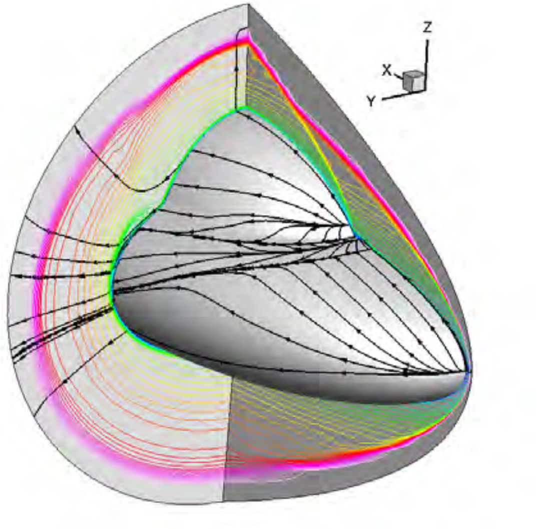
The flux evaluation is based on the integral solution of the kinetic model:

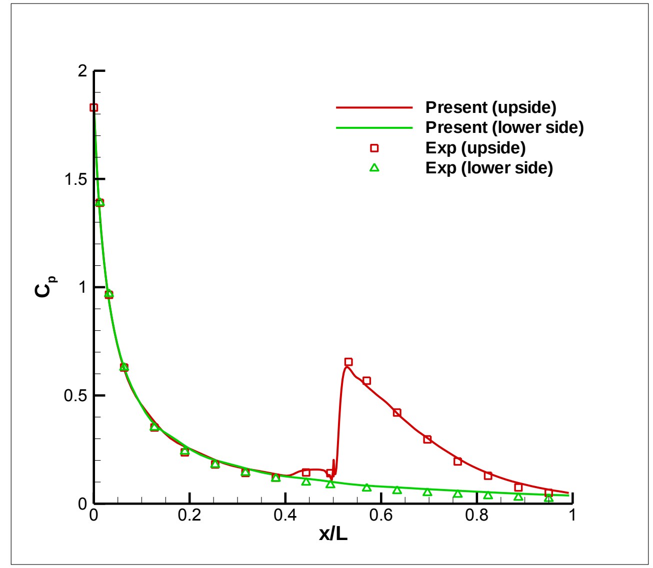
$$f_{j+1/2,k} = \frac{1}{\tau}\int_0^t g(x', t', u_k, \xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_{0,k}(x_{j+1/2} - u_k t)$$

Known in continuum flow regime

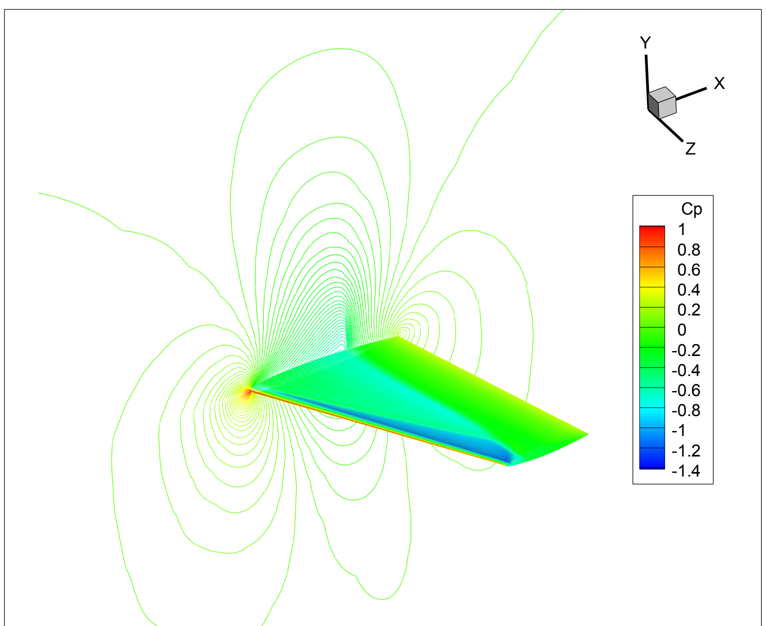
Update of conservative variables (marco):

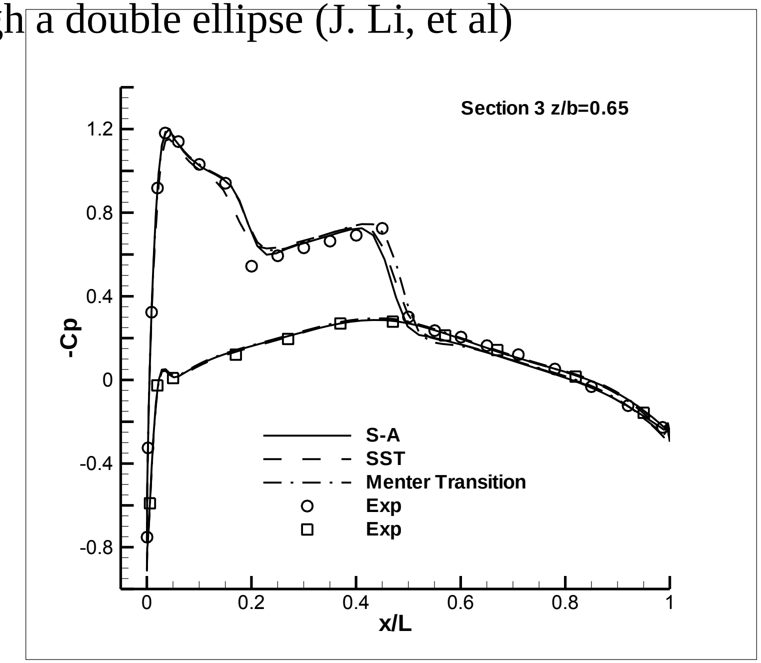
$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int u_k \psi (f_{j-1/2,k} - f_{j+1/2,k}) du_k d\xi dt$$





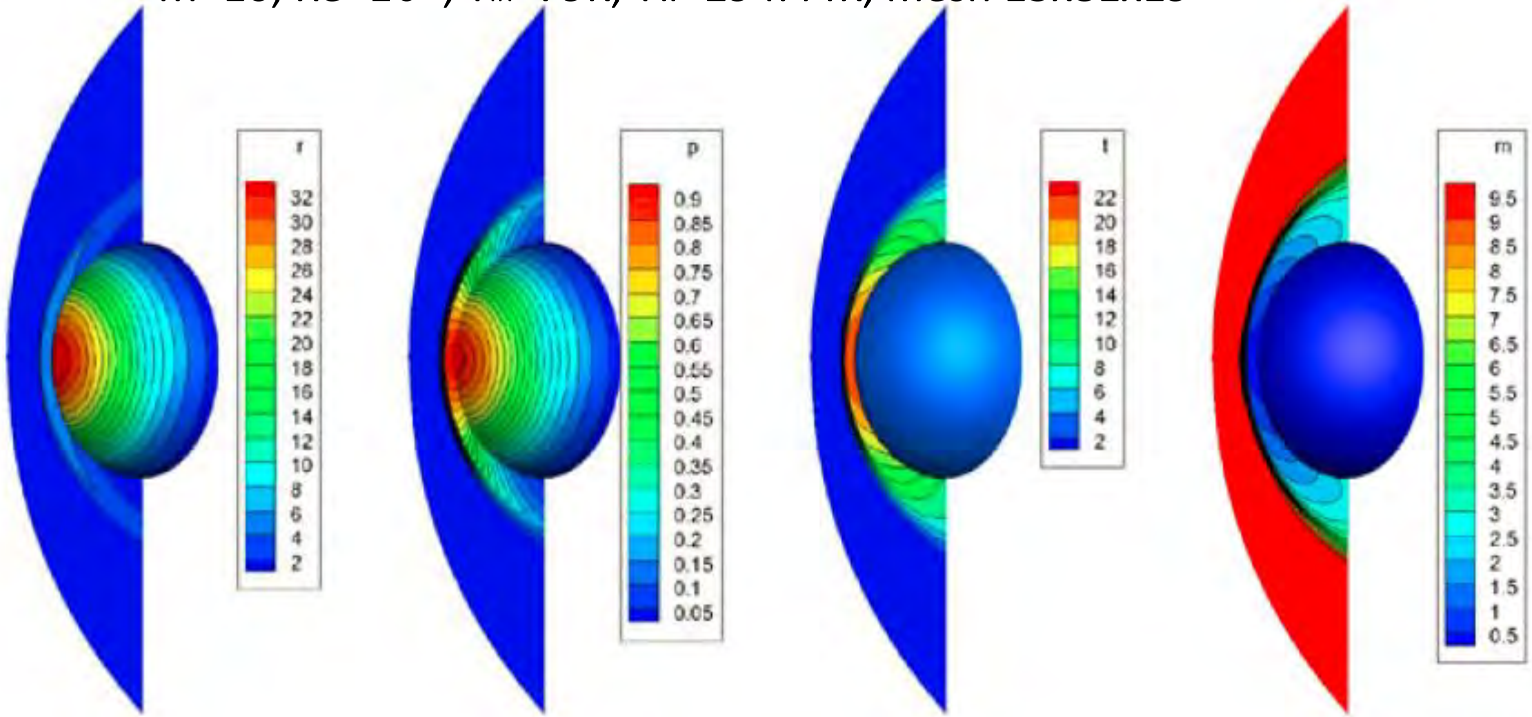
High Mach number flow passing through a double ellipse (J. Li, et al)

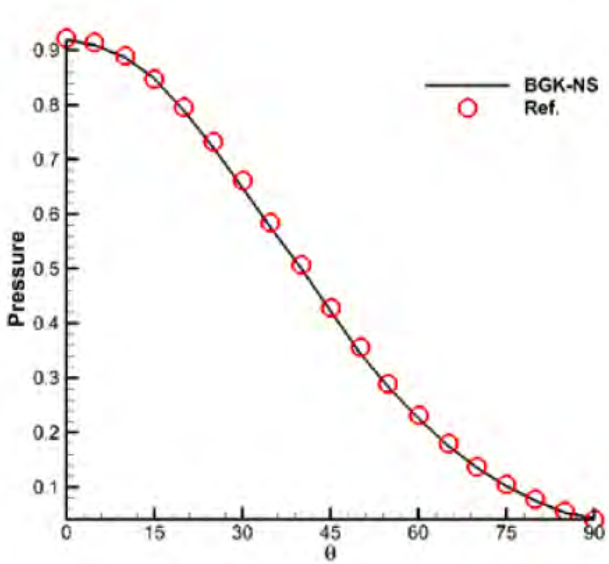


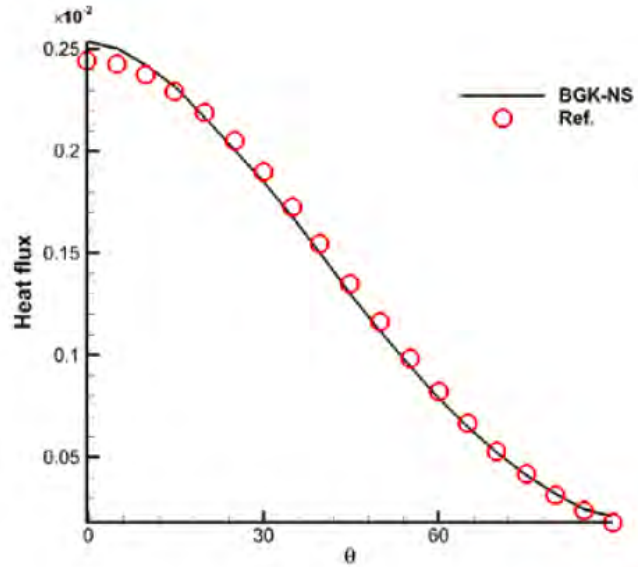


M6 airfoil (Y.H. Qian, et al)

M=10, Re=10^6, Tin=79K, Tw=294.44K, mesh 15x81x19



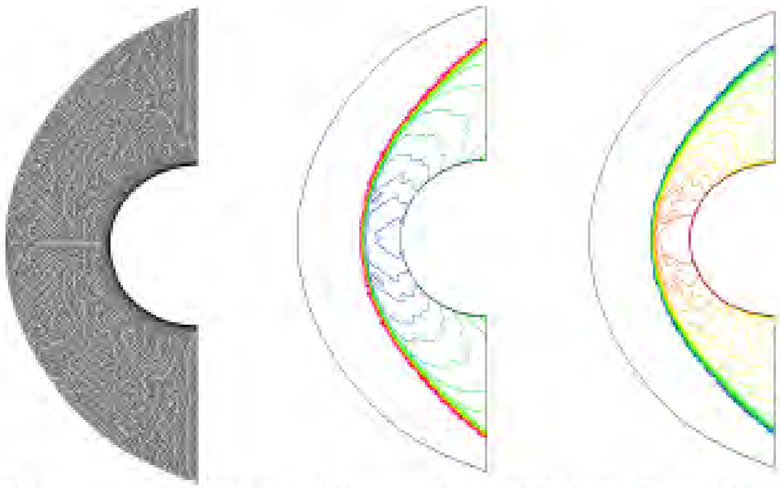




Li Jing

$$M_\infty = 8.03, T_\infty = 124.94K, T_w = 294K, R_e = 1.835 \times 10^5$$

LDG(P1)

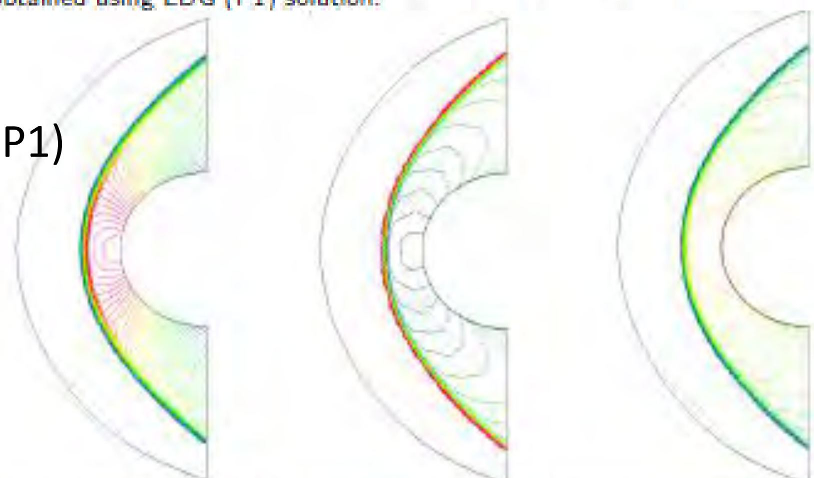


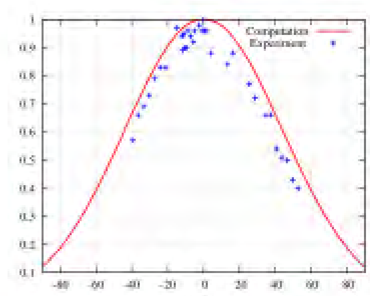
Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. 1, No. 3, pp. 301-318 (2009)

Hong Luo[1,*], Luqing Luo[1] and Kun Xu[2]

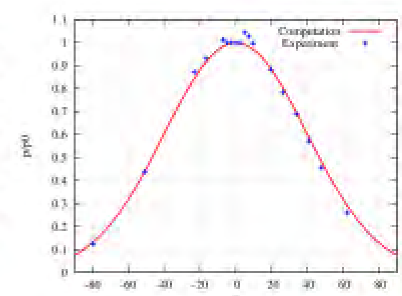
Figure 12: Computed mesh (left), computed Mach number (middle) and temperature (right) contours in the flow field obtained using LDG (P1) solution.

BGKDG(P1)



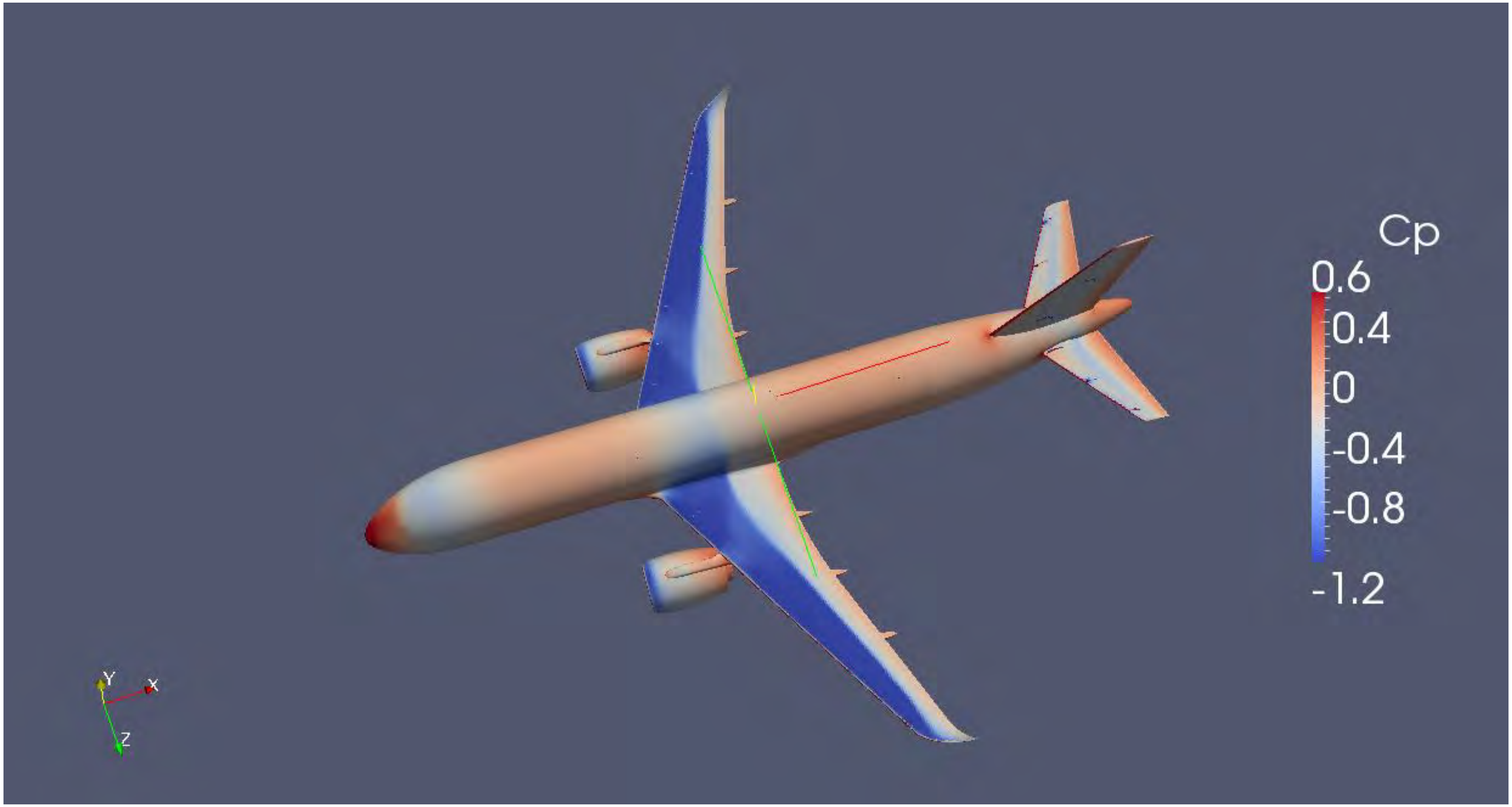


Heat flux



pressure

l: Computed pressure (left), Mach number (middle) and temperature (right) contours in the flow
iined using BGKDG (P1) solution.


Cp
0.6
0.4
0
-0.4
-0.8
-1.2
Y
X
Z

Physical process from a discontinuity (continuum flow regime)

Gas kinetic scheme

Particle free transport

↓

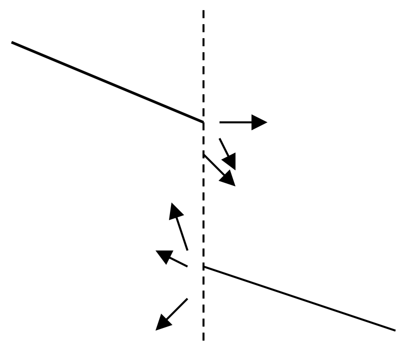
collision

↓

NS

↓

Euler



Godunov method

?

↑

NS

↑ **Riemann solver**

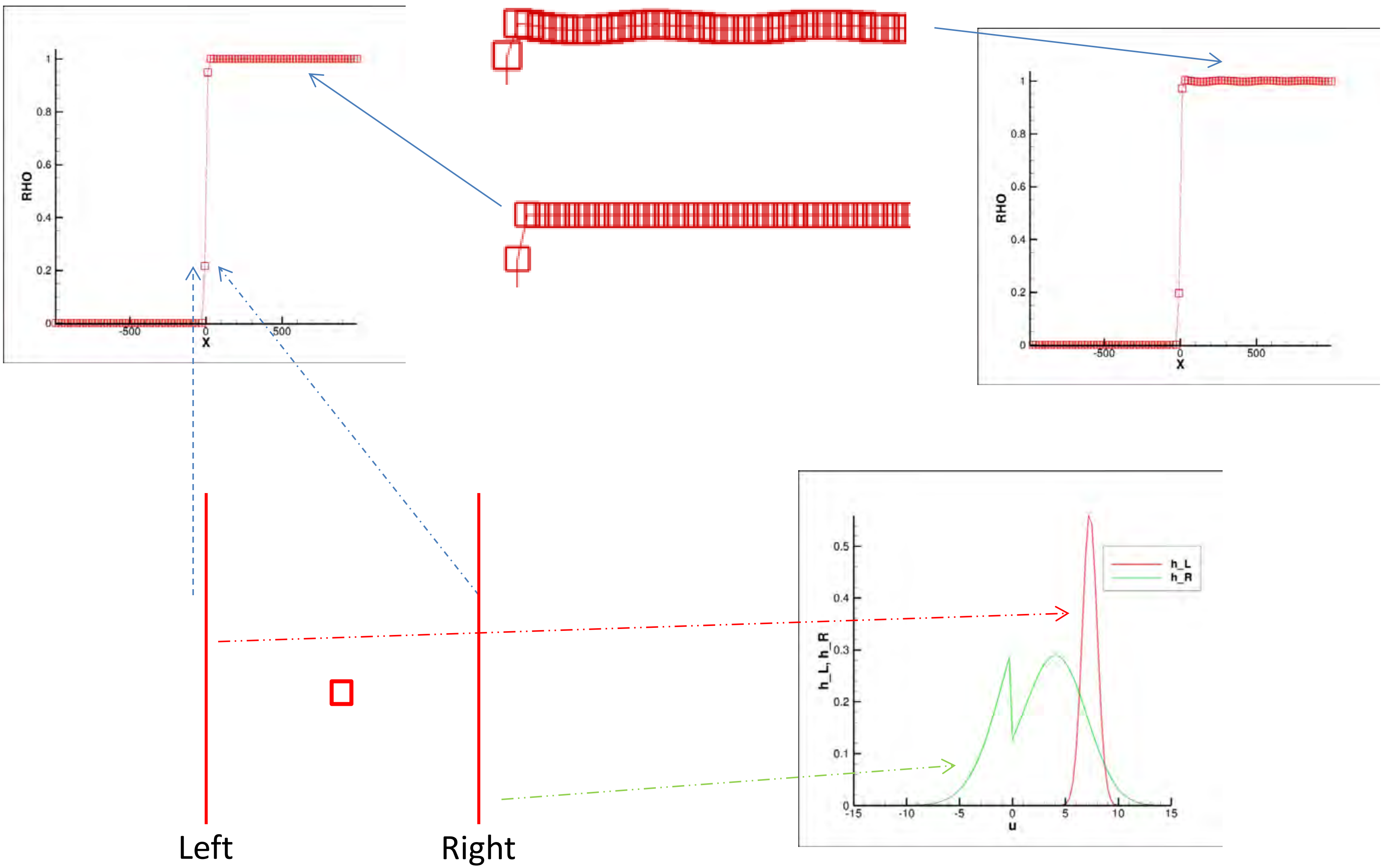
Euler

(infinite number of collisions)

Mach 8 shock wave NS solution (mesh size >> particle mean free path)

GKS

Godunov (inviscid + viscous)

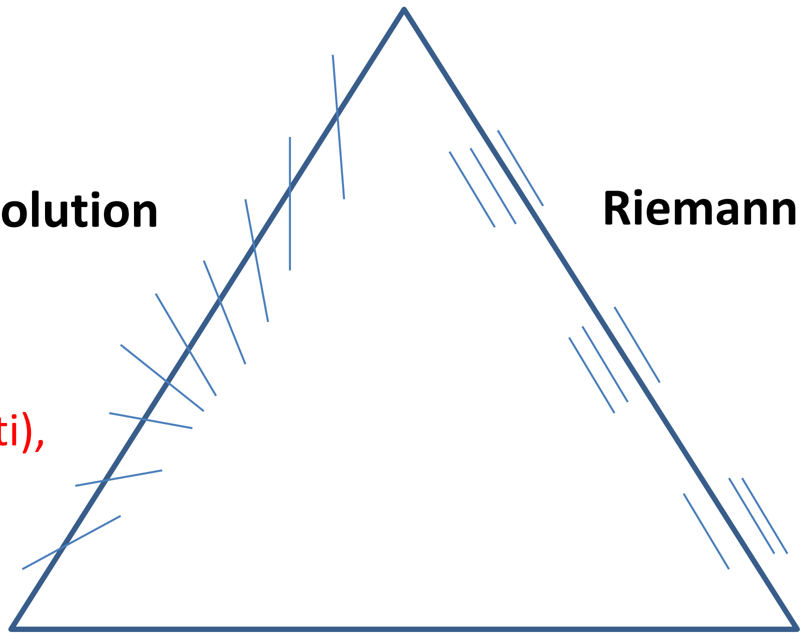


Comparison of gas evolution model

Gas-Kinetic Scheme vs Riemann solver

gas-kinetic evolution

Riemann solver evolution

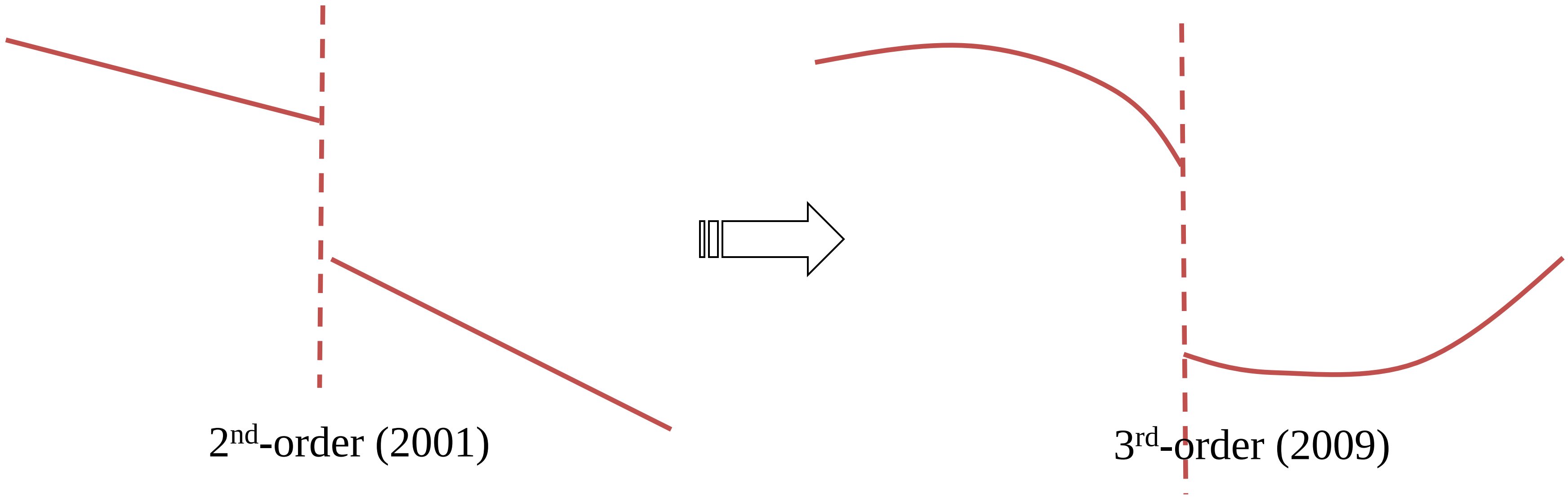


Space & time,
inviscid & viscous,
direction & direction (multi),
kinetic & Hydrodynamic,
are fully coupled !

High-order Gas-kinetic scheme: one step integration along the cell interface.

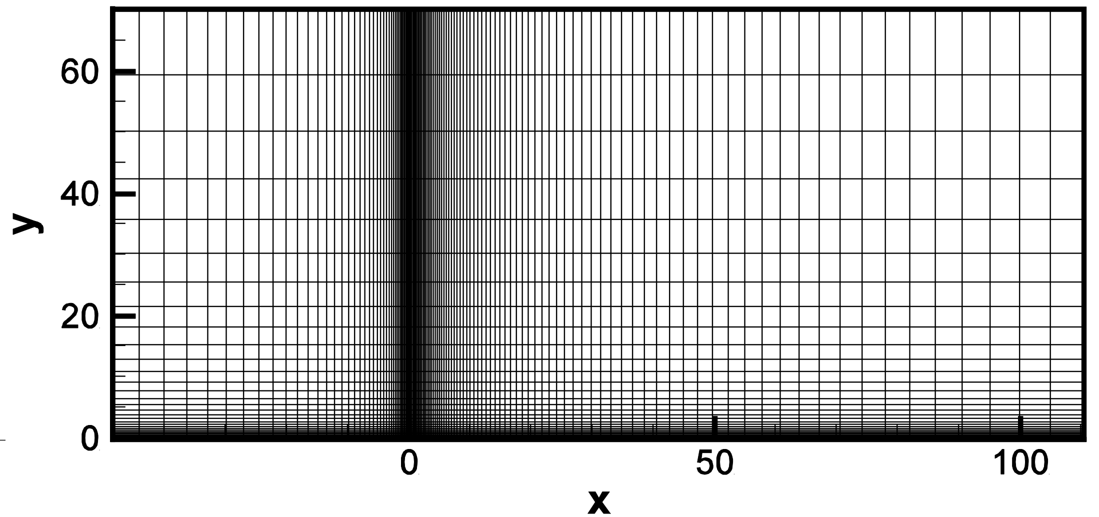
Gauss-points: Riemann solvers for others

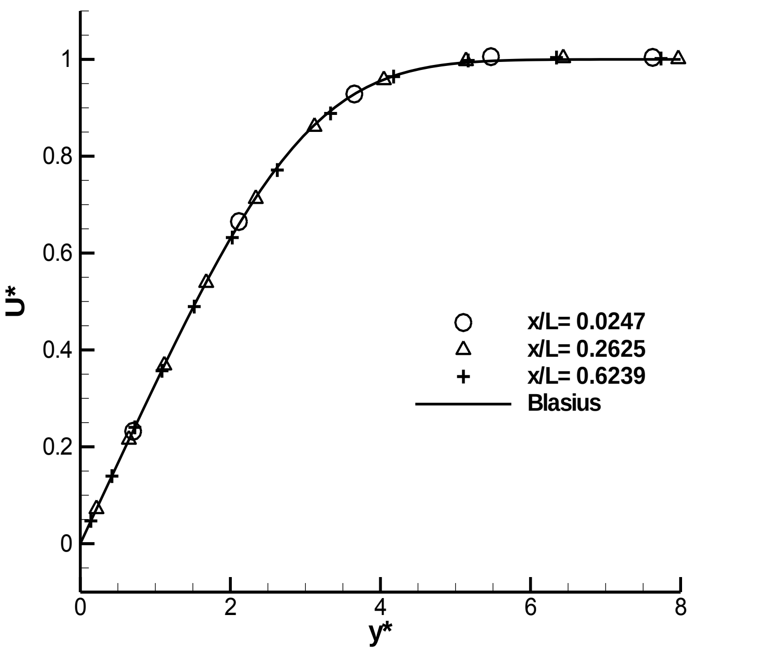
High-order Gas-kinetic Scheme

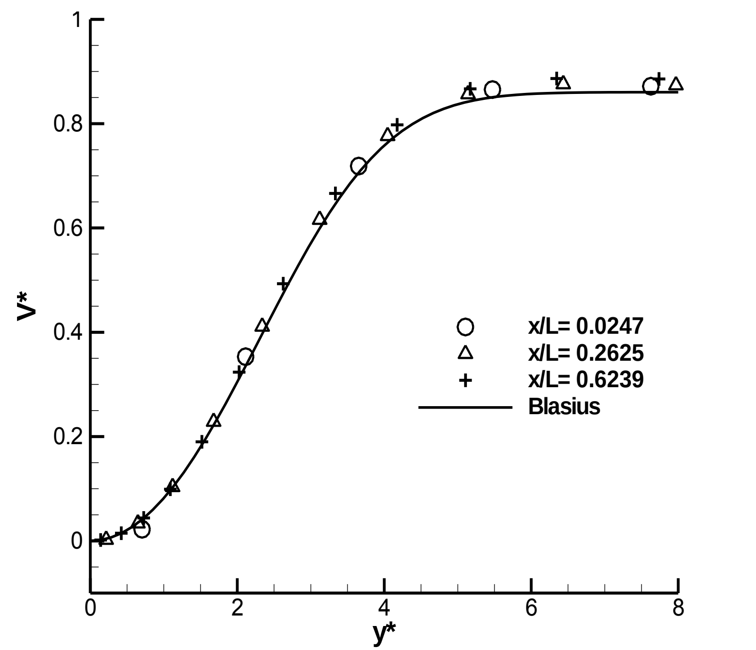


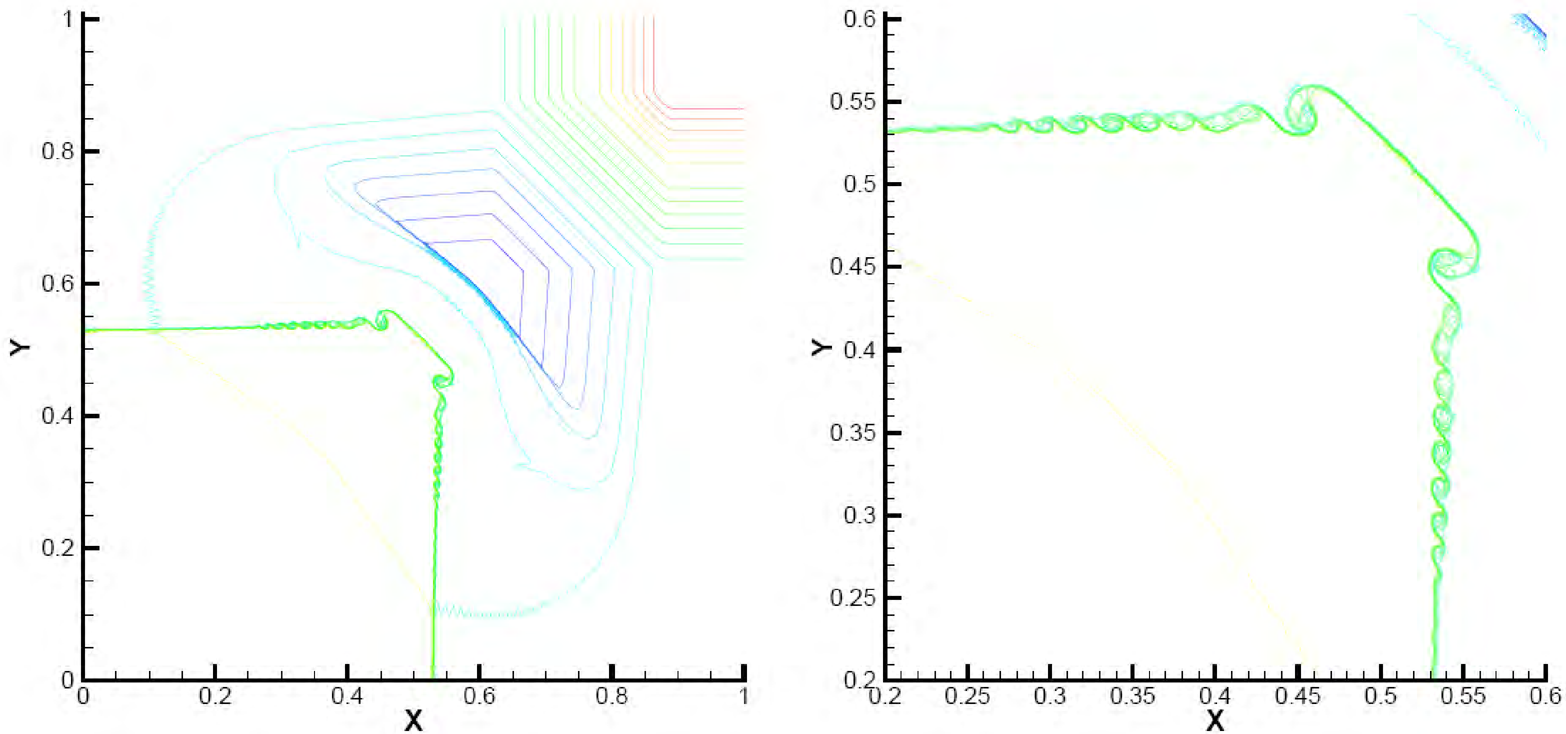
Laminar Boundary Layer

$$Re = 10^5$$







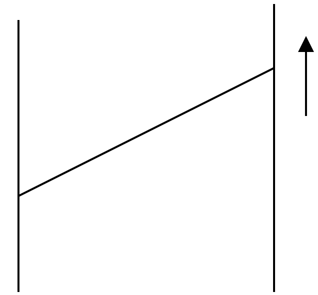


800x800 mesh points

Riemann problem IV

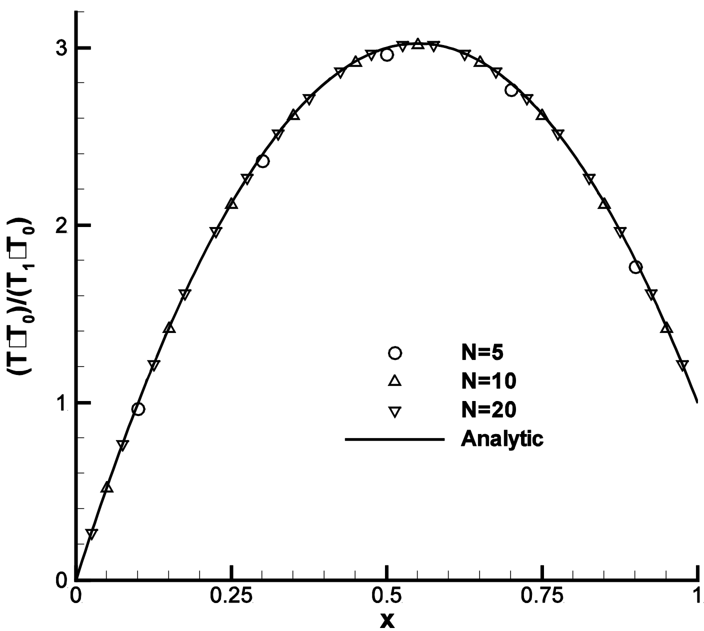
$$(\rho_1,\, U_1,\, V_1,\, p_1) = (1,\, 0.1,\, 0.1,\, 1), \qquad (\rho_2,\, U_2,\, V_2,\, p_2) = (0.5197,\, -0.6259,\, 0.1,\, 0.4),$$
$$(\rho_3,\, U_3,\, V_3,\, p_3) = (0.8,\, 0.1,\, 0.1,\, 0.4), \quad (\rho_4,\, U_4,\, V_4,\, p_4) = (0.5197,\, 0.1,\, -0.6259,\, 0.4).$$

Couette Flow with a Temperature Gradient

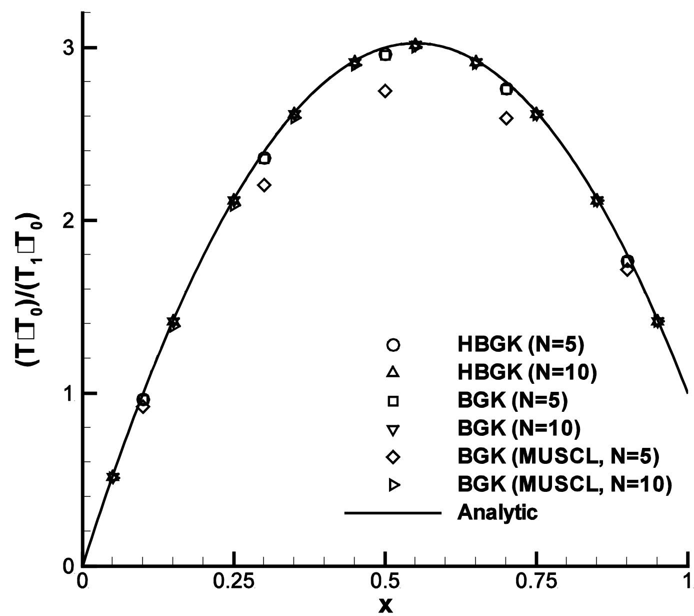


Exact solution: $$\frac{T-T_0}{T_1-T_0}=\frac{x}{H}+\frac{\Pr Ec}{2}\frac{x}{H}\left(1-\frac{x}{H}\right)$$

$$H = 1,\ \mu = 5\times 10^{-3},\ \Pr = 2/3,\ Ec = U^2/C_P(T_1 - T_0) = 20,\ M = 0.1$$



Convergence Study



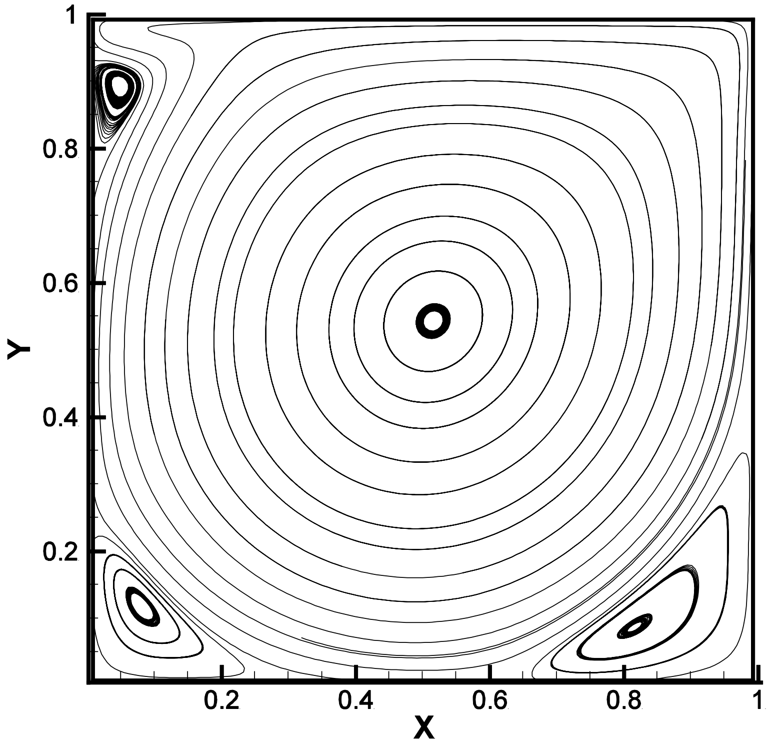
Different schemes

Based on the same 5^{th} WENO reconstruction

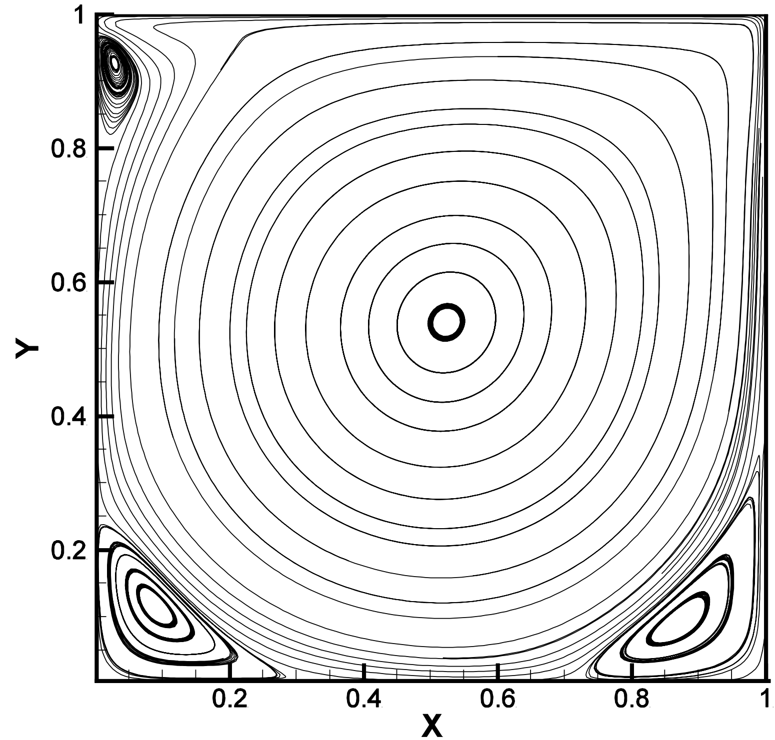
numerical results comparison between

Traditional WENO scheme (characteristic splitting)
WENO-GKS (gas-kinetic evolution model)

Cavity Flow at Re=3200 with 65 x 65 mesh points

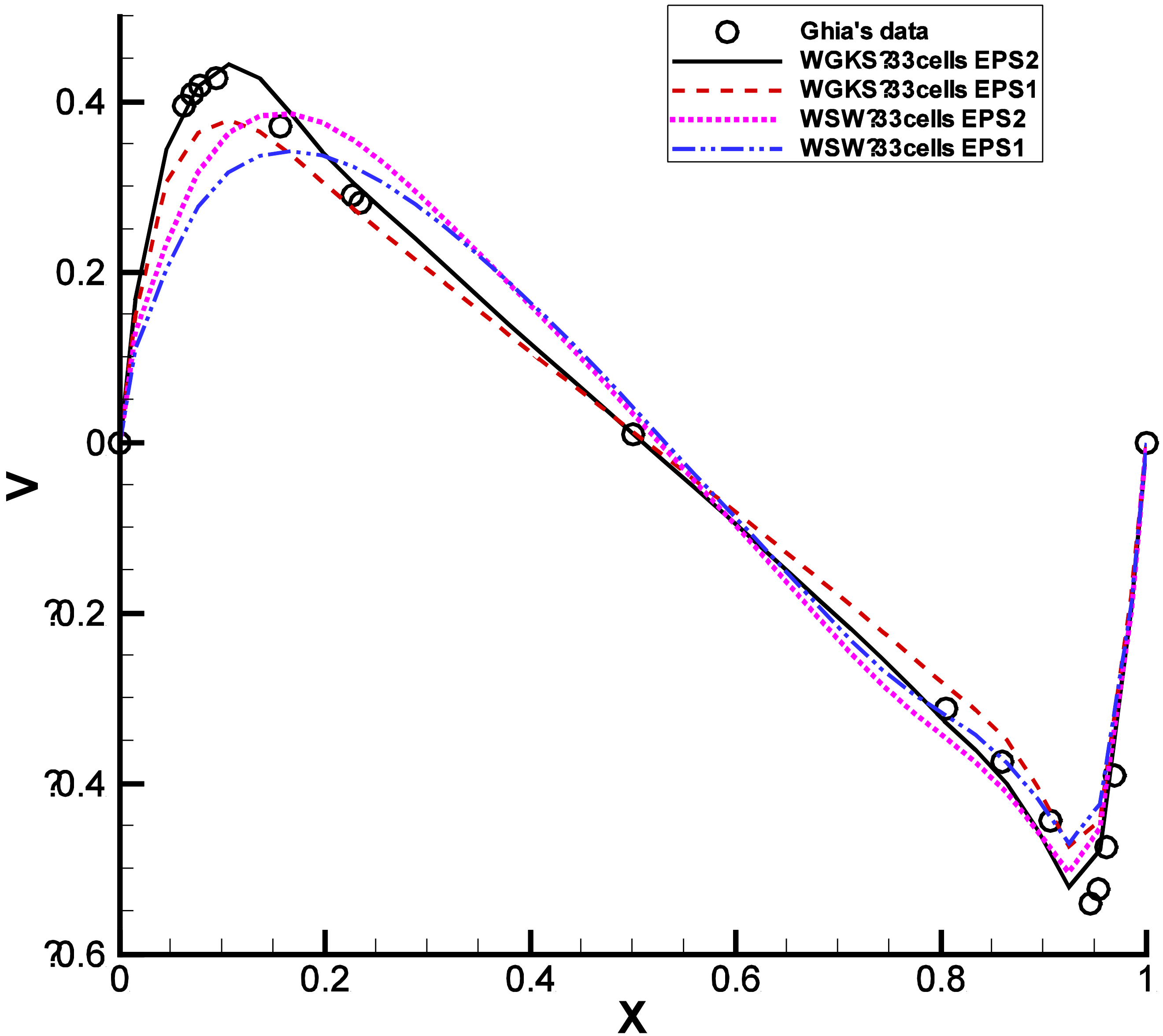


GKS

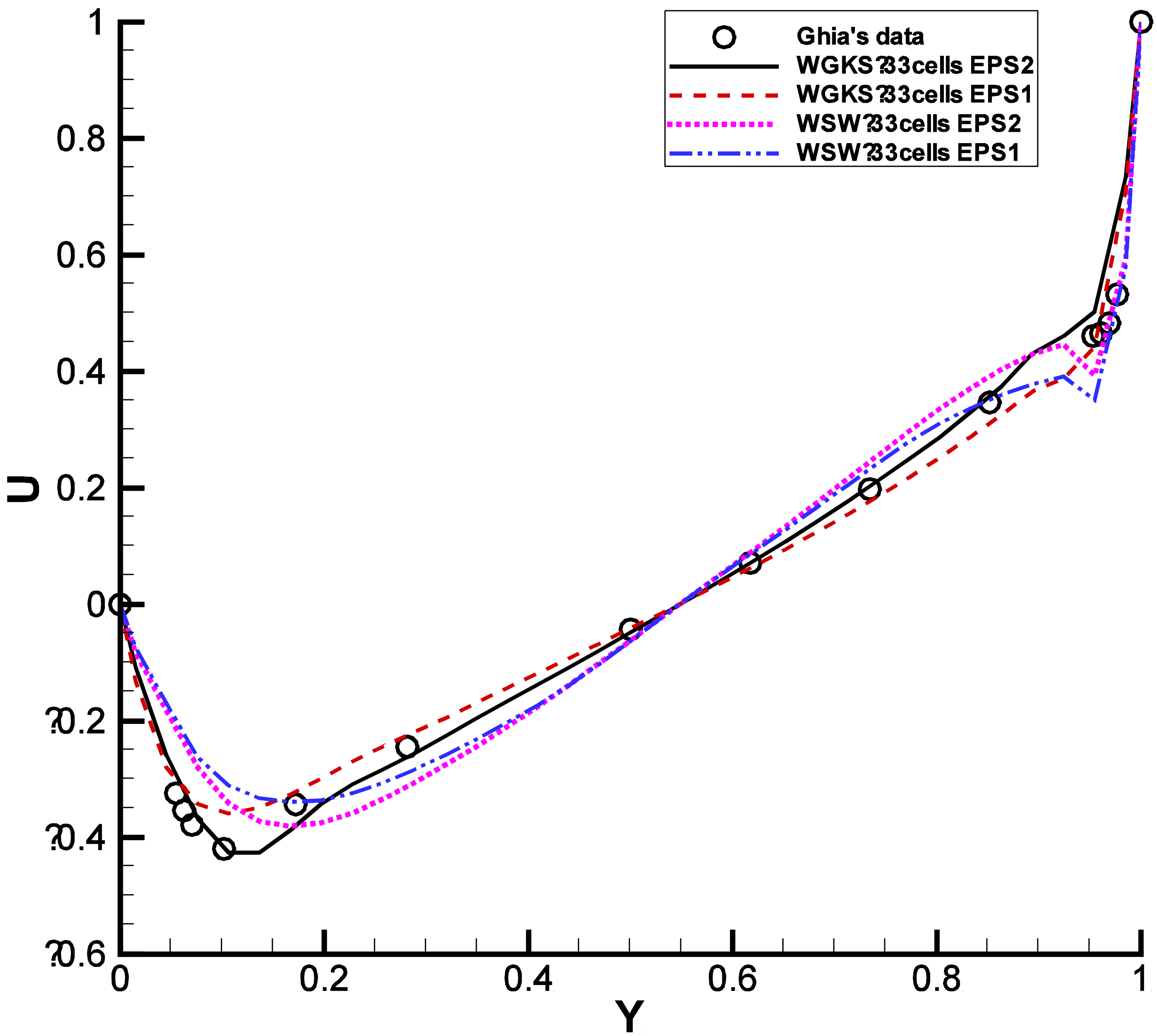


WENO-5

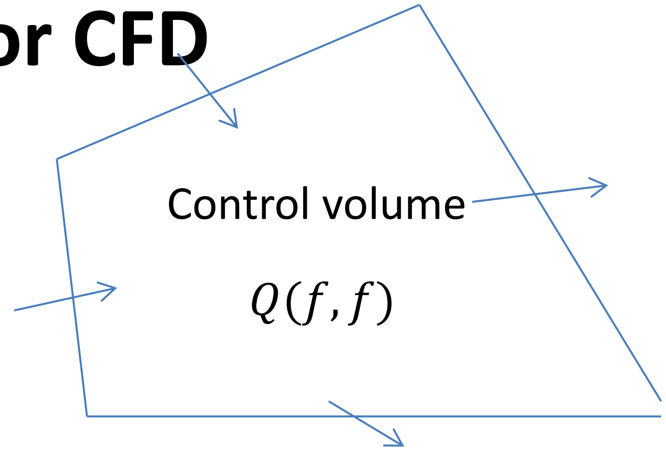
33x33 mesh points



33x33 mesh points



Direct Modeling for CFD



$\Delta x \not\to 0, \quad \Delta t \not\to 0$

Governing equations in discretized space:

micro

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

macro

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

+ Modeling the physical process

hydrodynamic

kinetic

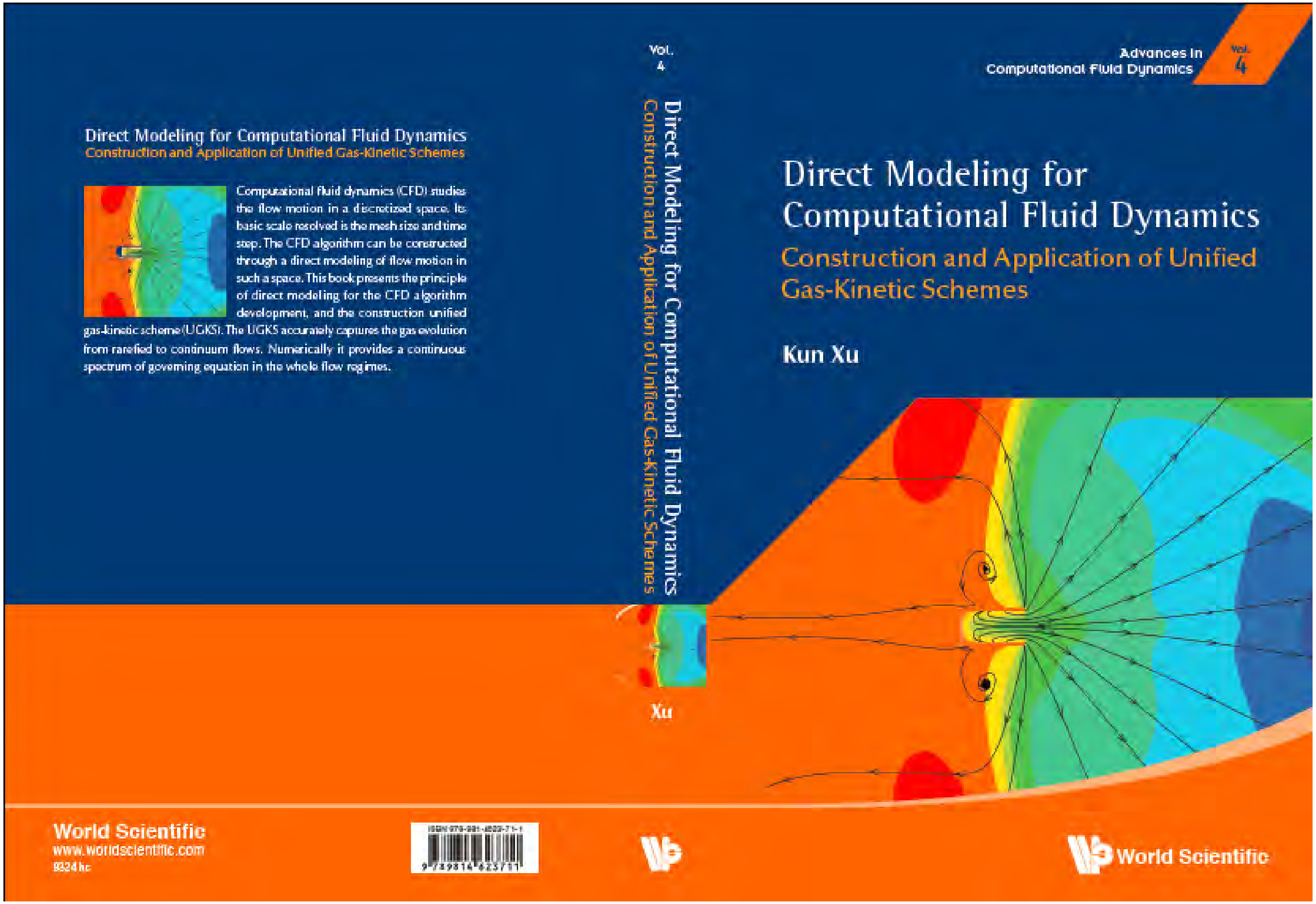
$$f(x,y,t,u,v,\xi) = \frac{1}{\tau}\int_0^t g(x',y',t',u,v,\xi)e^{-(t-t')/\tau}dt' + e^{-t/\tau}f_0(x-ut, y-vt)$$

Current Research Topics & Conclusion

- **Neutron and radiation transports,**
- **Plasma simulation**
- **Non-equilibrium thermodynamics**

  (use UGKS as a tool to explore …, such as checking *Onsager reciprocal relations*)
- **…**
- **UGKS is very effective to get numerical solutions for multiscale transport process**

Thanks !


Direct Modeling for Computational Fluid Dynamics
Construction and Application of Unified Gas-Kinetic Schemes
Computational fluid dynamics (CFD) studies the flow motion in a discretized space. Its basic scale resolved is the mesh size and time step. The CFD algorithm can be constructed through a direct modeling of flow motion in such a space. This book presents the principle of direct modeling for the CFD algorithm development, and the construction unified gas-kinetic scheme (UGKS). The UGKS accurately captures the gas evolution from rarefied to continuum flows. Numerically it provides a continuous spectrum of governing equation in the whole flow regimes.
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Direct Modeling for Computational Fluid Dynamics
Construction and Application of Unified Gas-Kinetic Schemes
Xu
Advances in Computational Fluid Dynamics
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Construction and Application of Unified Gas-Kinetic Schemes
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