Direct Modeling for Computational Fluid Dynamics and Unified Gas-kinetic Scheme

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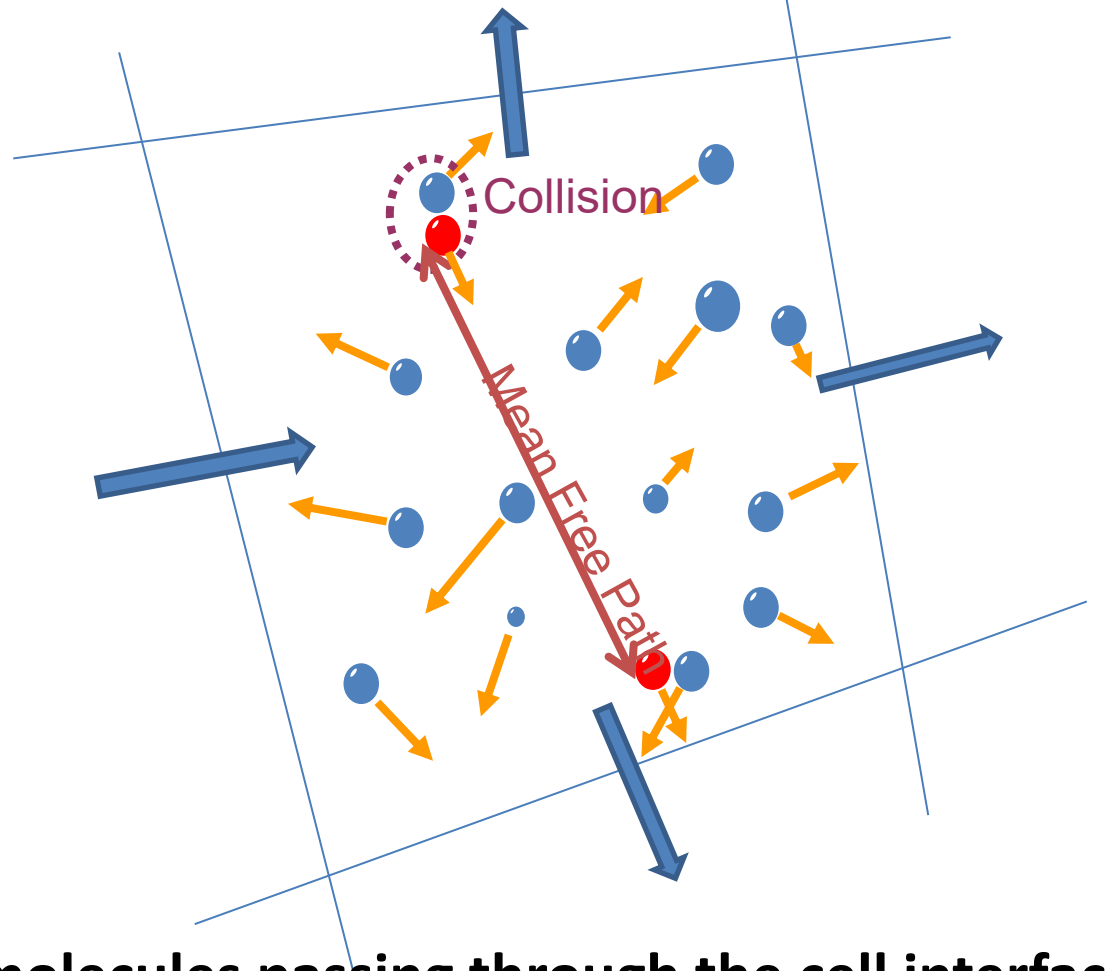
Contents

- The direct modeling in gas-kinetic scheme (GKS) for continuum and rarefied flows
- Examples
- Remarks on CFD method again
- Conclusion

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

Fundamental Physical Laws in Discretized Space

f : gas distribution function,

W : conservative macroscopic variables

governing equations (micro):

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

governing equations (macro):

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

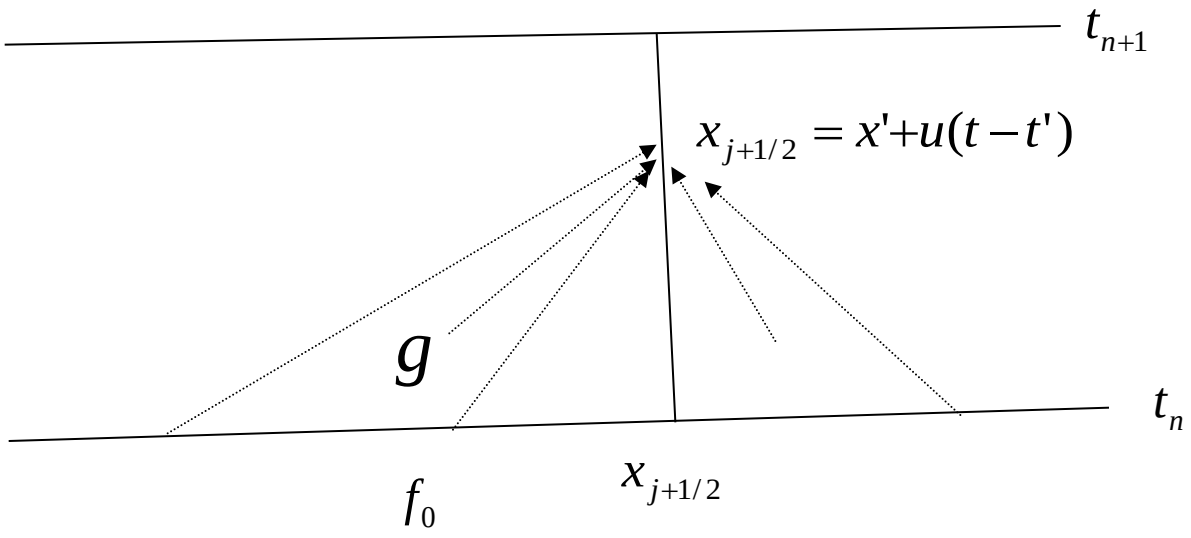
For the update of conservative flow variables, we only need to know the fluxes across a cell interface!

PDE-based modeling: use PDE's local solution to model the physical process of gas molecules passing through the cell interface

The physical modeling of particles distribution function at a cell interface

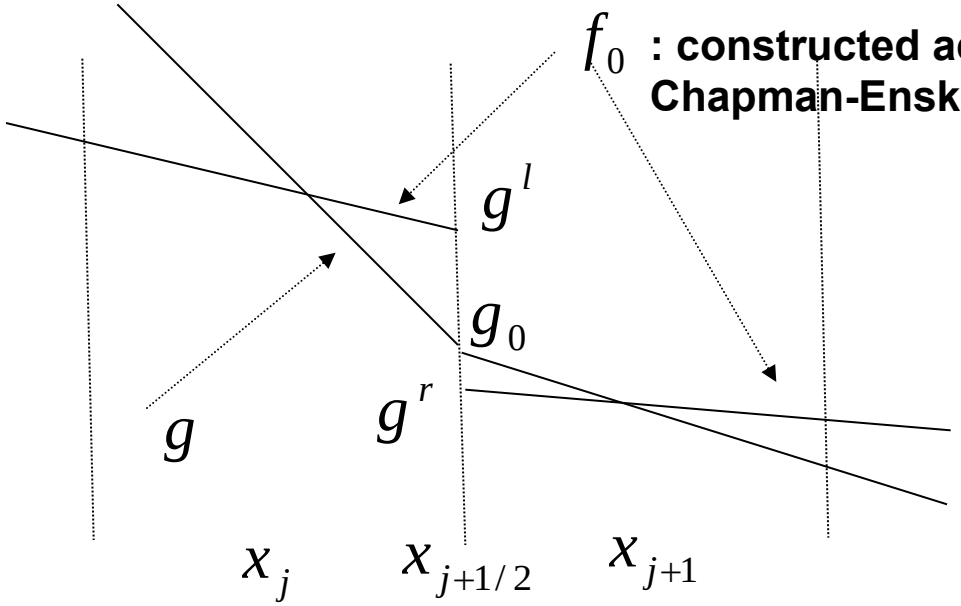
$$f(x_{j+1/2}, t, u, v, \xi) = \frac{1}{\tau}\int_0^t g(x', t', u, v, \xi)e^{-(t-t')/\tau}dt' + e^{-t/\tau}f_0(x_{j+1/2} - ut)$$

where $x' = x_{j+1/2} - u(t - t')$ is the particle trajectory.



Previous approach for continuum flows

(*ignore small scale non-equilibrium effect*)



Unified Gas-kinetic Scheme (UGKS)

(Be able to capture equilibrium and non-equilibrium flow distributions in different domains)

UGKS Scheme:

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:

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

$$= \tilde{g}_{j+1/2,k} + \tilde{f}_{j+1/2,k}$$

No need to use Chapman-Enskog expansion

Updated (UGKS)

where $\tilde{g}_{j+1/2,k}$ can be evaluated using continuum particle velocity space (same as kinetic-NS), and $\tilde{f}_{j+1/2,k}$ is evaluated in a discretized velocity space.

Update of conservative variables (marco):

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

UGKS Numerical Steps

(micro-scale)

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

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

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:

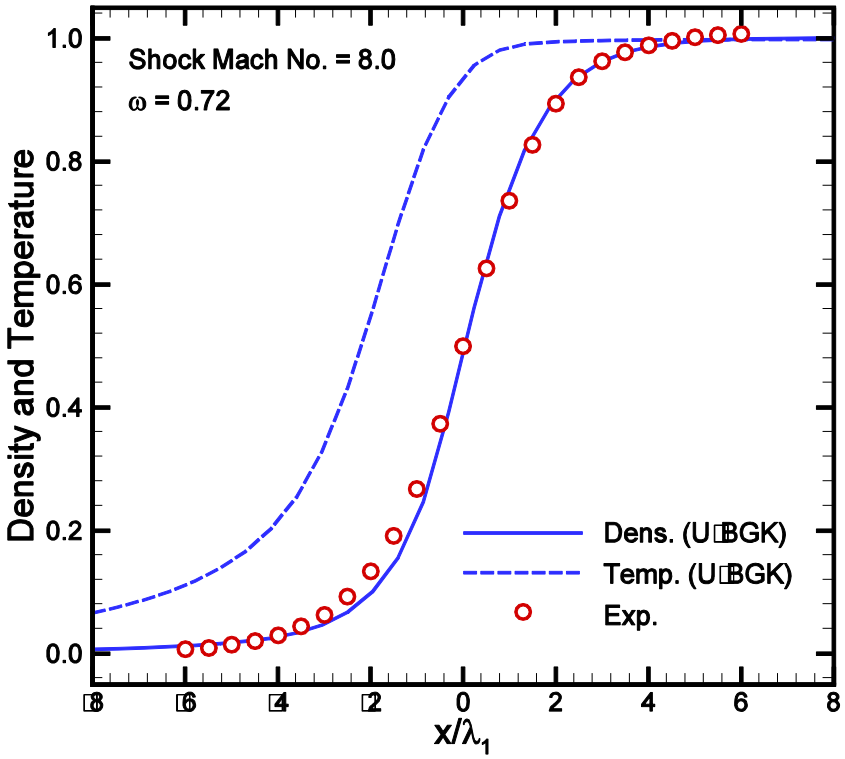
$$\left(1 + \frac{\Delta t}{2\tau_j^{n+1}}\right) f_{j,k}^{n+1} = f_{j,k}^{n} + \frac{1}{\Delta x}\left(\int_{t^n}^{t^{n+1}} u_k(\tilde{g}_{j-1/2,k} - \tilde{g}_{j+1/2,k})dt + \int_{t^n}^{t^{n+1}} u_k(\tilde{f}_{j-1/2,k} - \tilde{f}_{j+1/2,k})dt \right)$$

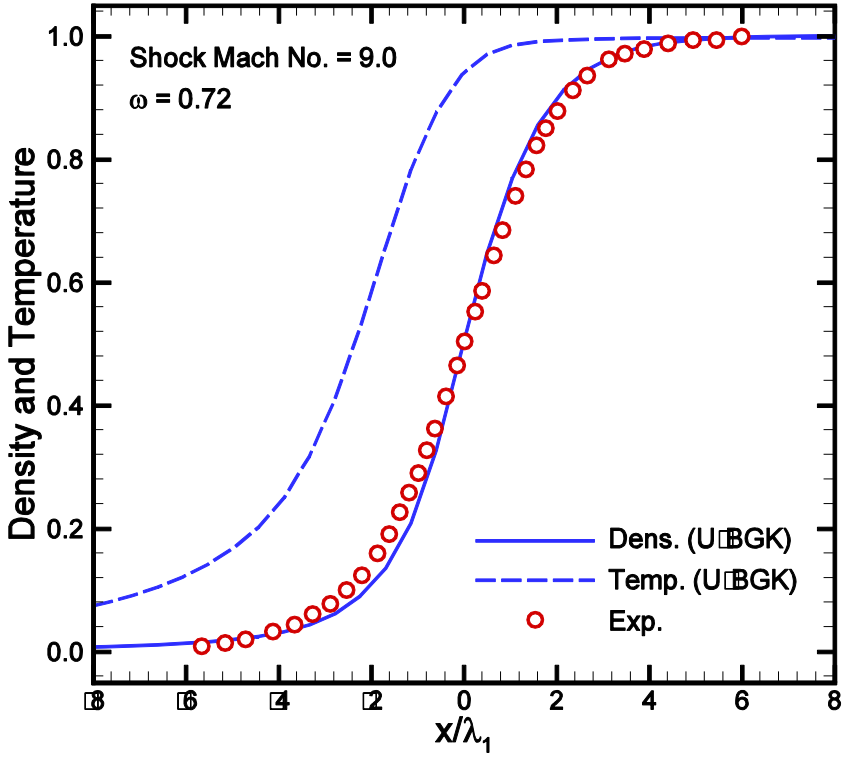
$$+ \frac{\Delta t}{2}\left(\frac{g_{j,k}^{n+1}}{\tau_j^{n+1}} + \frac{g_{j,k}^{n} - f_{j,k}^{n}}{\tau_j^{n}} \right)$$

shock structure calculations

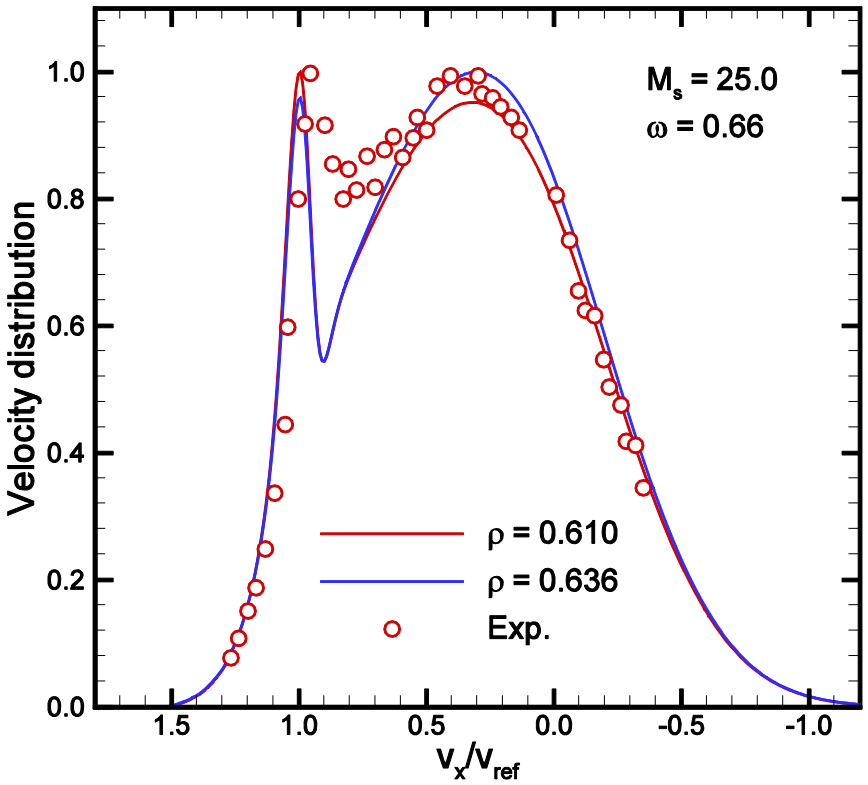
Mach 8 and 9 argon shock structure vs. experiments

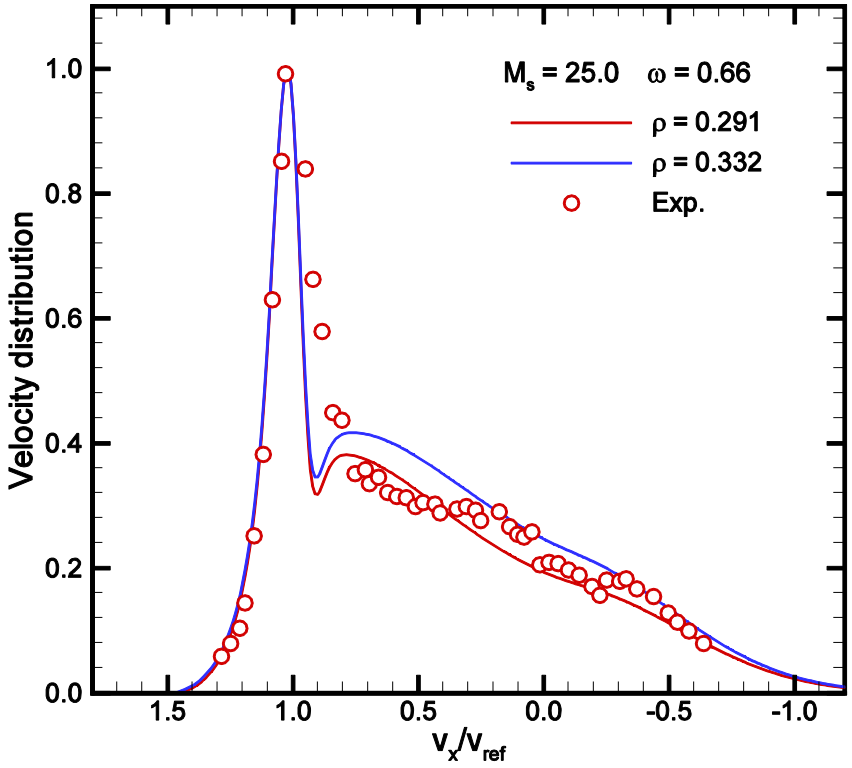
$$\mu \sim T^{\omega}$$

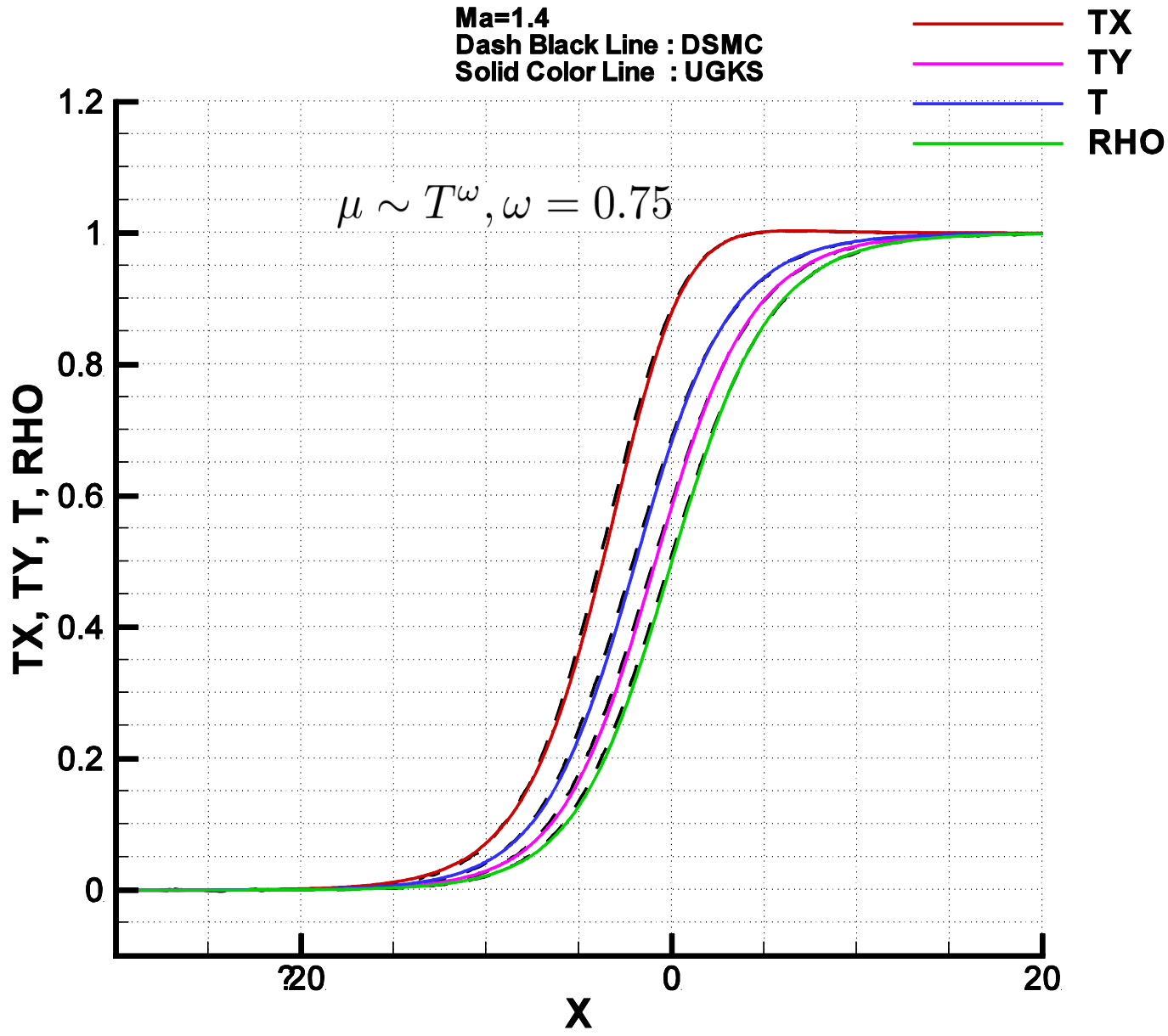


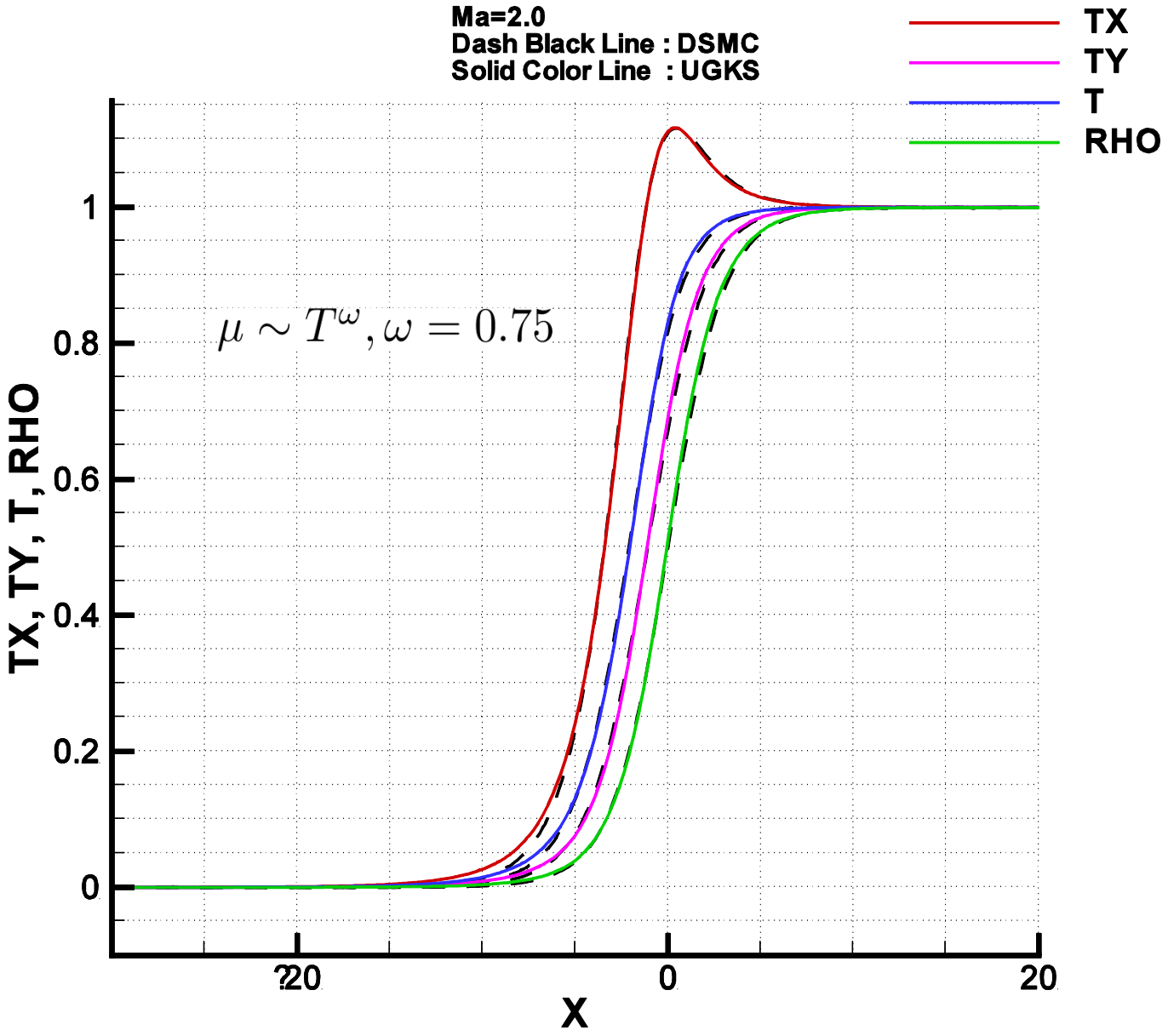


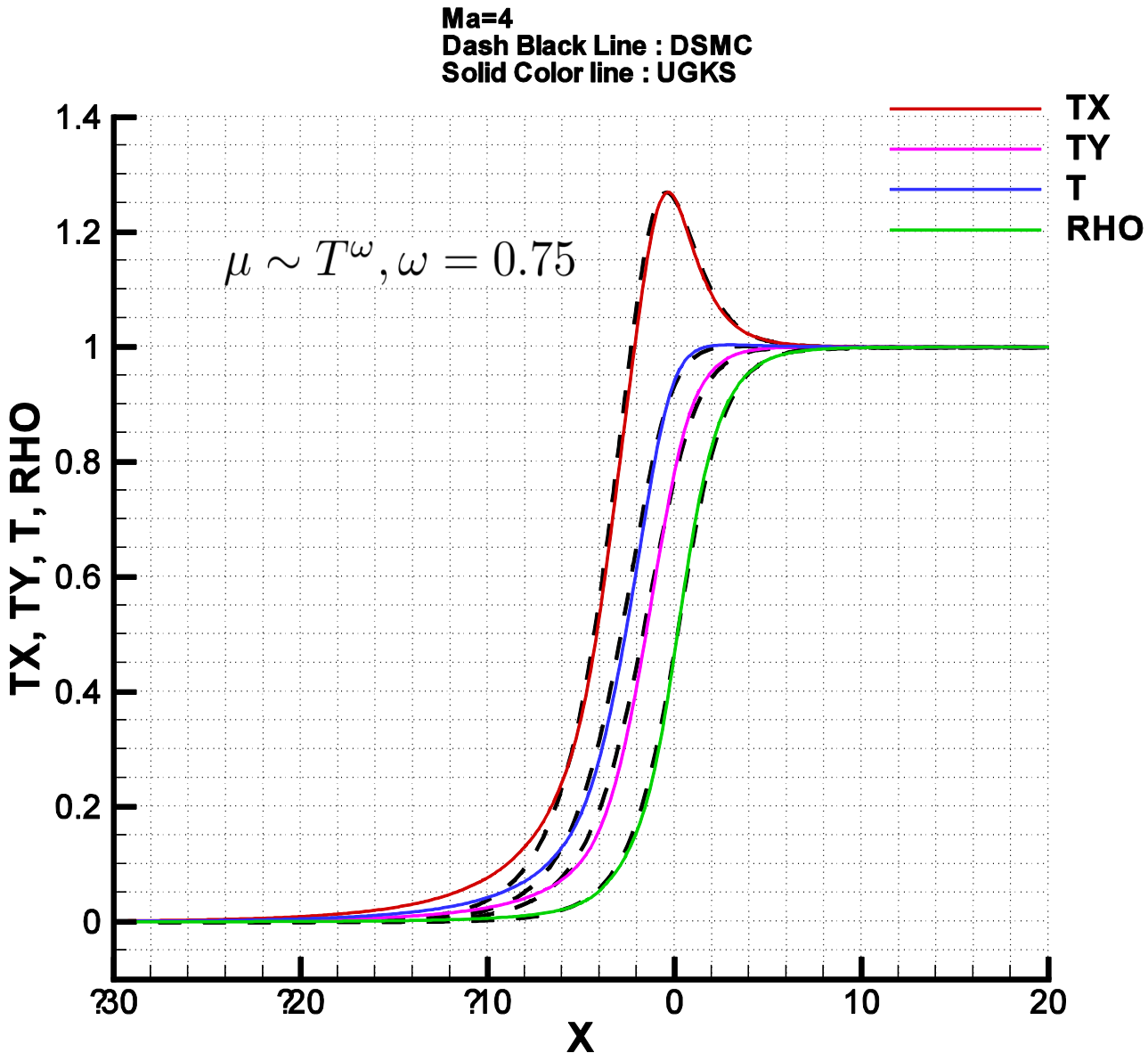
Distribution functions inside M=25 helium shock structure

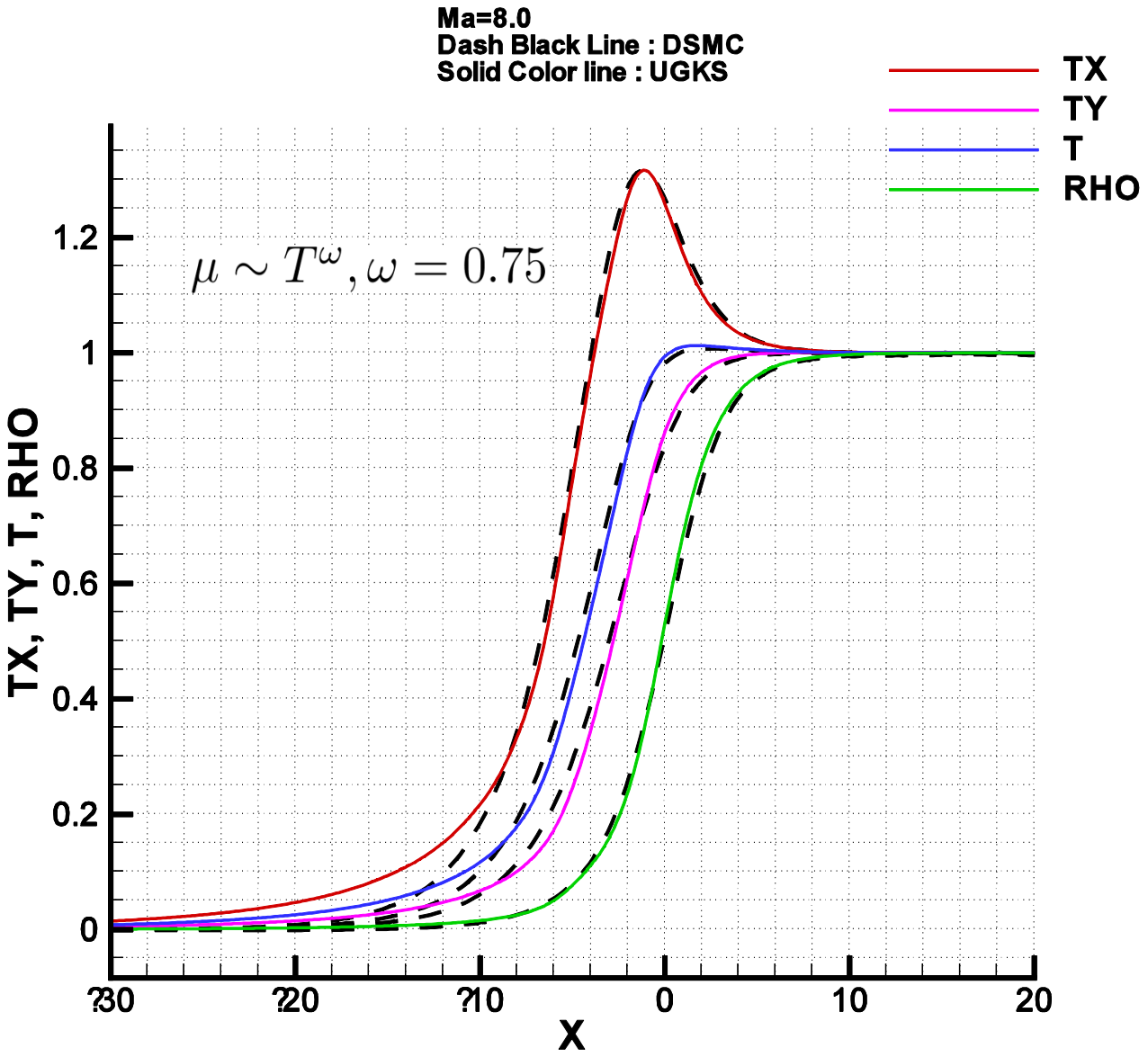





Ma=1.4
Dash Black Line : DSMC
Solid Color Line : UGKS
TX
TY
T
RHO
$\mu \sim T^{\omega}, \omega = 0.75$
TX, TY, T, RHO
1.2
1
0.8
0.6
0.4
0.2
0
-20
0
20
X

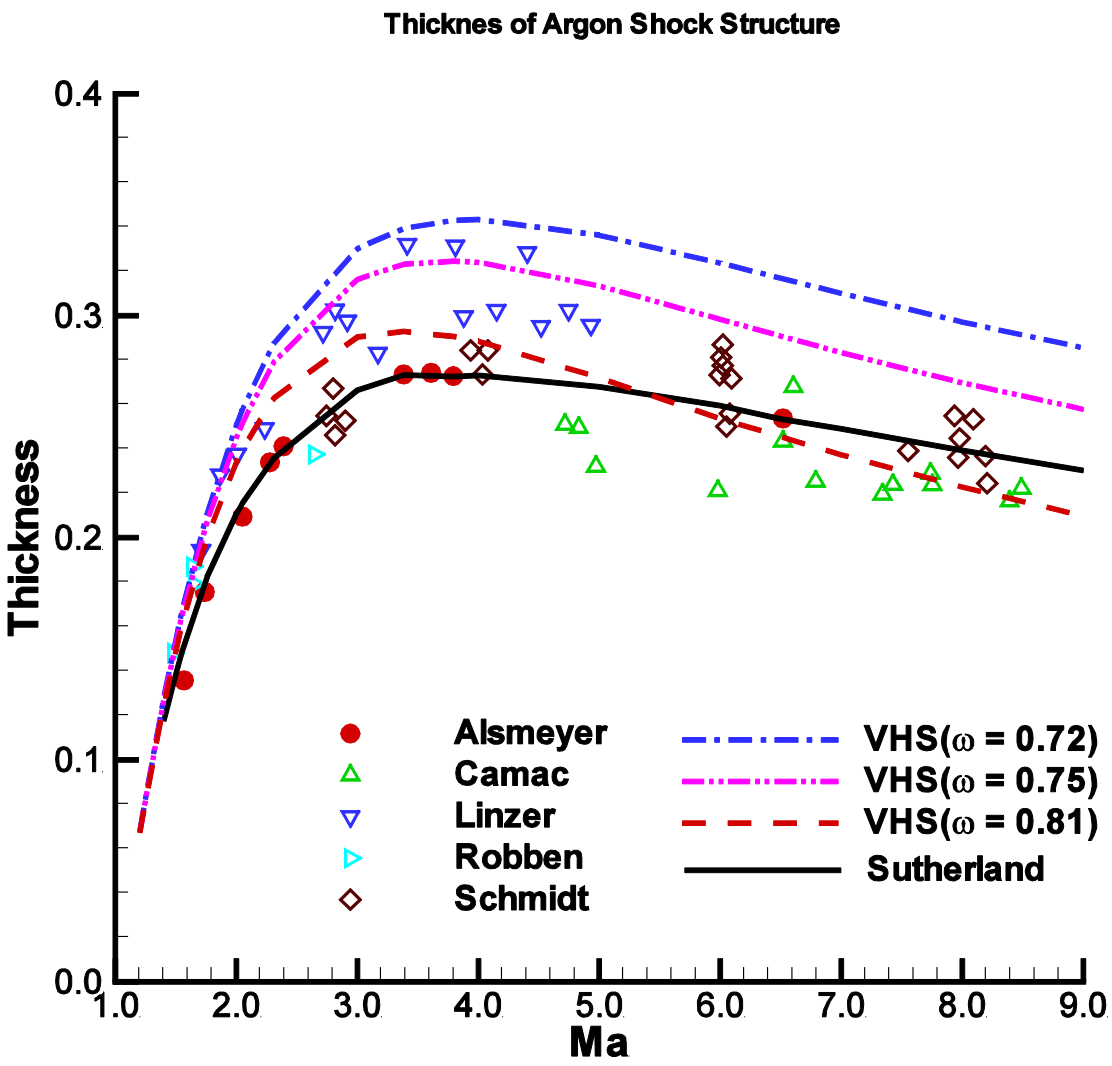

Ma=2.0
Dash Black Line : DSMC
Solid Color Line : UGKS
TX
TY
T
RHO
$\mu \sim T^{\omega}, \omega = 0.75$
TX, TY, T, RHO
1
0.8
0.6
0.4
0.2
0
-20
0
20
X

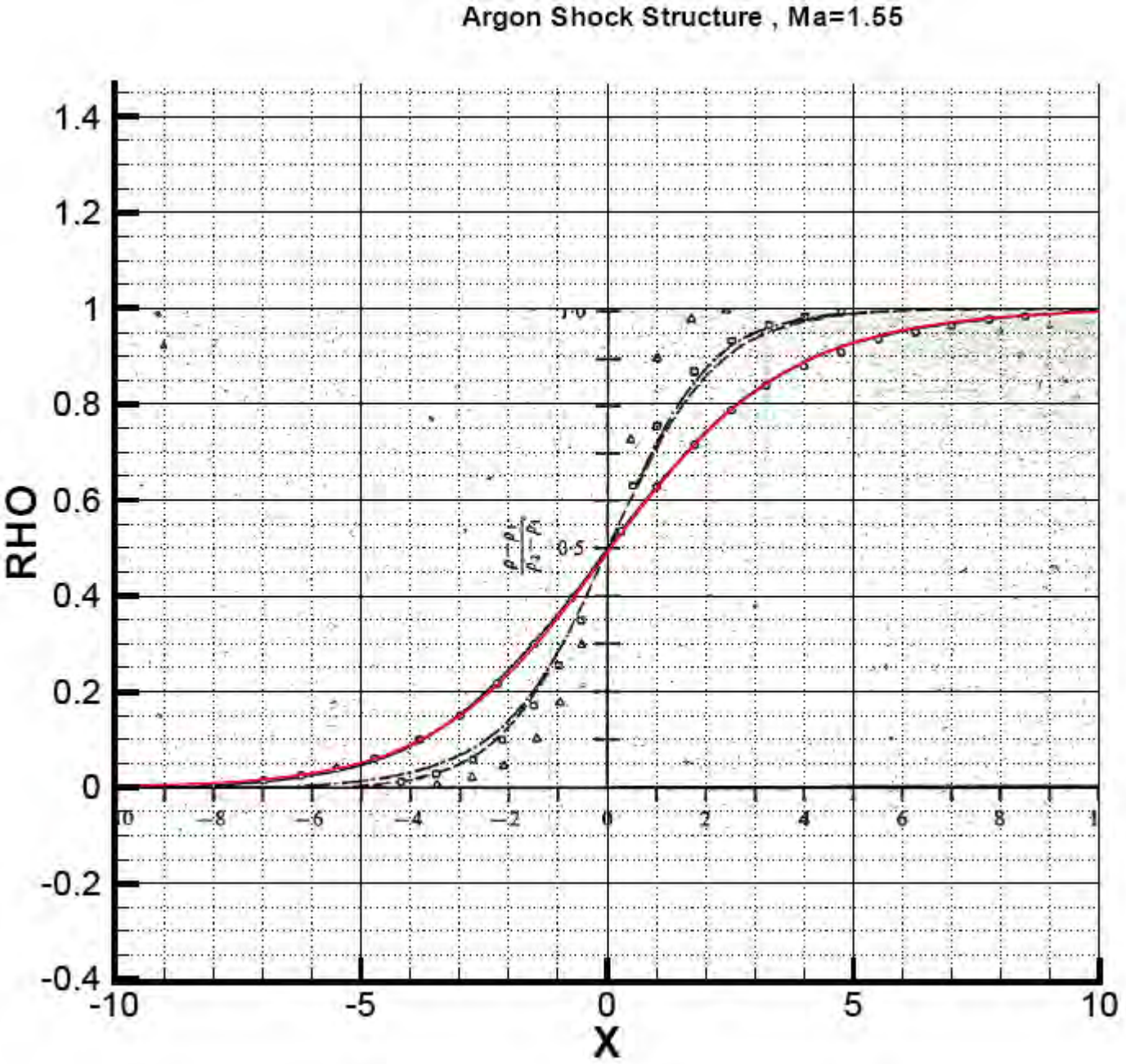

Ma=4
Dash Black Line : DSMC
Solid Color line : UGKS
$\mu \sim T^{\omega}, \omega = 0.75$
TX
TY
T
RHO
TX, TY, T, RHO
X
1.4
1.2
1
0.8
0.6
0.4
0.2
0
?30
?20
?10
0
10
20


Ma=8.0
Dash Black Line : DSMC
Solid Color line : UGKS
TX
TY
T
RHO
$\mu \sim T^{\omega}, \omega = 0.75$
TX, TY, T, RHO
1.2
1
0.8
0.6
0.4
0.2
0
?30
?20
?10
0
10
20
X

Shock thickness: Sutherland

$$\tau = \mu_s / p$$



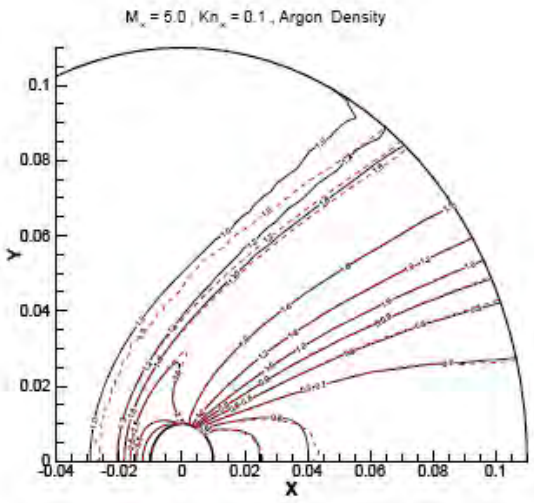

Argon Shock Structure , Ma=1.55
RHO
X
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-10
-5
0
5
10

Deduced experimental inflow conditions

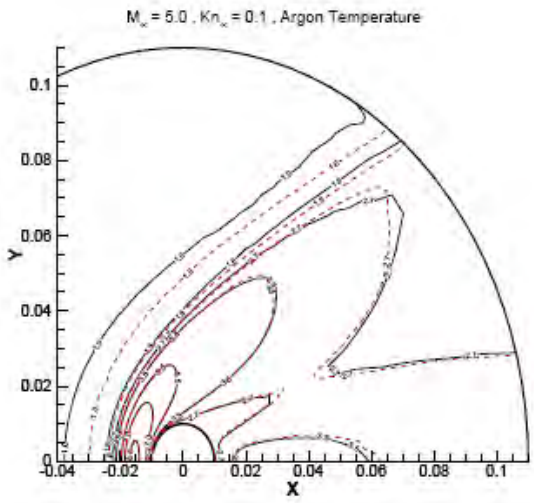
Ma	T_norm	upstream T	downstream T
1.40	1.39	120.00	167.02
1.50	1.49	120.00	179.38
1.55	1.55	120.00	185.73
1.76	1.78	120.00	213.90
2.00	2.08	120.00	249.38
2.05	2.14	120.00	257.24
2.31	2.51	120.00	300.89
3.00	3.67	120.00	440.00
3.38	4.43	120.00	531.45
3.80	5.37	120.00	644.94
4.00	5.86	110.00	644.96
5.00	8.68	100.00	868.00
6.00	12.12	95.00	1151.38
6.50	14.07	92.00	1294.78
7.00	16.18	90.00	1456.53
8.00	20.87	82.00	1711.51
9.00	26.19	77.00	2016.26

Flow passing through a cylinder

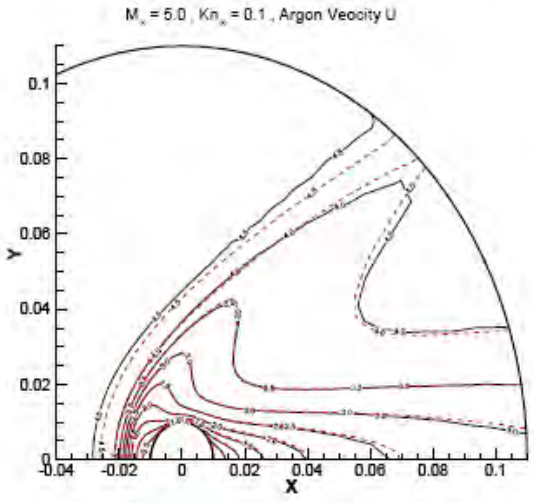
M=5.0, Kn=0.1



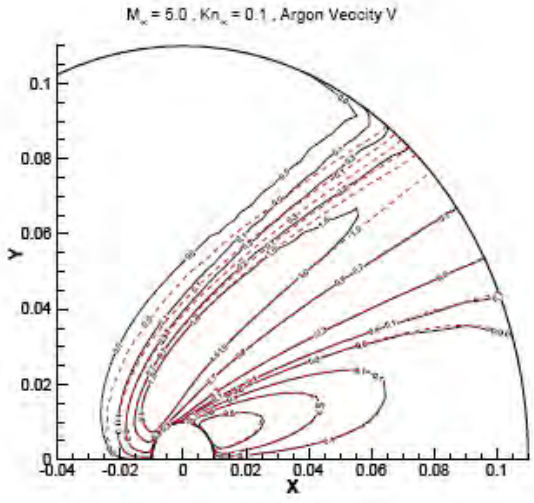
(a)



(b)

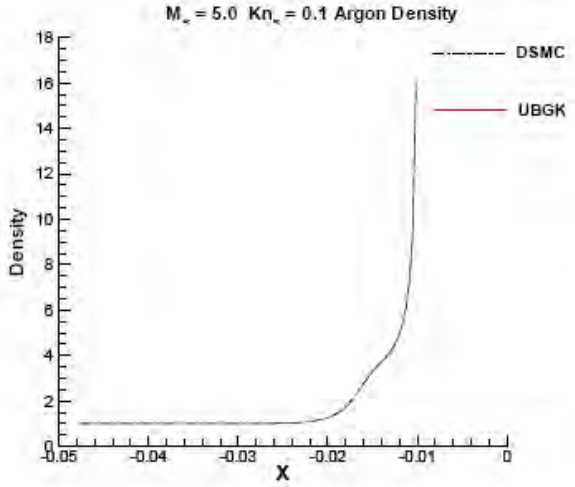


(c)

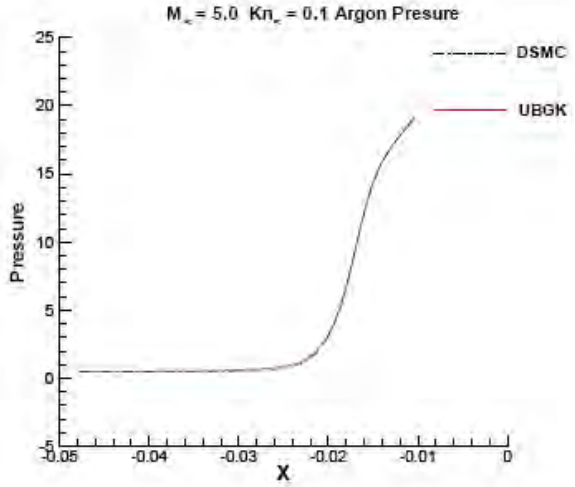


(d)

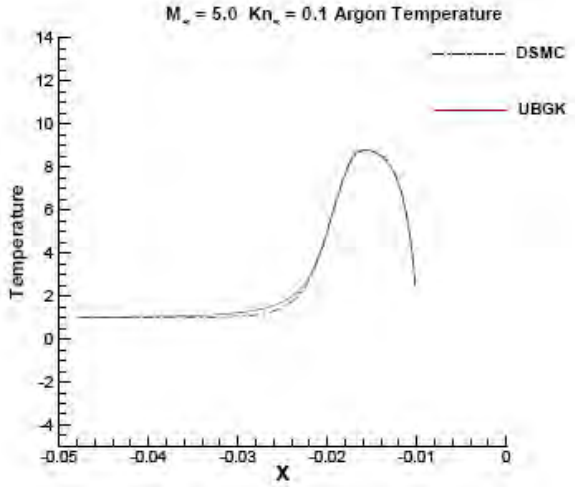
DSMC solution provided by Q.H. Sun


M∞ = 5.0 Kn∞ = 0.1 Argon Density
DSMC
UBGK
Density
X

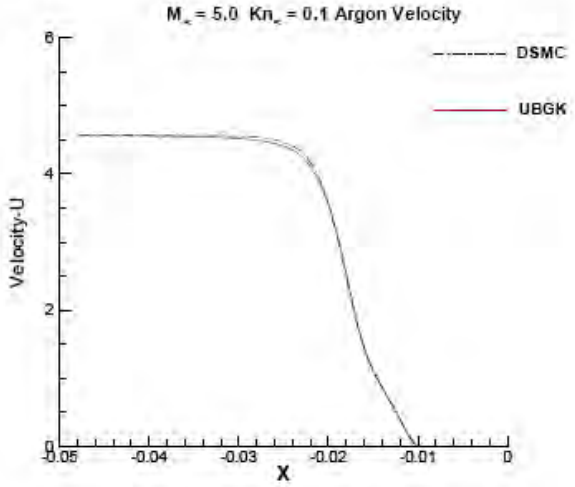
(a)


M∞ = 5.0 Kn∞ = 0.1 Argon Presure
DSMC
UBGK
Pressure
X

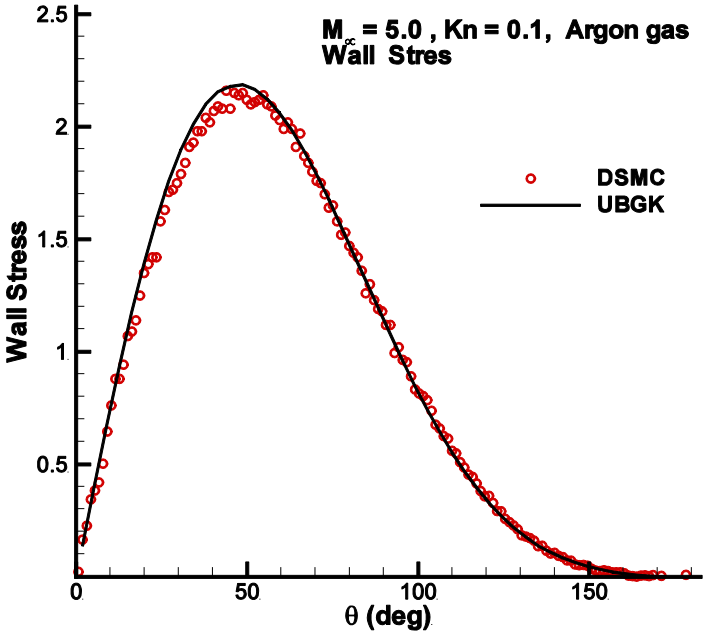
(b)

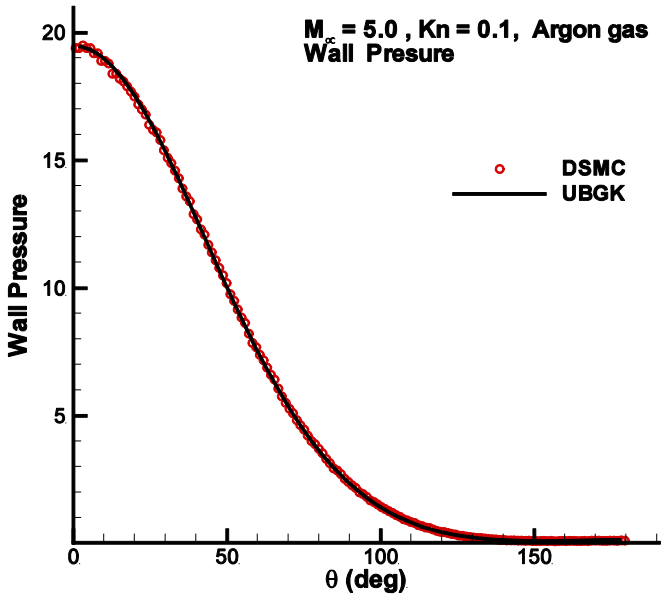

M∞ = 5.0 Kn∞ = 0.1 Argon Temperature
DSMC
UBGK
Temperature
X

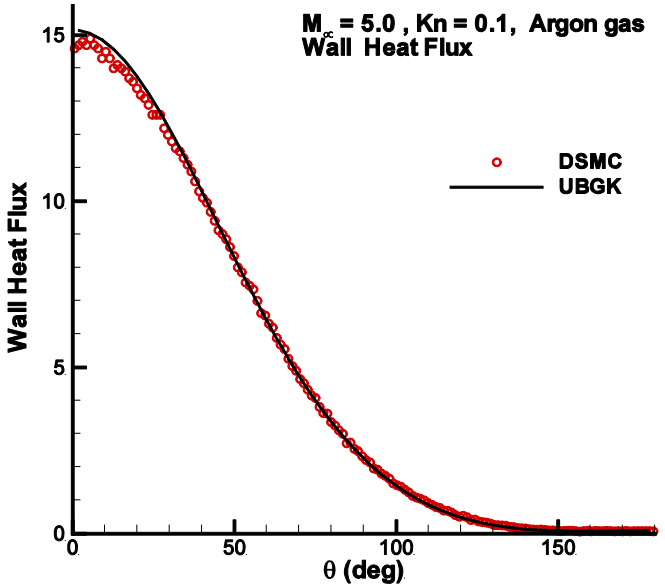
(c)


M∞ = 5.0 Kn∞ = 0.1 Argon Velocity
DSMC
UBGK
Velocity-U
X

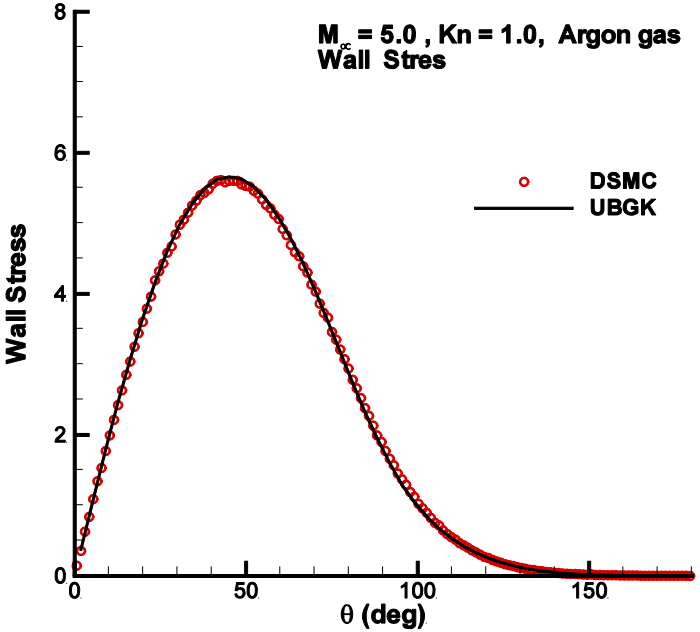
(d)

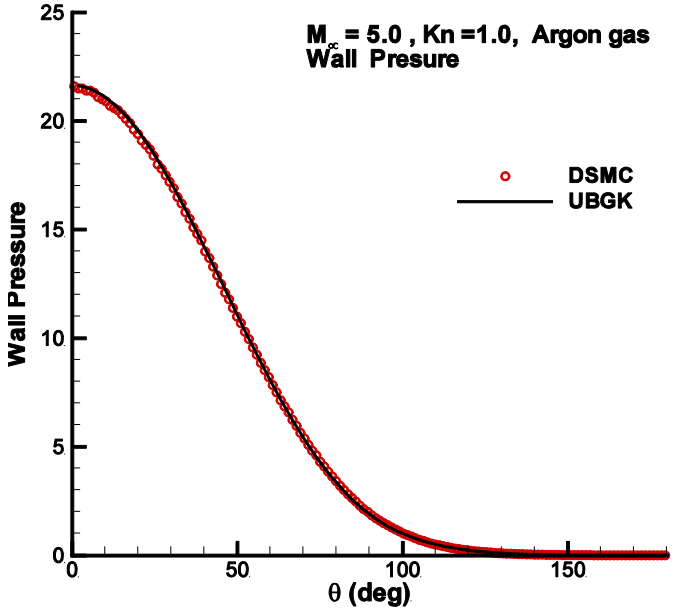

M∞ = 5.0 , Kn = 0.1, Argon gas
Wall Stres
DSMC
UBGK
Wall Stress
θ (deg)
0
50
100
150
0.5
1
1.5
2
2.5

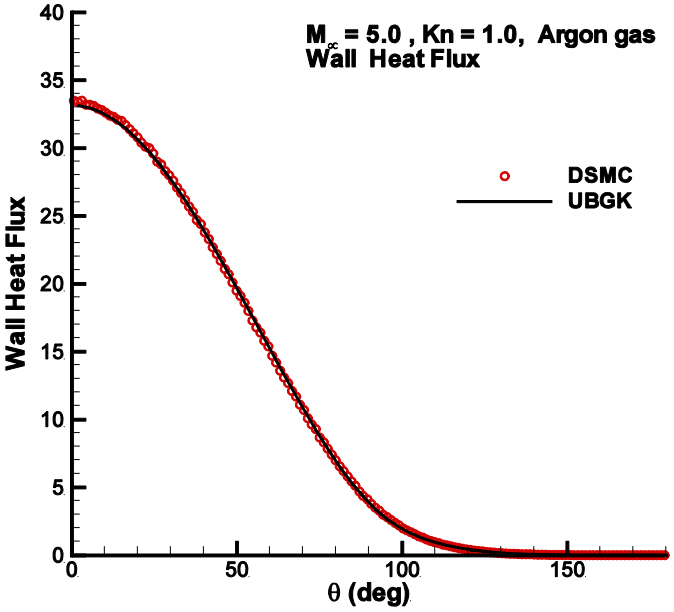

M∞ = 5.0 , Kn = 0.1, Argon gas
Wall Presure
DSMC
UBGK
Wall Pressure
θ (deg)
0
50
100
150
5
10
15
20


M∞ = 5.0 , Kn = 0.1, Argon gas
Wall Heat Flux
DSMC
UBGK
Wall Heat Flux
θ (deg)
0
50
100
150
5
10
15

M=5, Kn=0.1

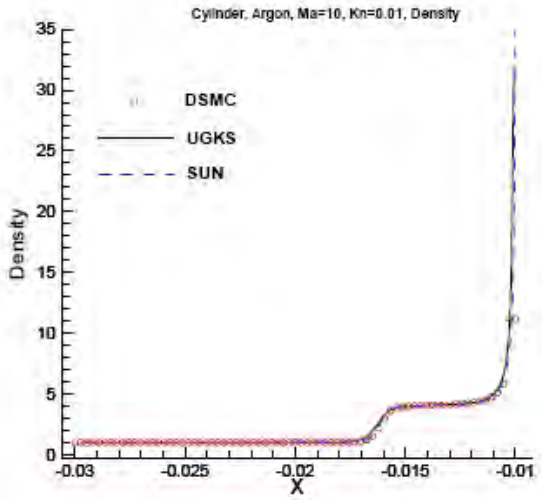

M∞ = 5.0 , Kn = 1.0, Argon gas
Wall Stres
DSMC
UBGK
Wall Stress
θ (deg)
0
2
4
6
8
0
50
100
150


M∞ = 5.0 , Kn =1.0, Argon gas
Wall Presure
DSMC
UBGK
Wall Pressure
θ (deg)
0
5
10
15
20
25
0
50
100
150

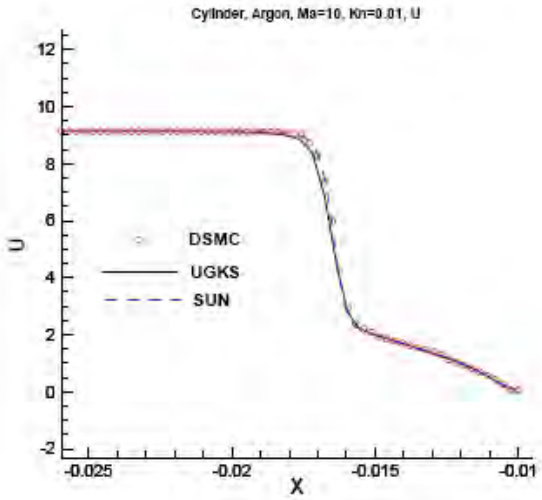

M∞ = 5.0 , Kn = 1.0, Argon gas
Wall Heat Flux
DSMC
UBGK
Wall Heat Flux
θ (deg)
0
5
10
15
20
25
30
35
40
0
50
100
150

M=5, Kn=1.0

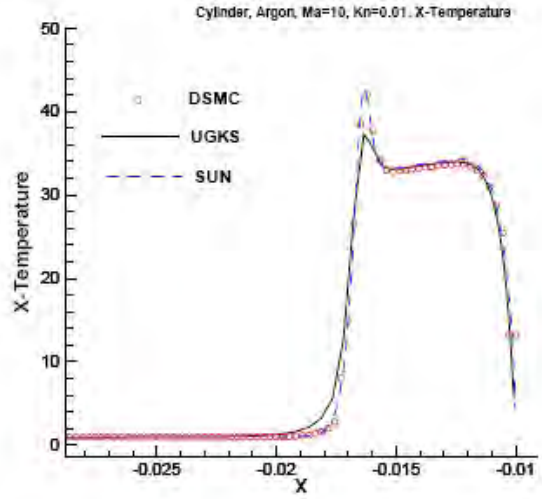
Hypersonic Flow Computations



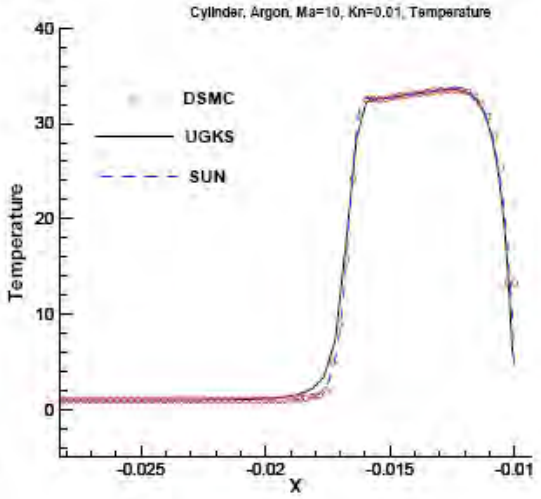
(a) Density



(b) Velocity

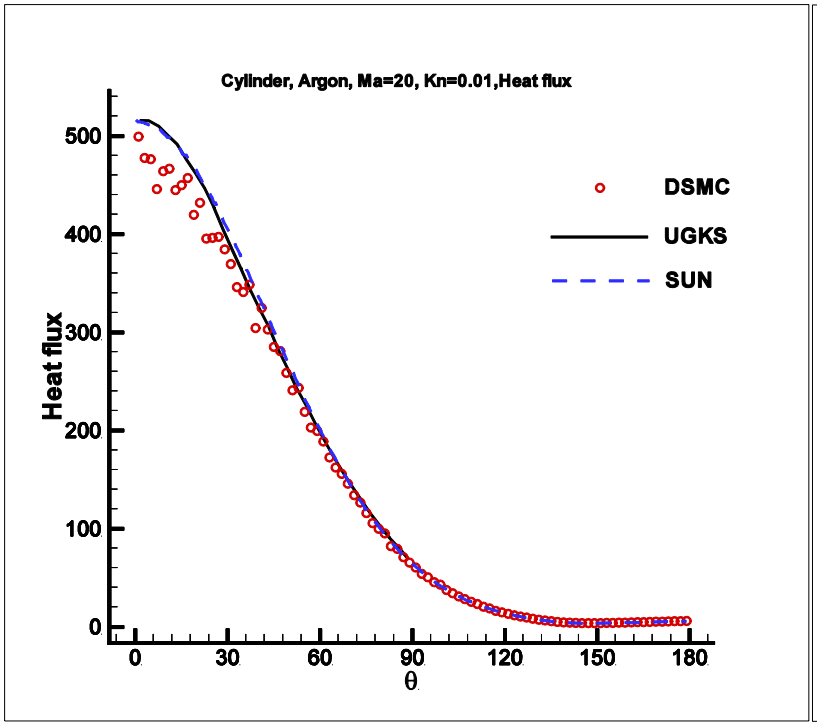


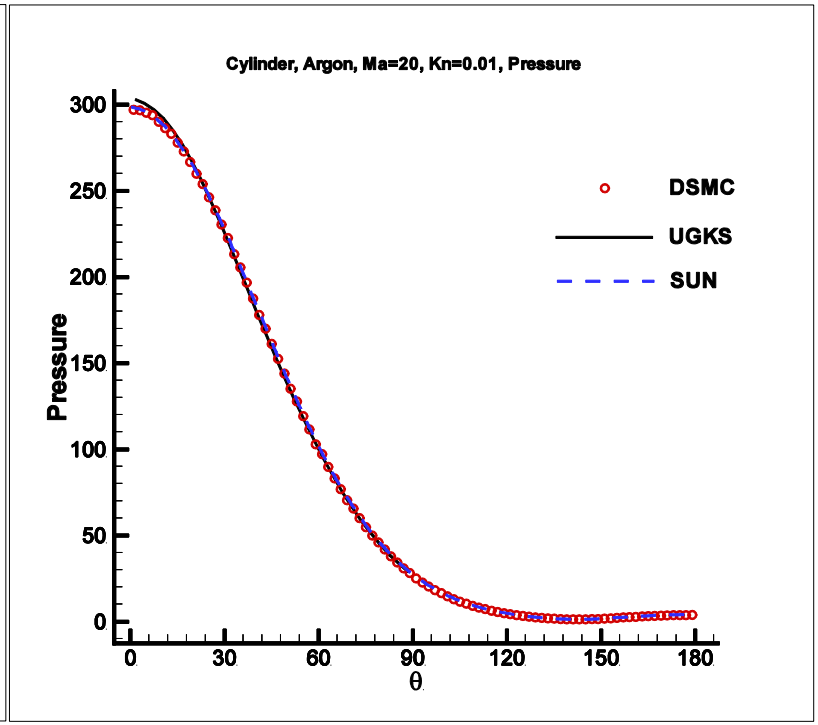
(c) Temperature-X

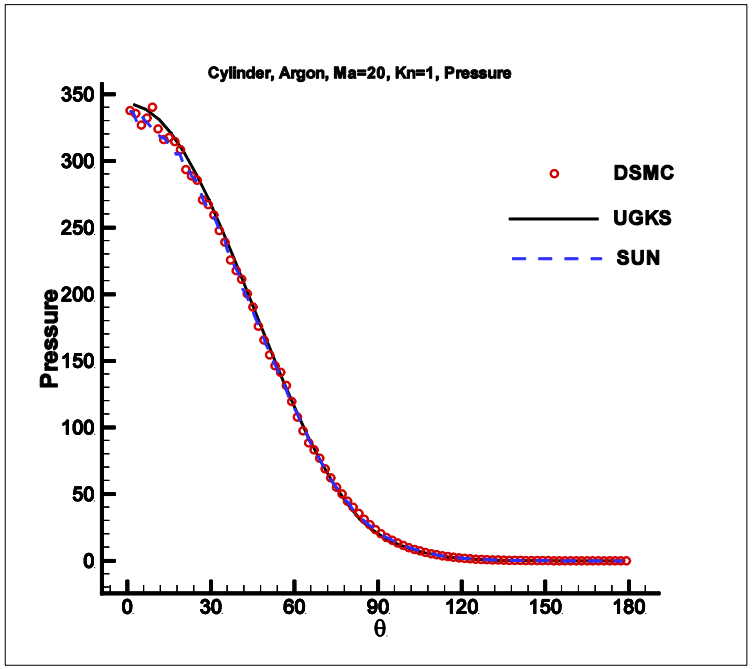


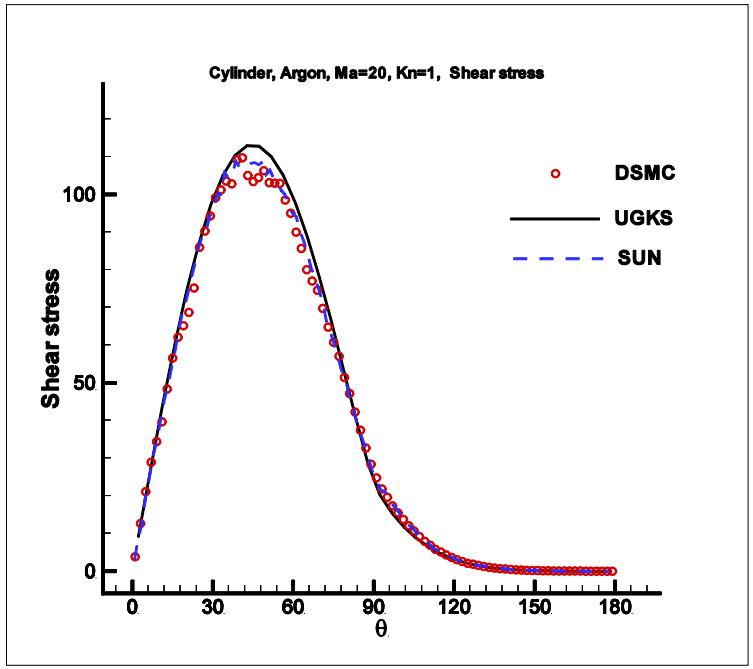
(d) Temperature

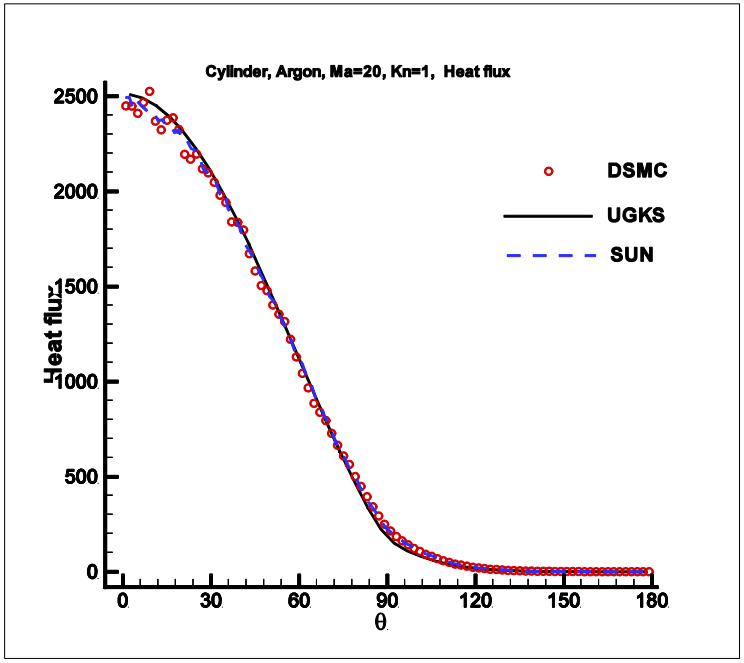
M=20, Kn=0.01


Cylinder, Argon, Ma=20, Kn=0.01,Heat flux
Heat flux
θ
DSMC
UGKS
SUN
0
100
200
300
400
500
0
30
60
90
120
150
180


Cylinder, Argon, Ma=20, Kn=0.01, Pressure
Pressure
θ
DSMC
UGKS
SUN
0
50
100
150
200
250
300
0
30
60
90
120
150
180


Cylinder, Argon, Ma=20, Kn=1, Pressure
Pressure
θ
DSMC
UGKS
SUN
0
50
100
150
200
250
300
350
0
30
60
90
120
150
180

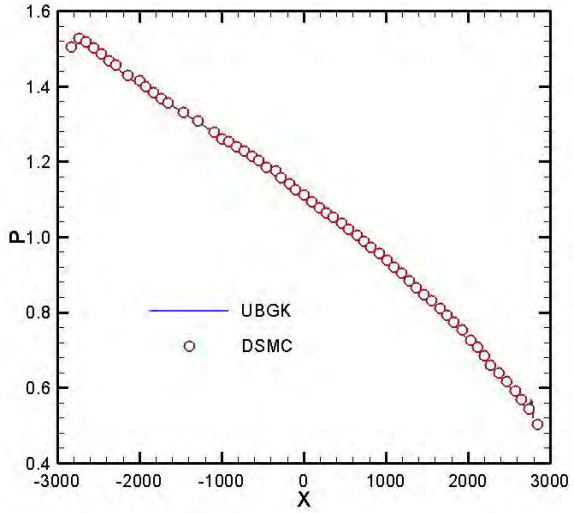

Cylinder, Argon, Ma=20, Kn=1, Shear stress
Shear stress
θ
DSMC
UGKS
SUN
0
50
100
0
30
60
90
120
150
180

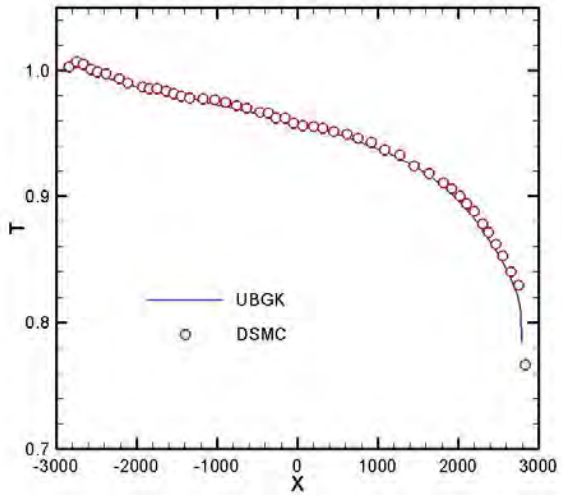

Cylinder, Argon, Ma=20, Kn=1, Heat flux
Heat flux
θ
DSMC
UGKS
SUN
0
500
1000
1500
2000
2500
0
30
60
90
120
150
180

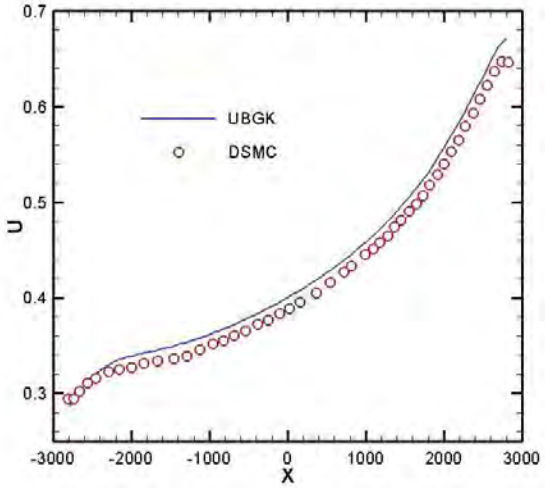
M=20, Kn=1

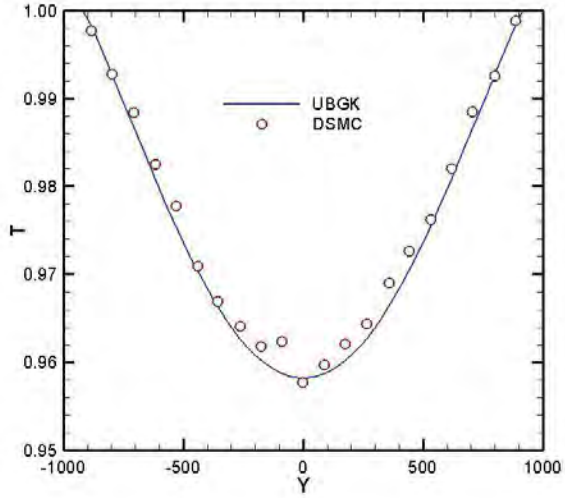
Micro-flows

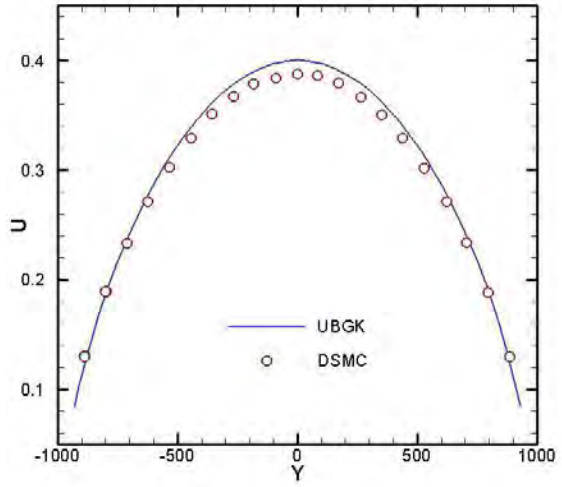
Pressure Driven Poiseuille Flow: Kn=0.1

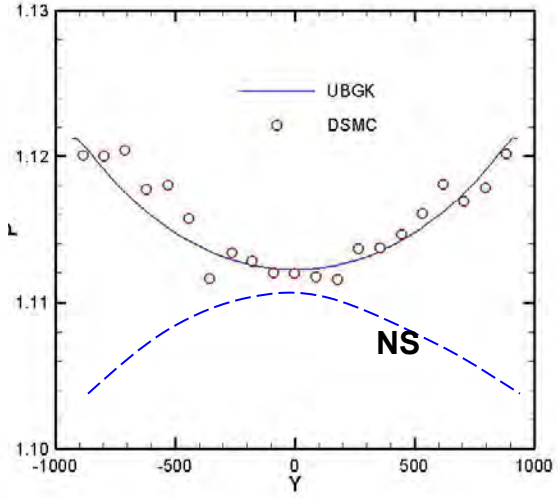




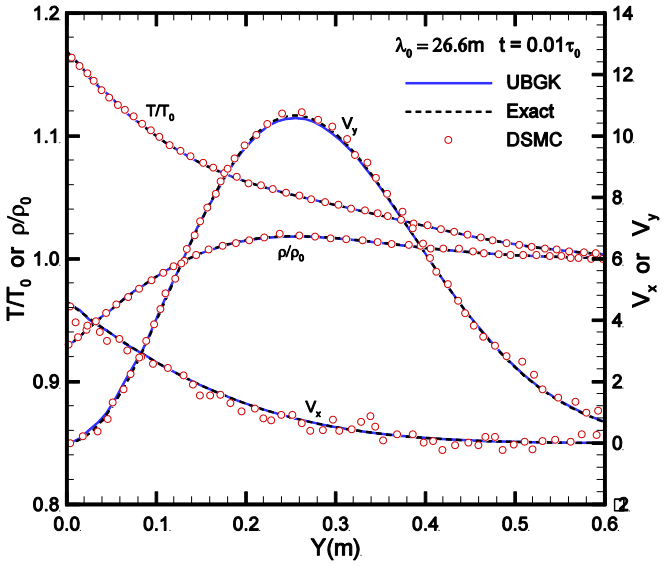


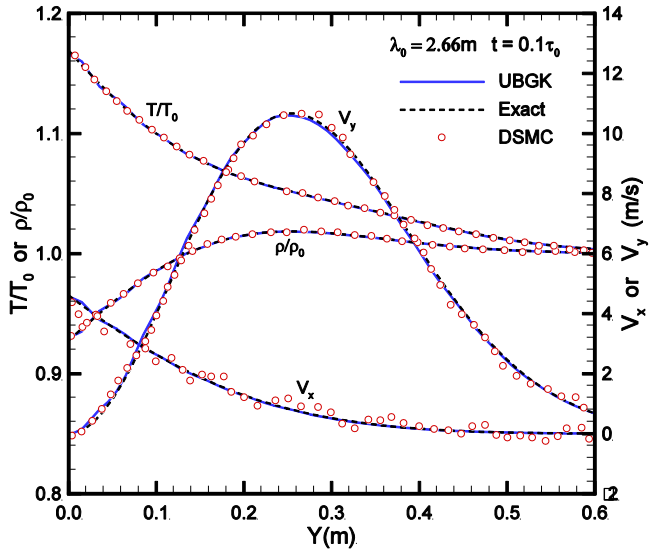


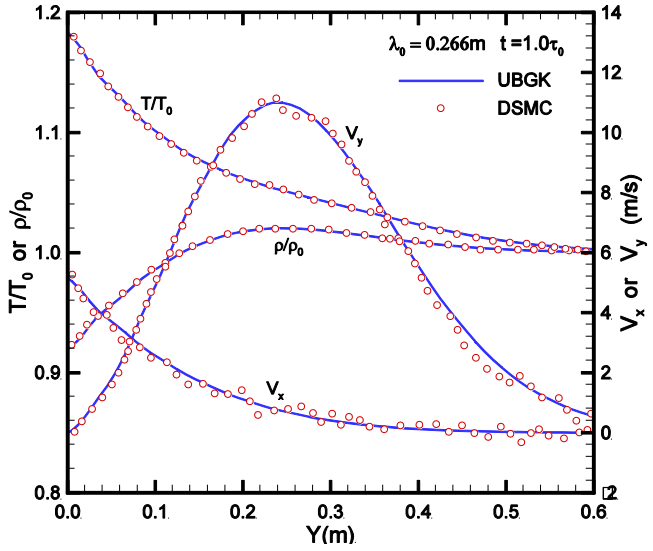


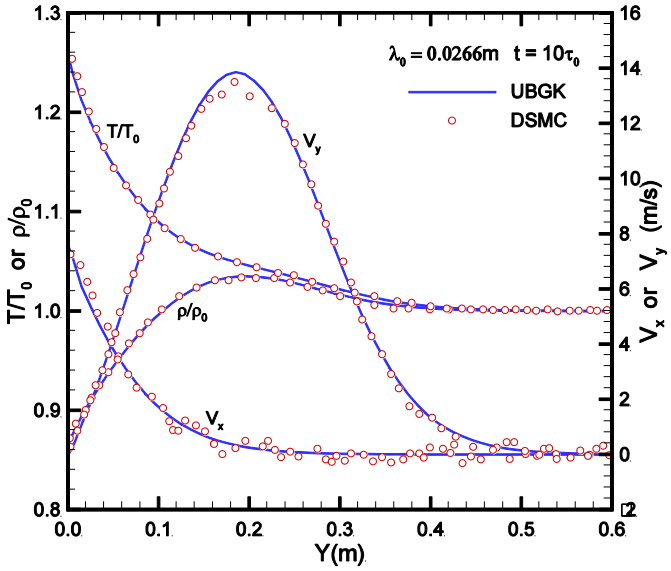


Rayleigh Problem

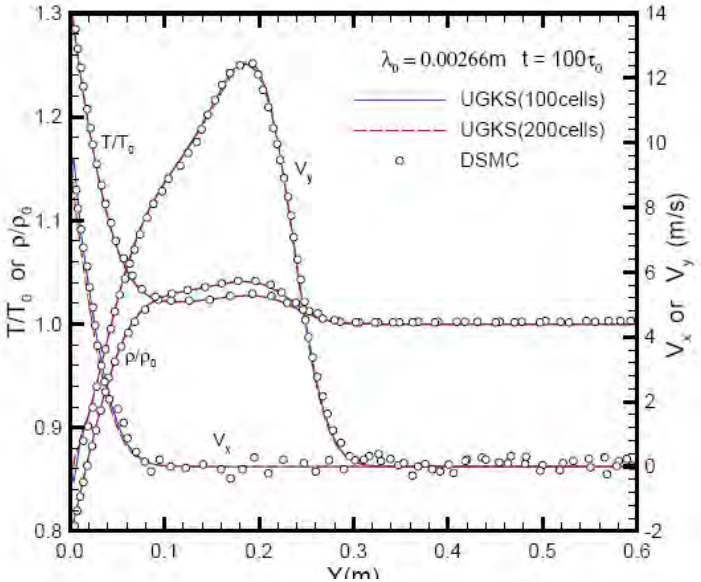




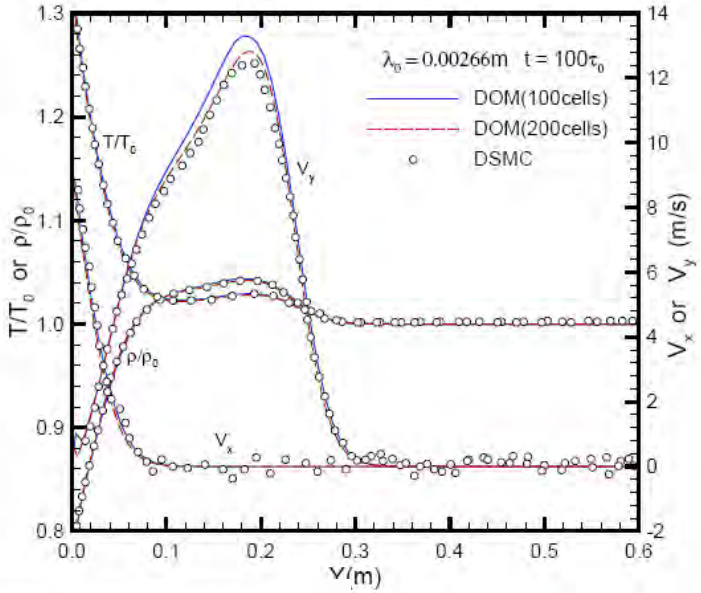


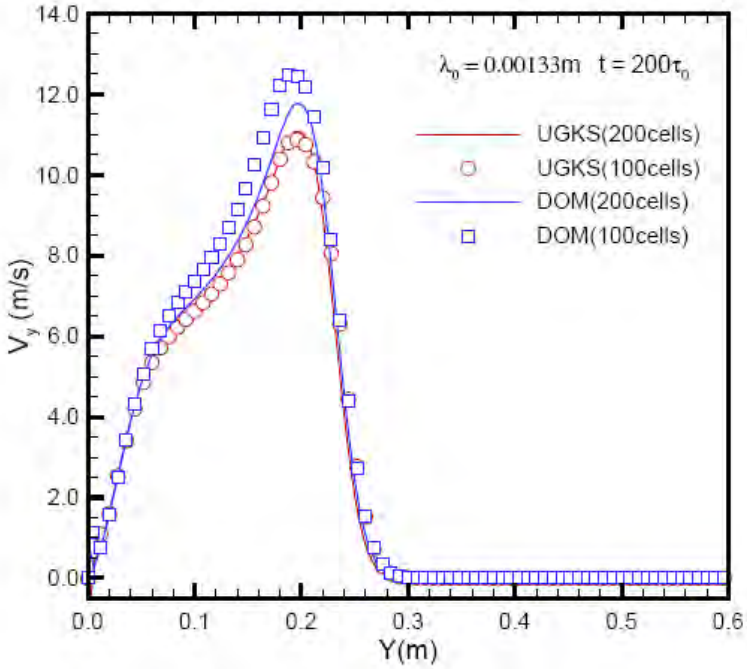


Unified

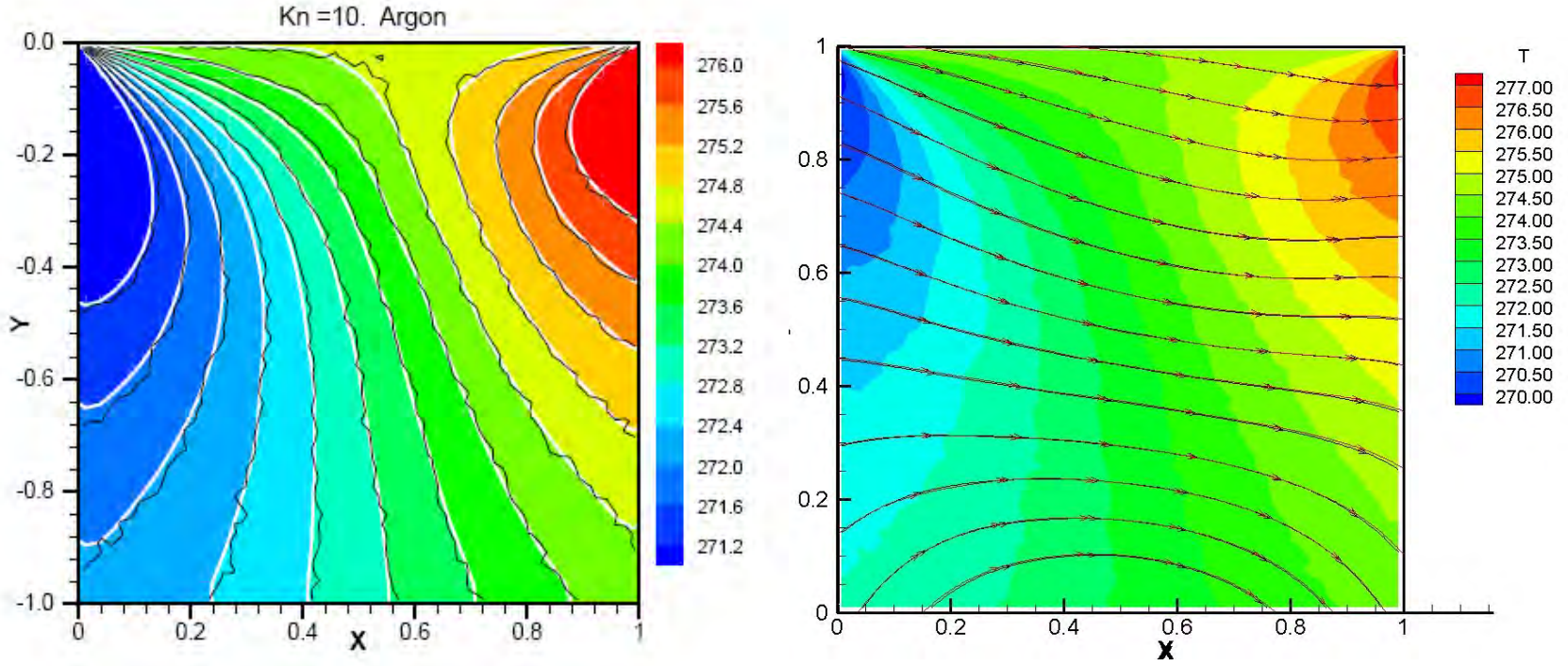

$\lambda_0 = 0.00266$m t = $100\tau_0$
UGKS(100cells)
UGKS(200cells)
DSMC
T/T0
ρ/ρ0
Vx
Vy
T/T0 or ρ/ρ0
Vx or Vy (m/s)
Y(m)

DOM

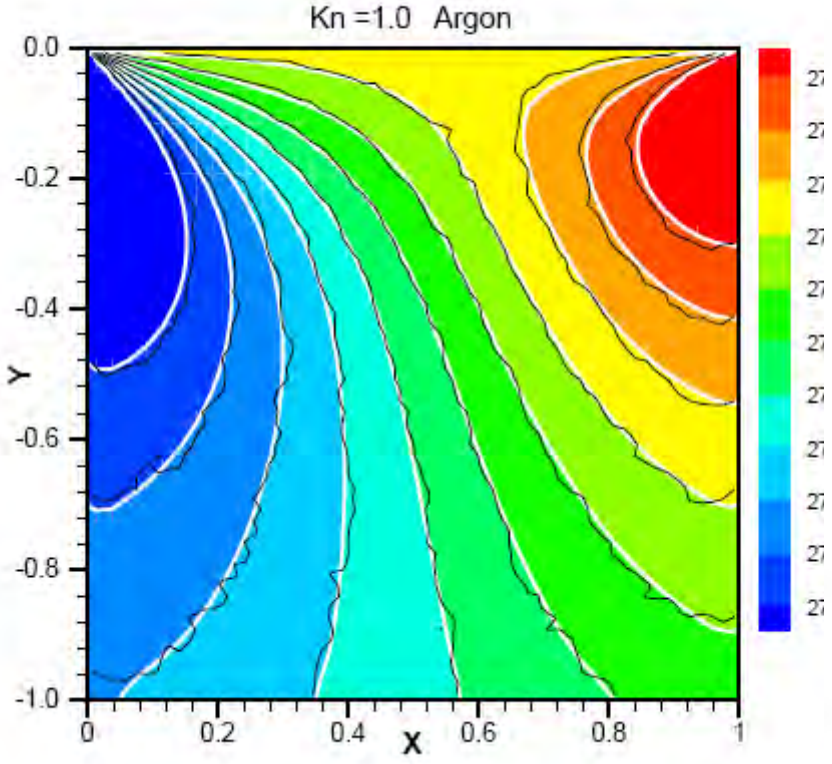

$\lambda_0 = 0.00266$m t = $100\tau_0$
DOM(100cells)
DOM(200cells)
DSMC
T/T0
ρ/ρ0
Vx
Vy
T/T0 or ρ/ρ0
Vx or Vy (m/s)
Y(m)

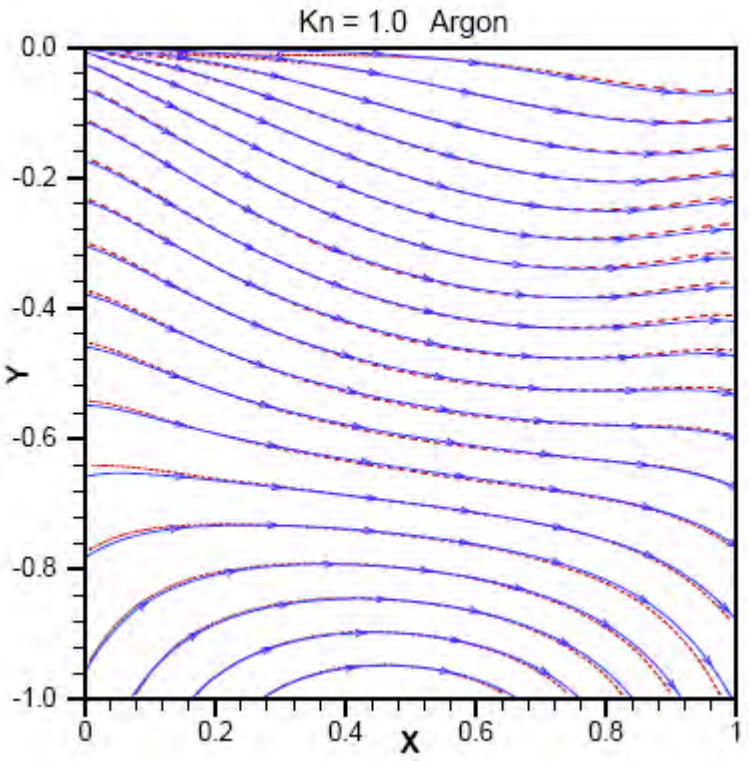

$\lambda_0 = 0.00133$m t = $200\tau_0$
UGKS(200cells)
UGKS(100cells)
DOM(200cells)
DOM(100cells)
Vy (m/s)
Y(m)

Knudsen *number: Kn=10*

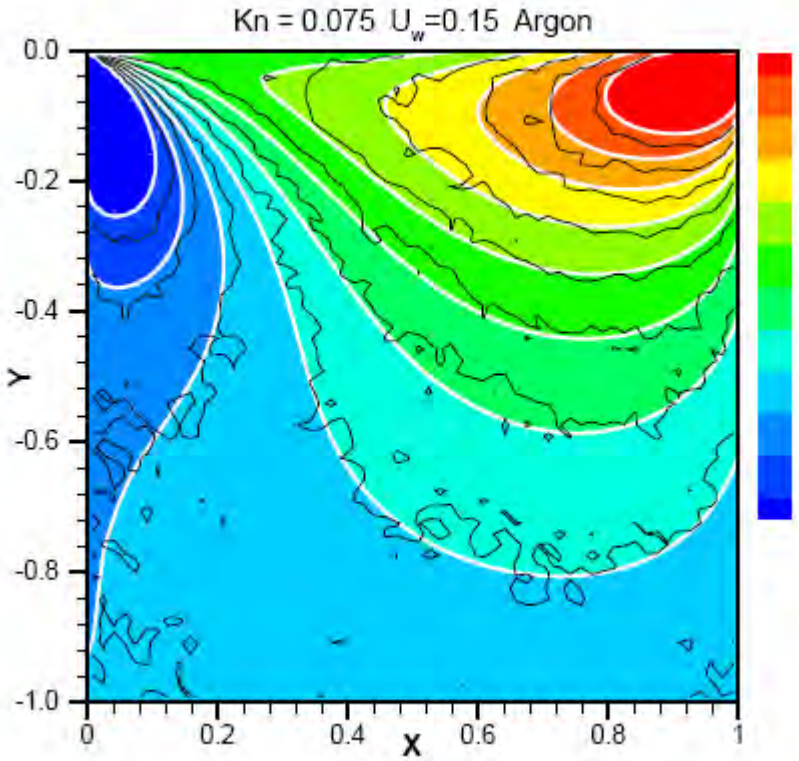


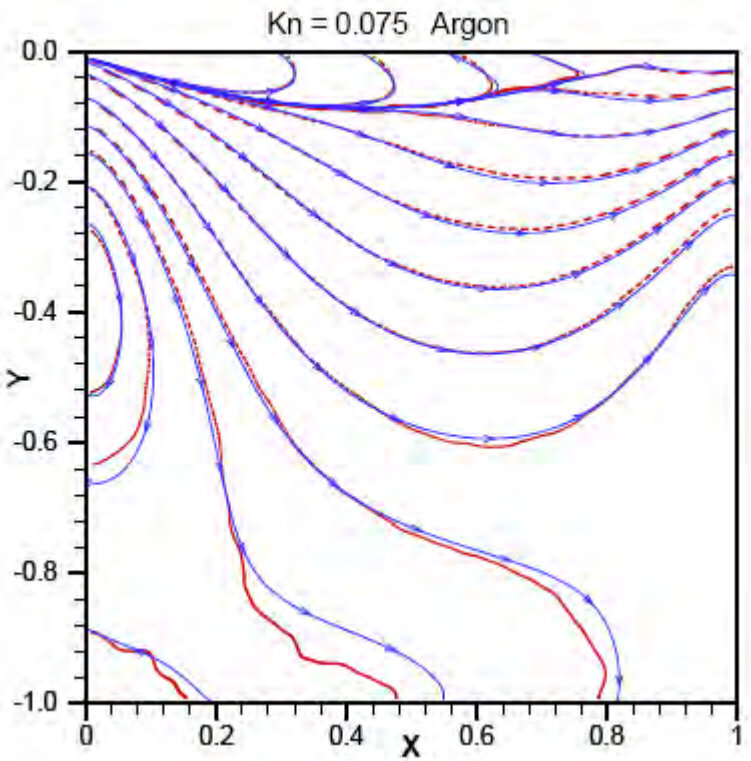
Kn=1.0 (transitional)





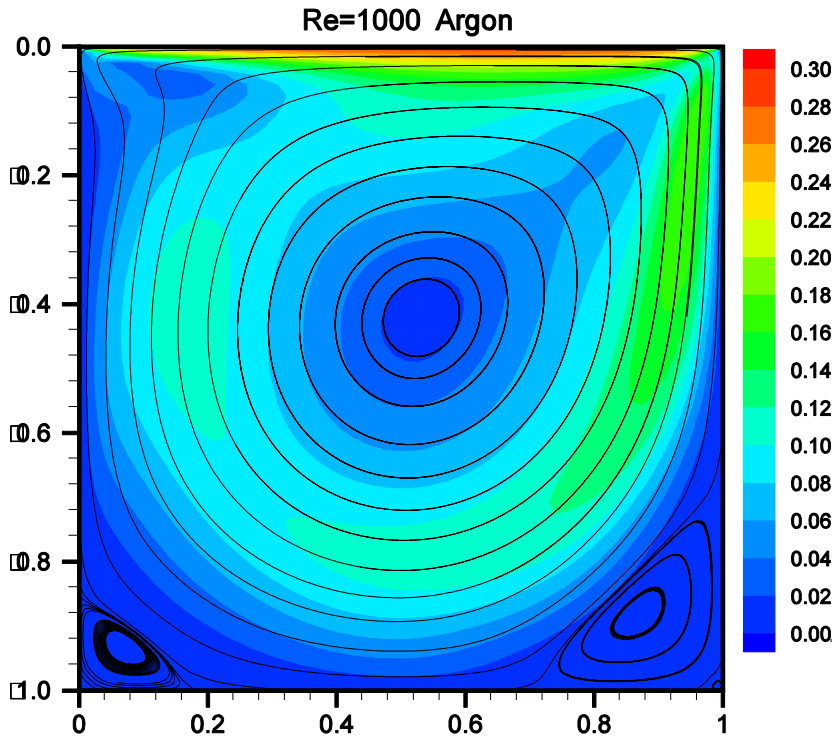
Kn=0.075 (near continuum)

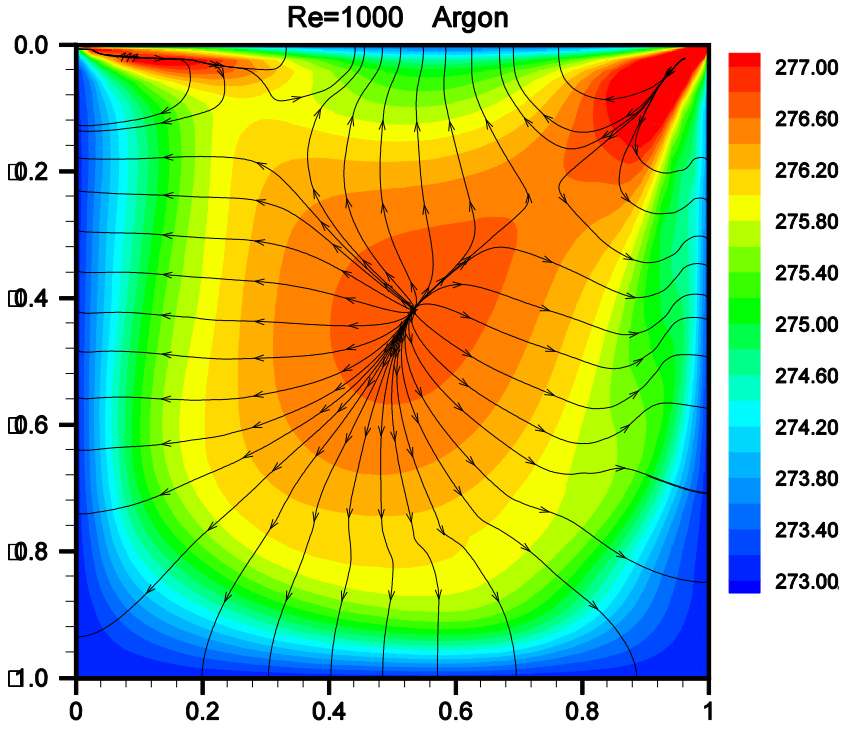




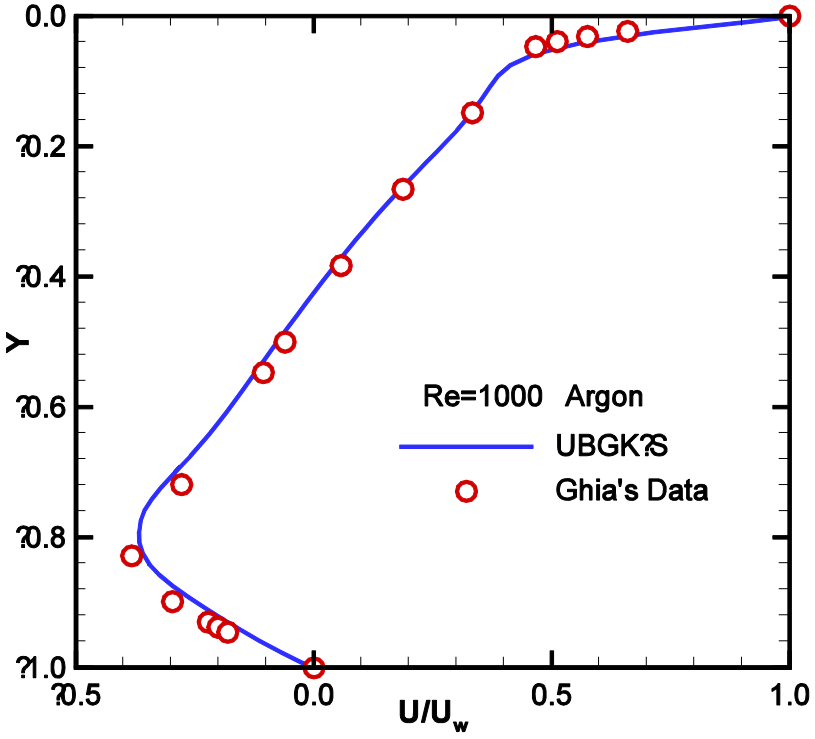
UGKS

Re=1000 (continuum)

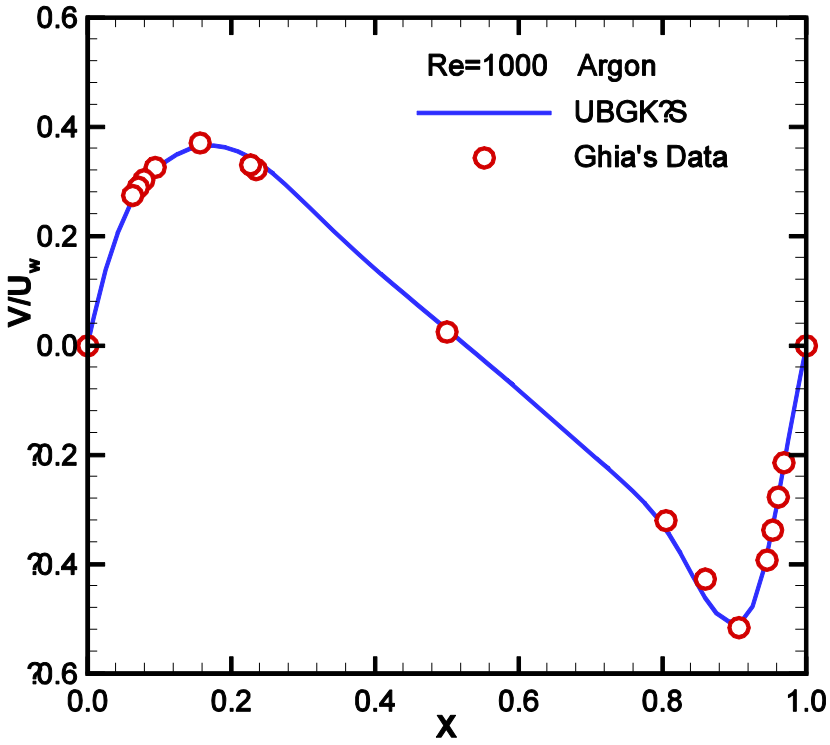




U-velocity

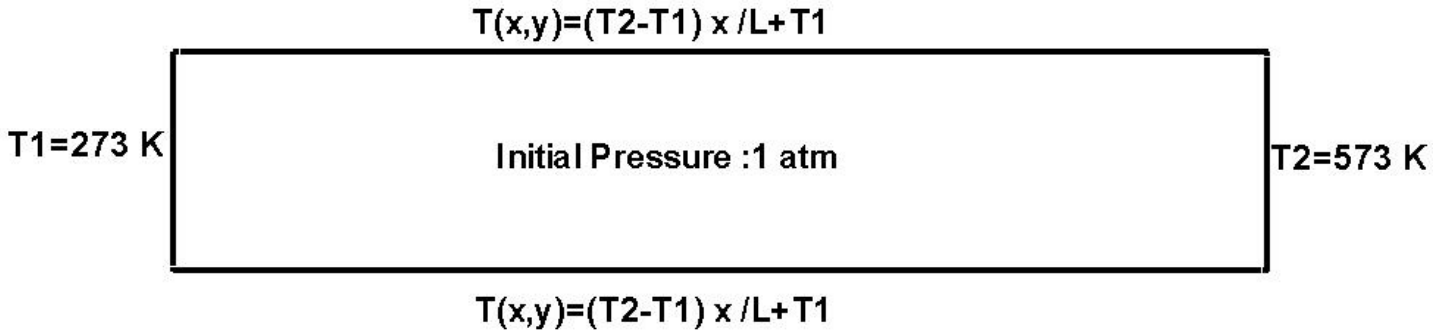


V-velocity

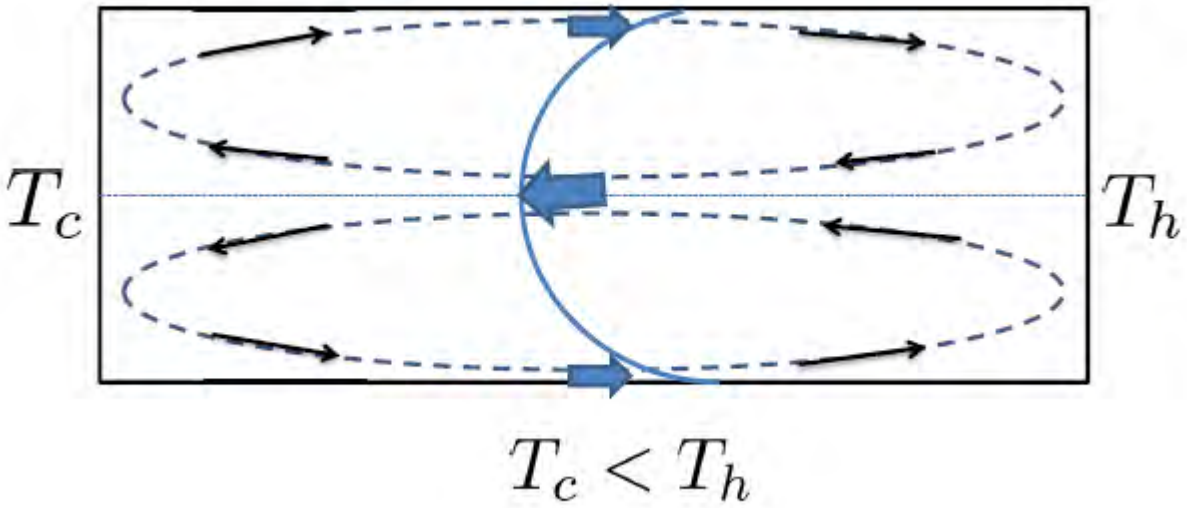


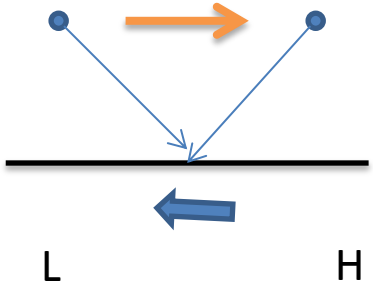
Thermal creep flows

Thermal Creep Flow

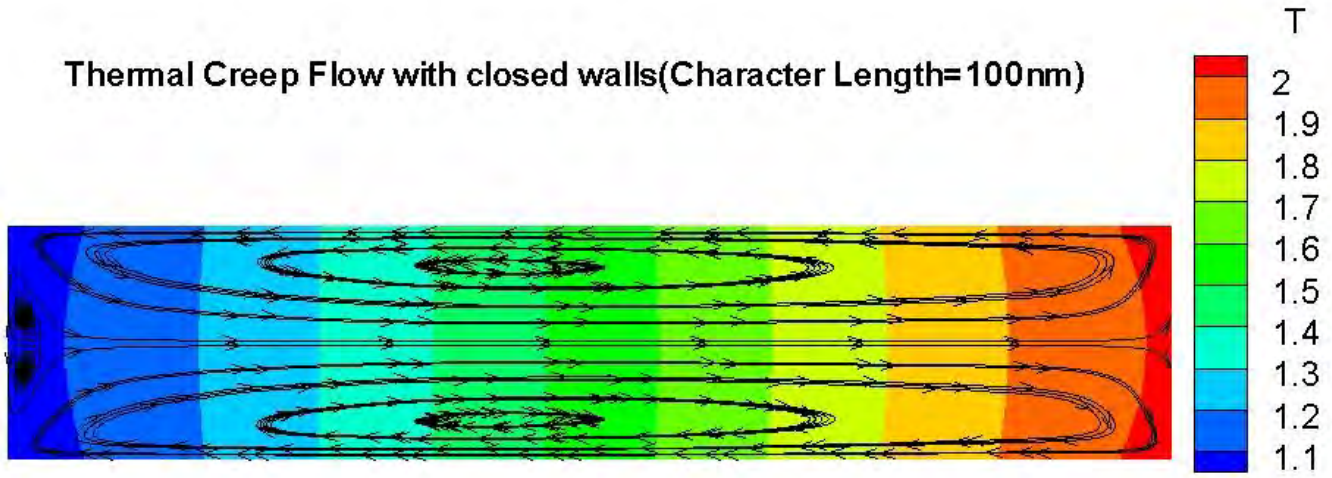


Thermal Creep Flow

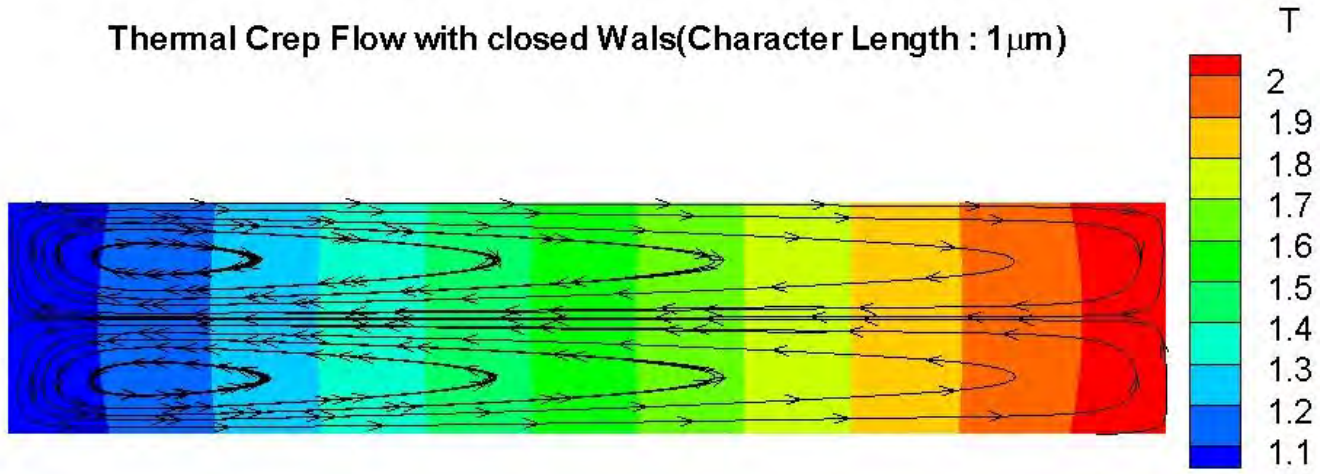




Kn=0.64

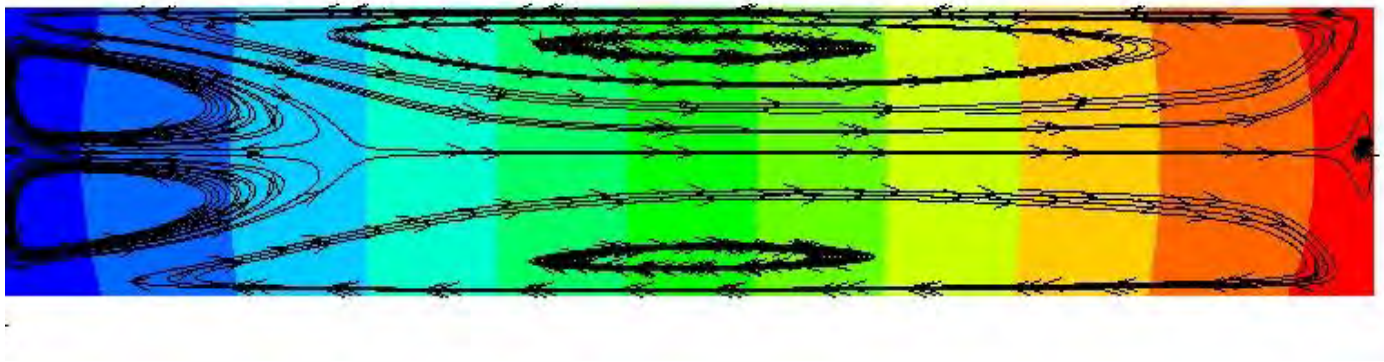


Kn=0.064

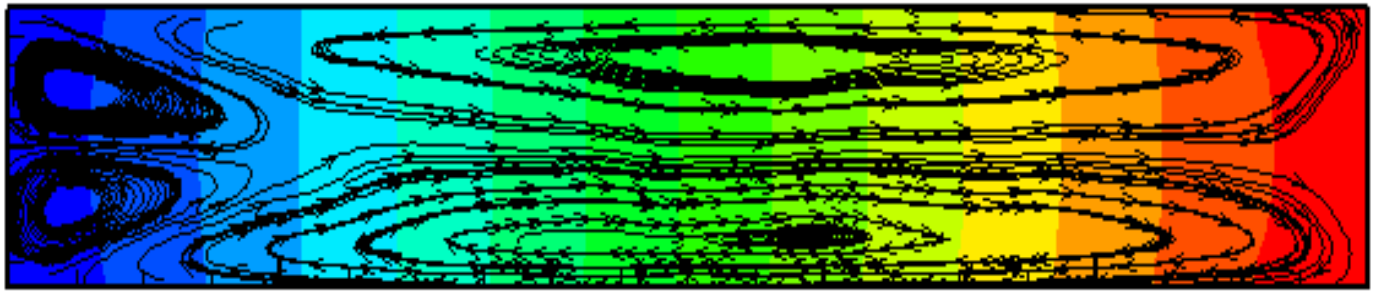


H=200nm Kn=0.32

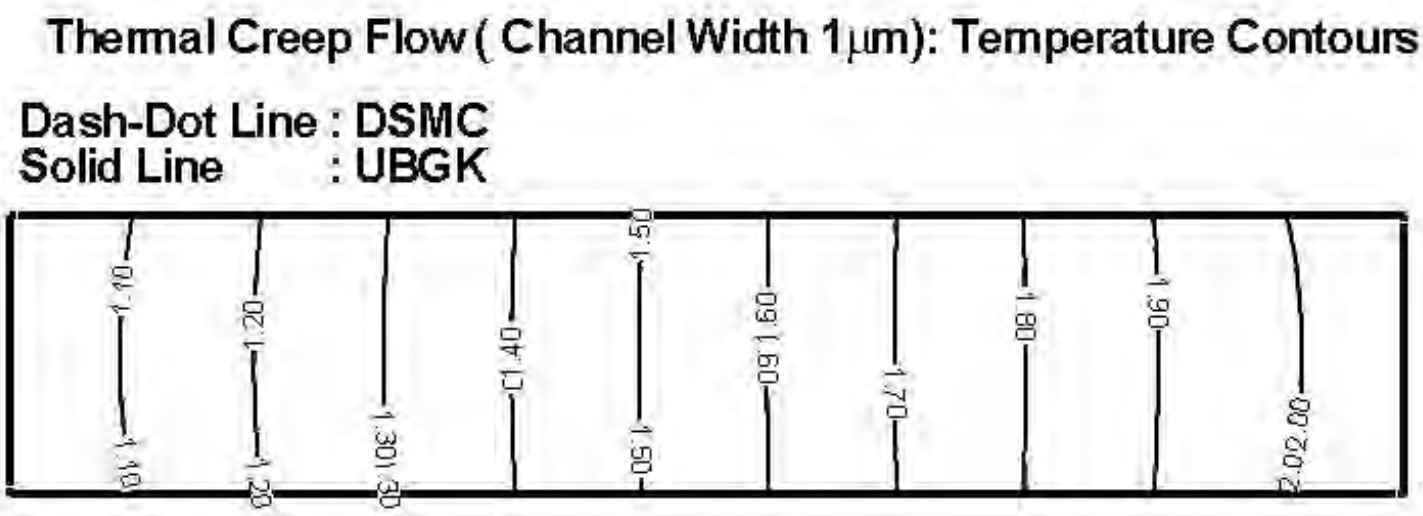
UGKS

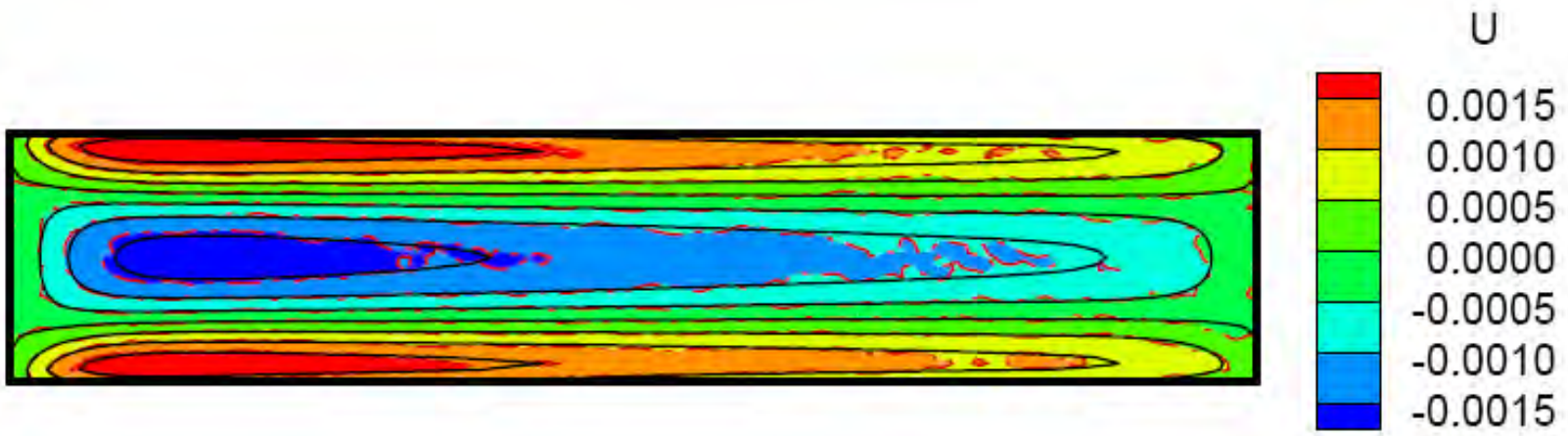


DSMC



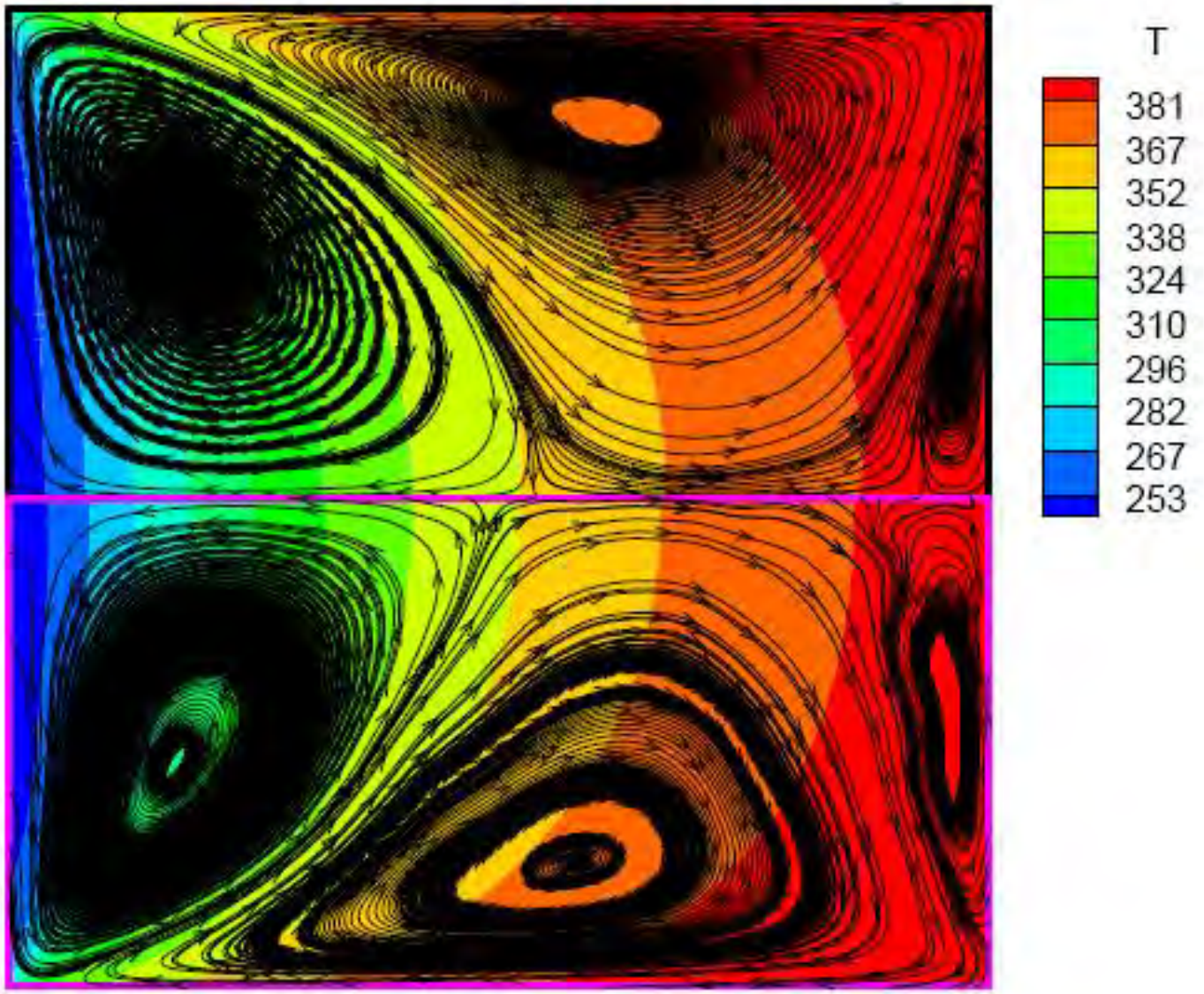
UGKS vs DSMC at Kn=0.064





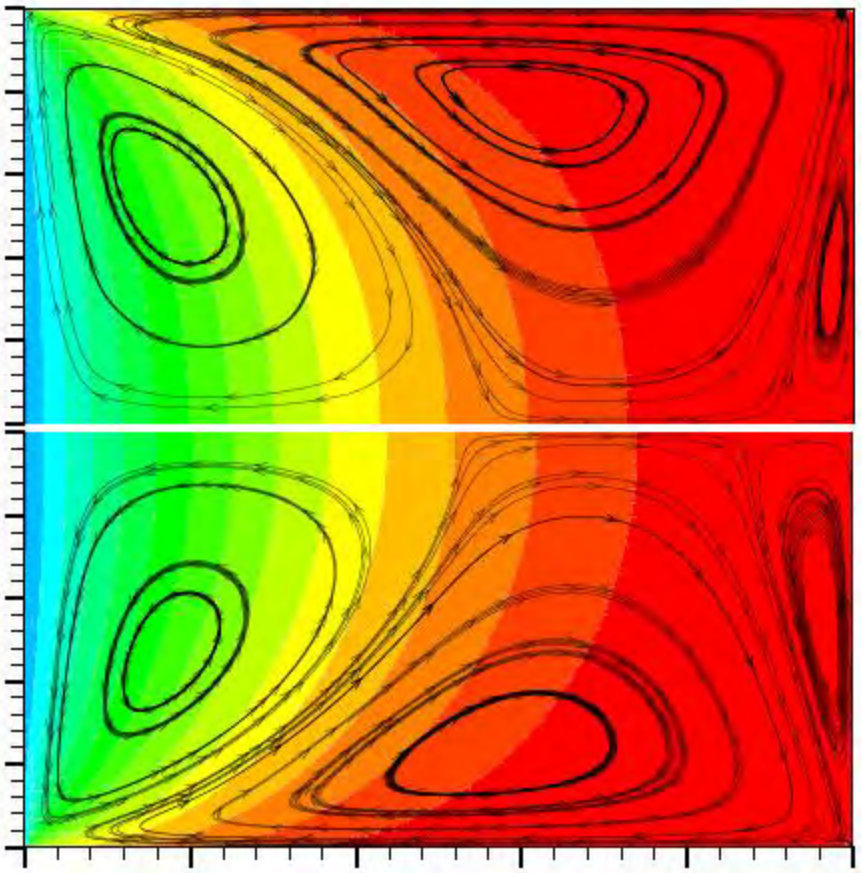
UBGK

DSMC



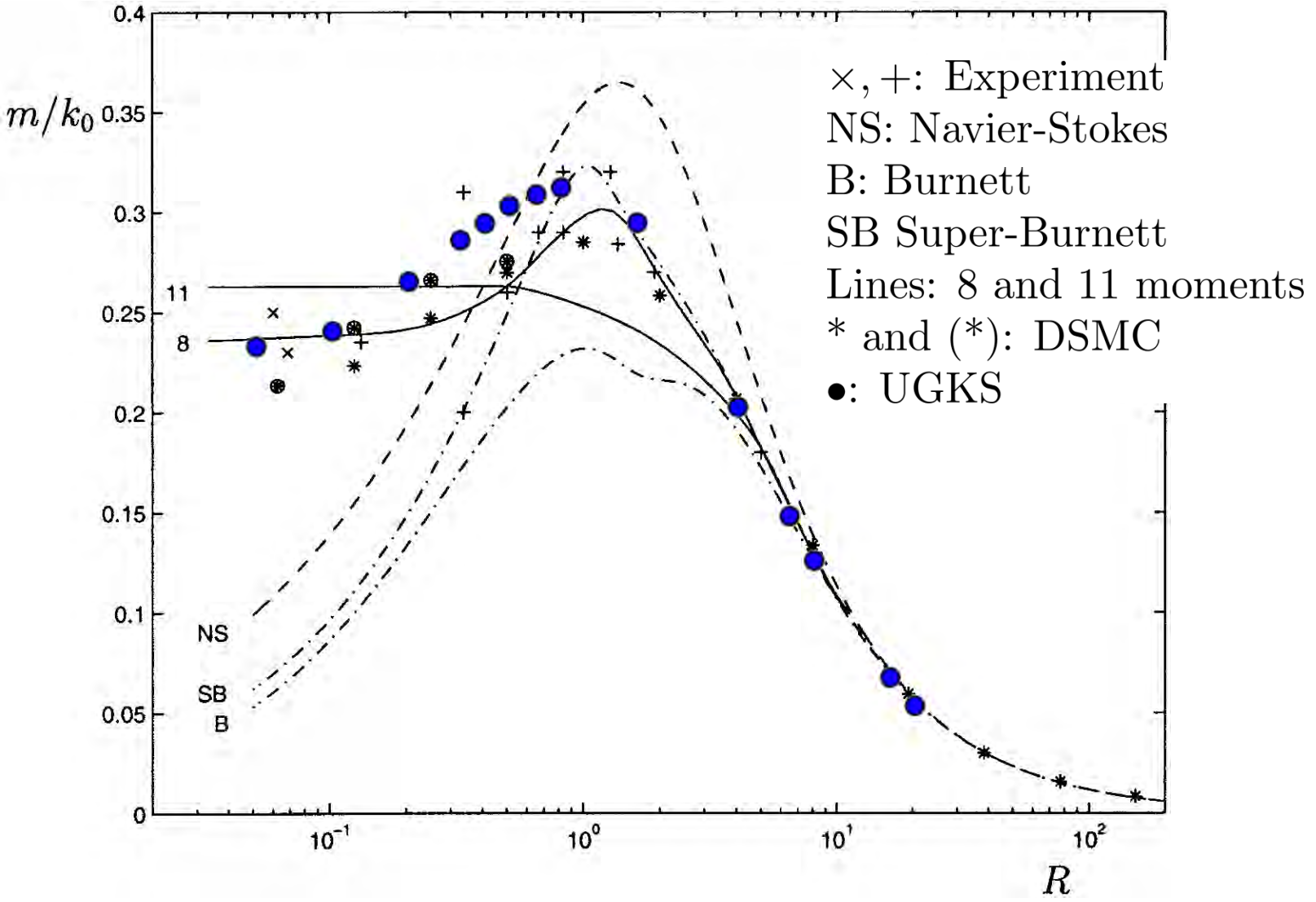
UGKS

Full Boltzmann solution

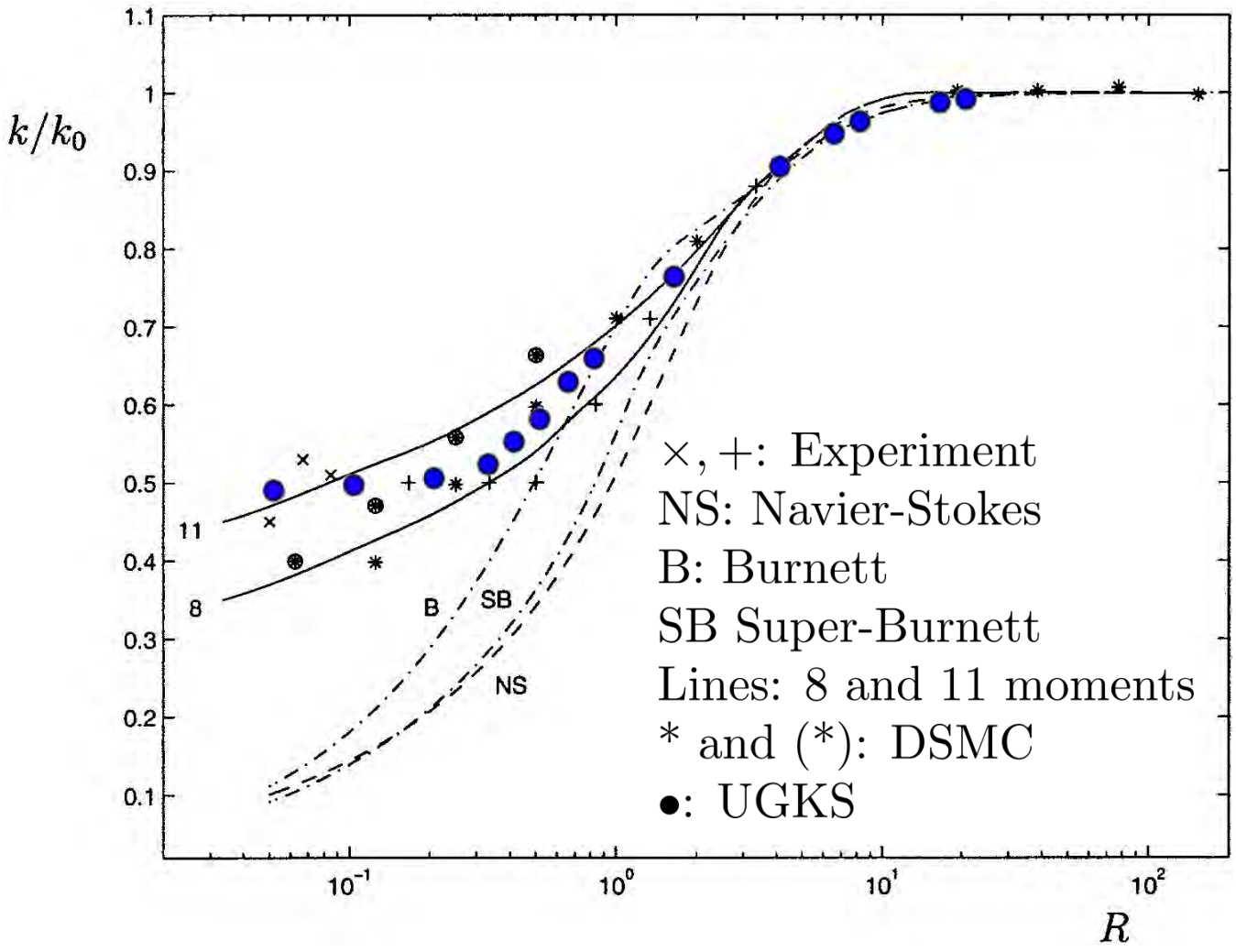


Sound wave propagation in simple gases

Absorption

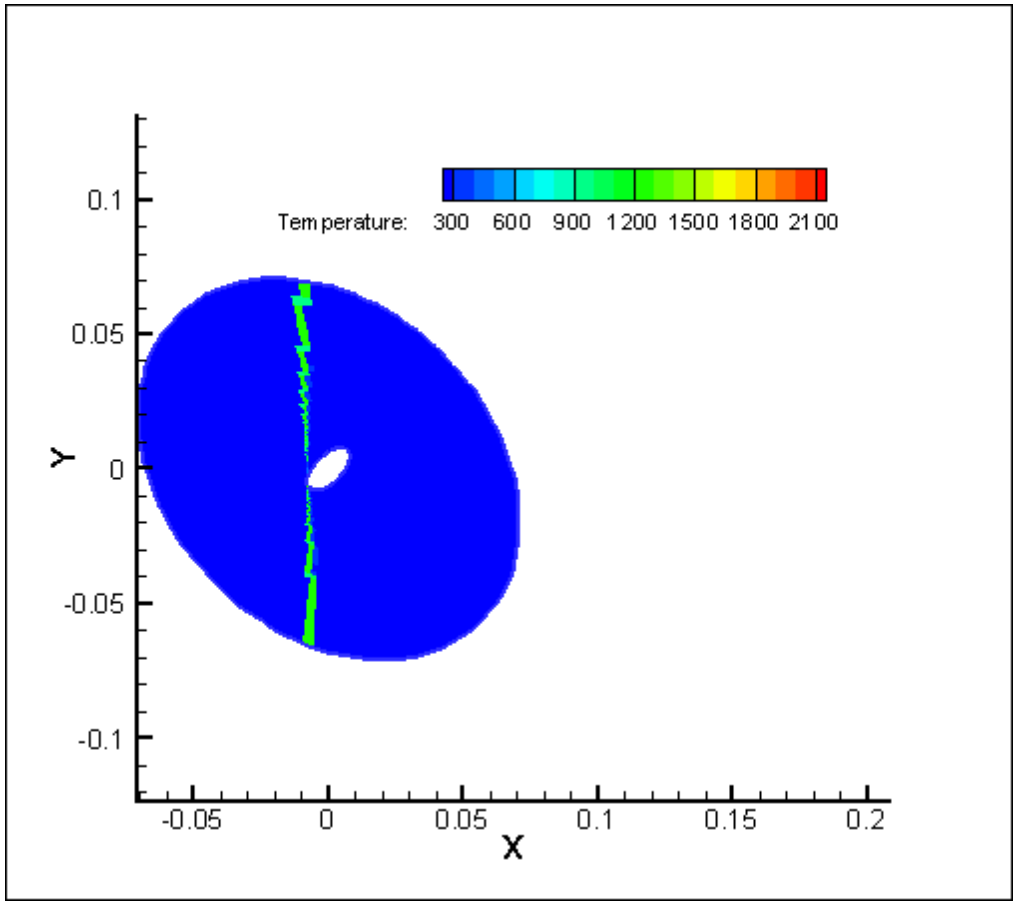

m/k_0
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
11
8
NS
SB
B
10^{-1}
10^{0}
10^{1}
10^{2}
R
×, +: Experiment
NS: Navier-Stokes
B: Burnett
SB Super-Burnett
Lines: 8 and 11 moments
* and (*): DSMC
●: UGKS

Speed

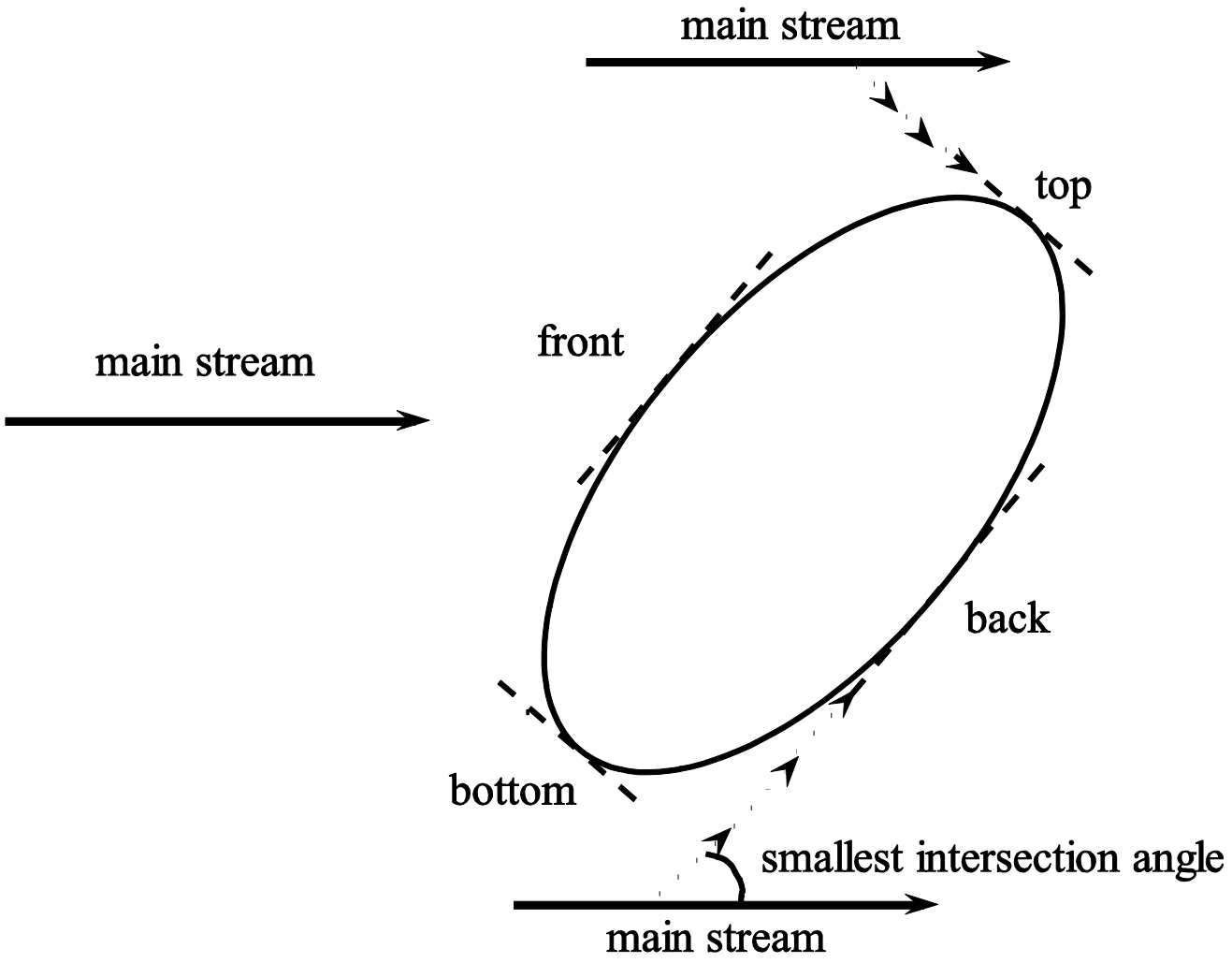

k/k_0
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
11
8
B
SB
NS
10^{-1}
10^{0}
10^{1}
10^{2}
R
×, +: Experiment
NS: Navier-Stokes
B: Burnett
SB Super-Burnett
Lines: 8 and 11 moments
* and (*): DSMC
●: UGKS

UGKS with moving mesh in physical space and particle velocity adaptation

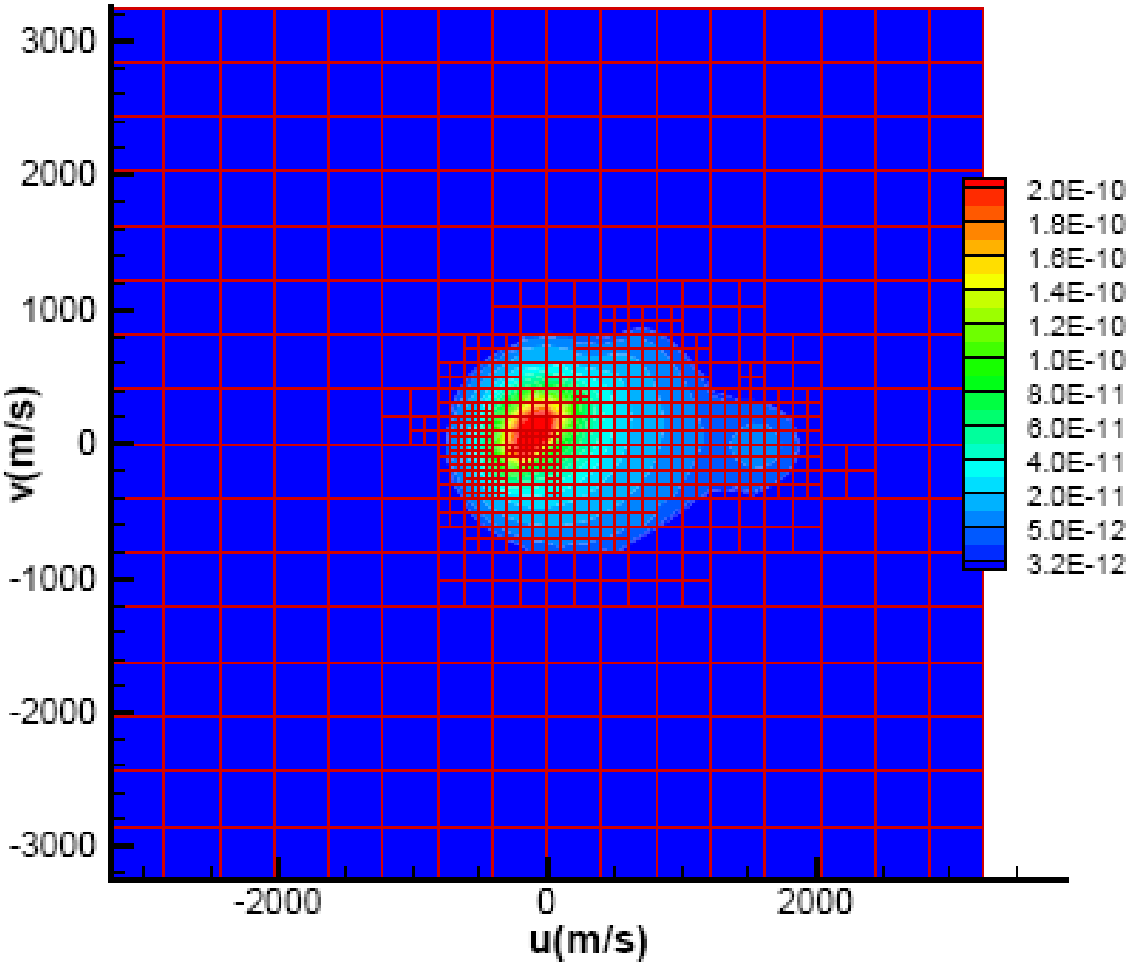
Hypersonic flight in rarefied environment



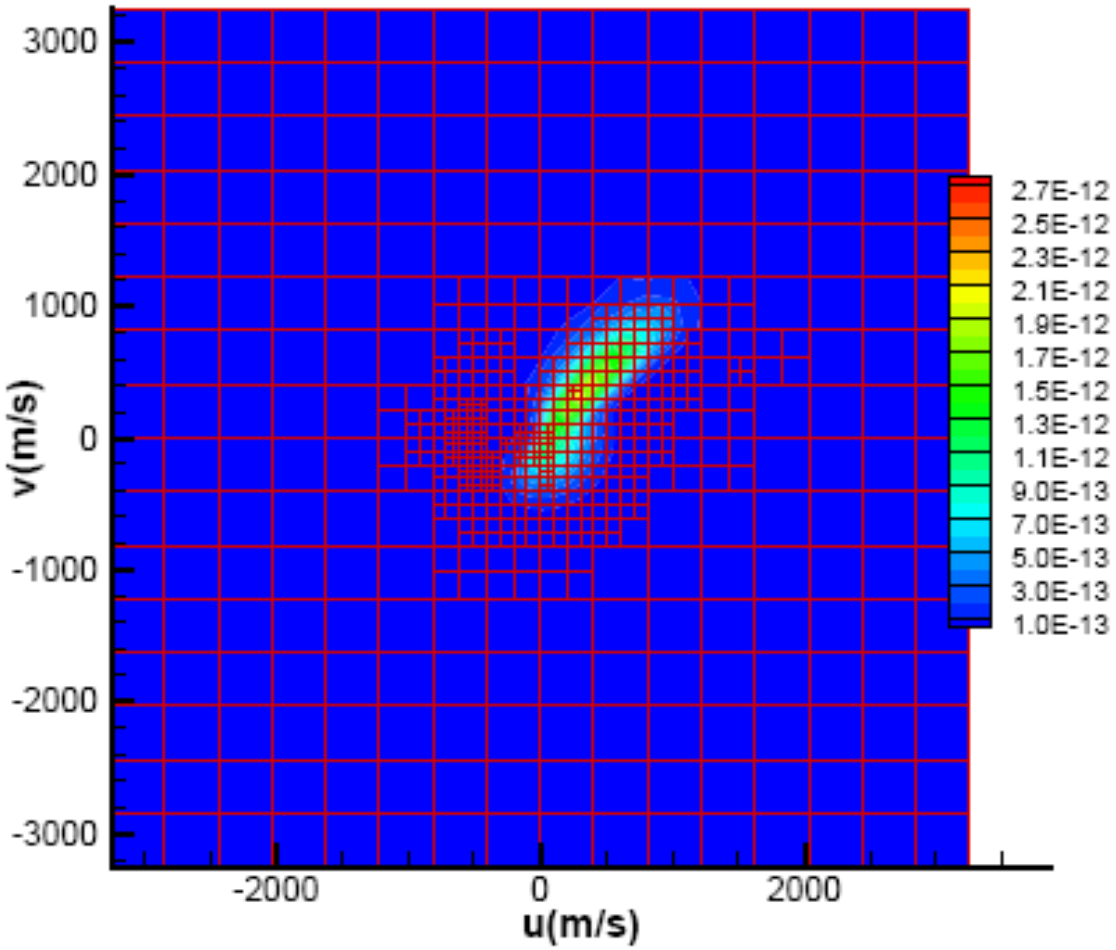
Typical particle velocity distribution function



In the front of the ellipse (upwind)



Behind the ellipse (downwind)

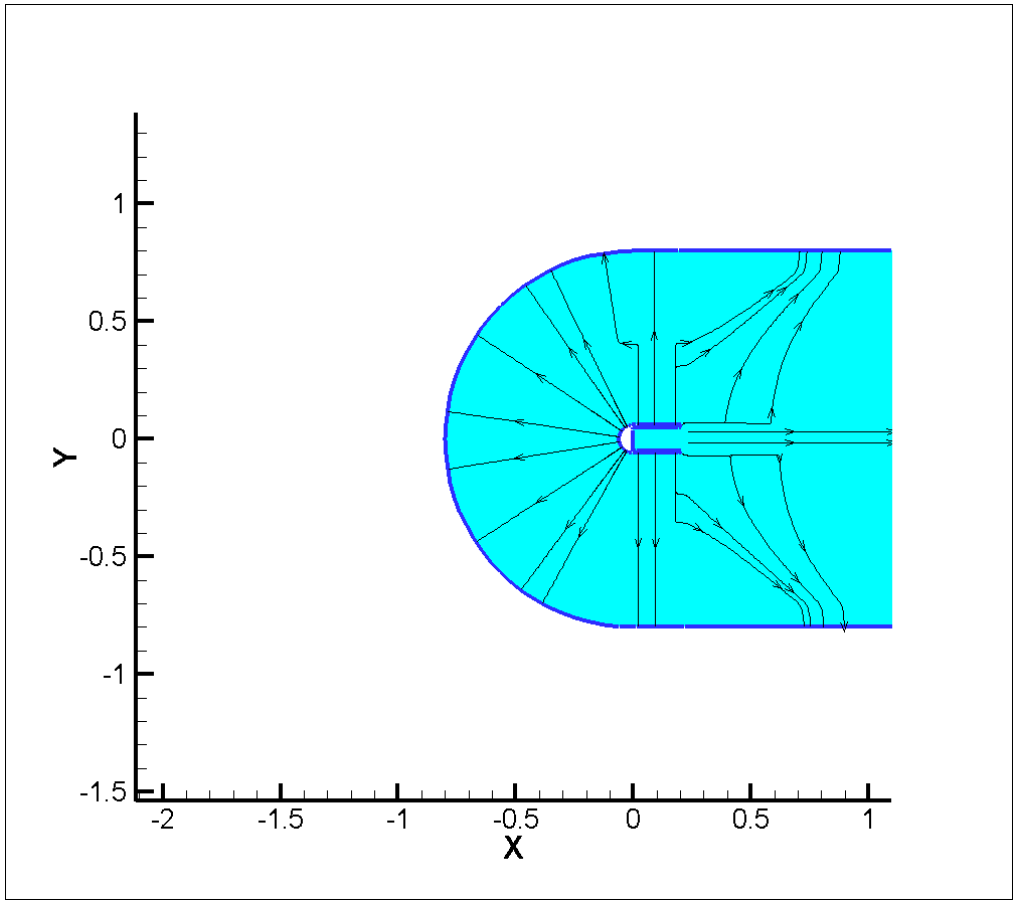


Efficiency

Mesh size in velocity space

760 （AUGKS） vs 64×64 （UGKS）

Expansion flow from a nozzle



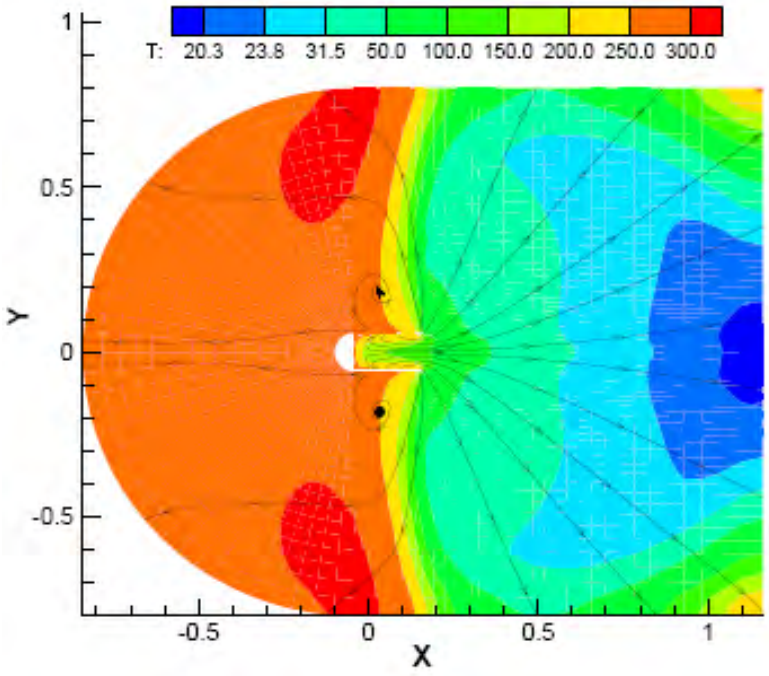
Density ratio

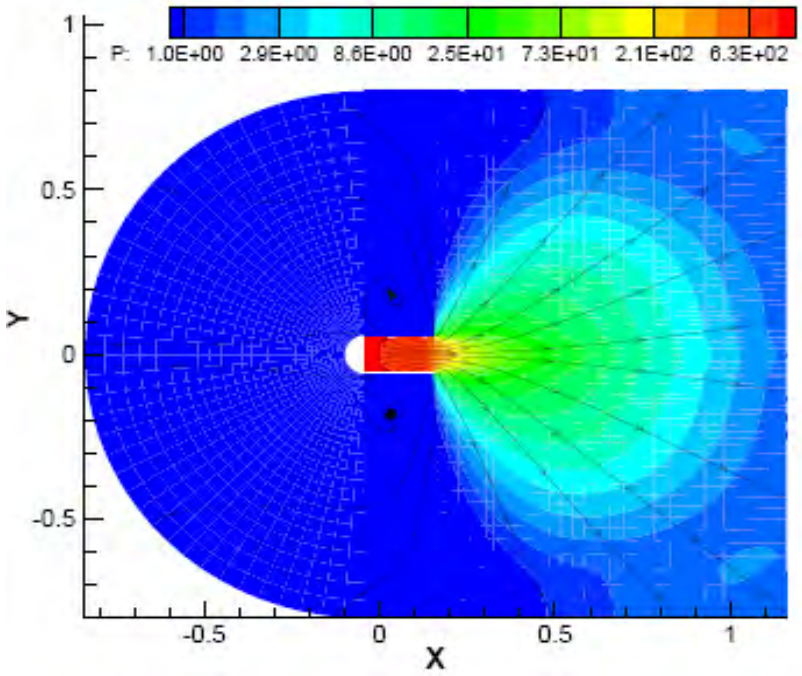
10000

Three stages of the expansion process

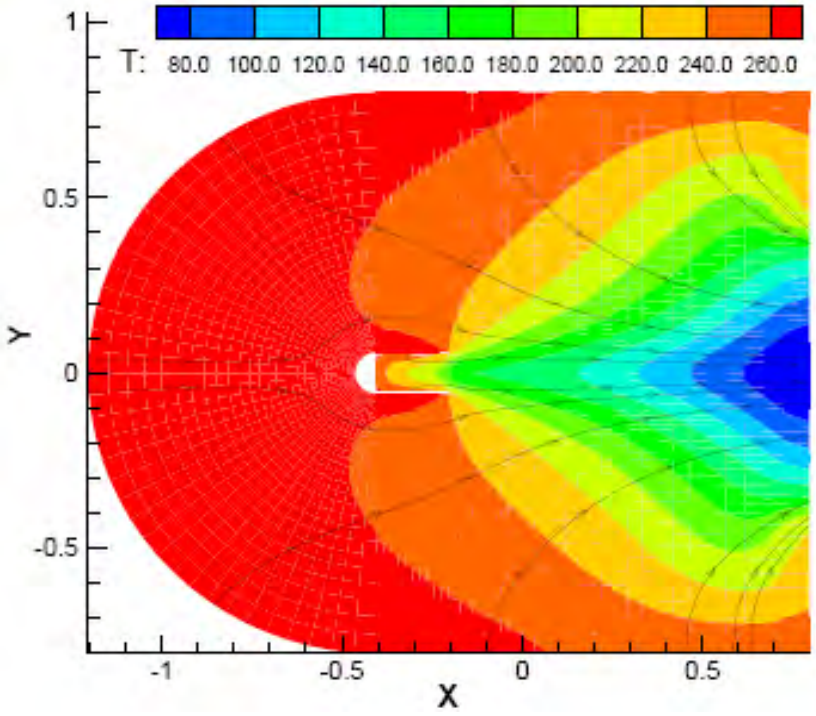
- Free expansion stage
- Jet-like stage
- Deceleration stage

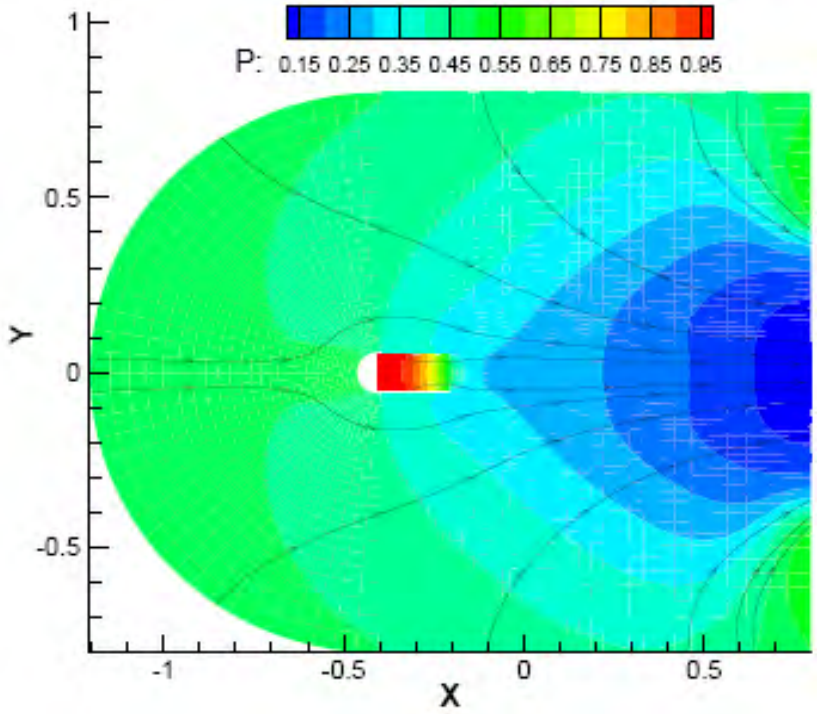
The flow field during free expansion stage



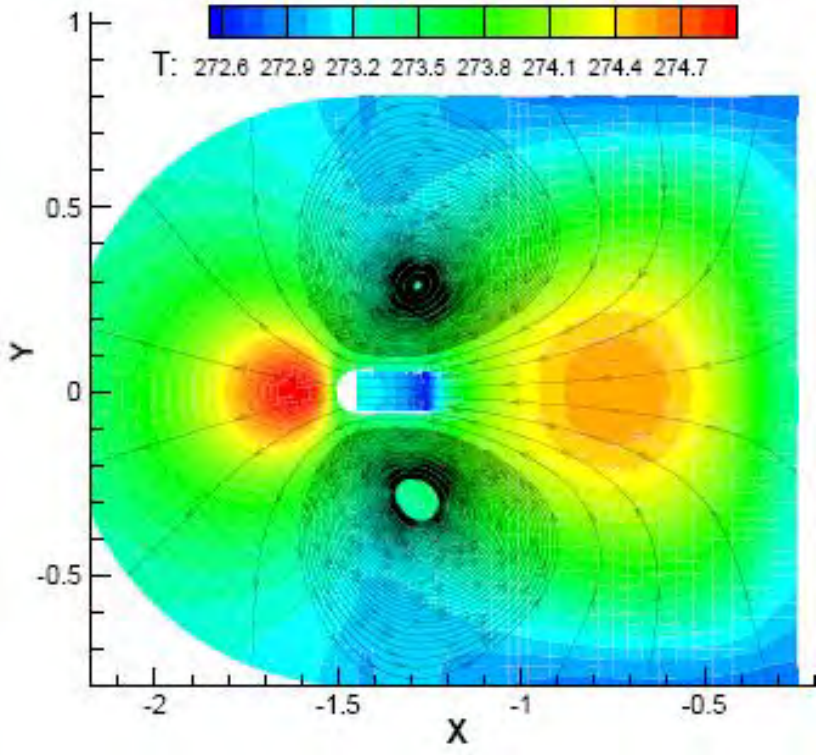


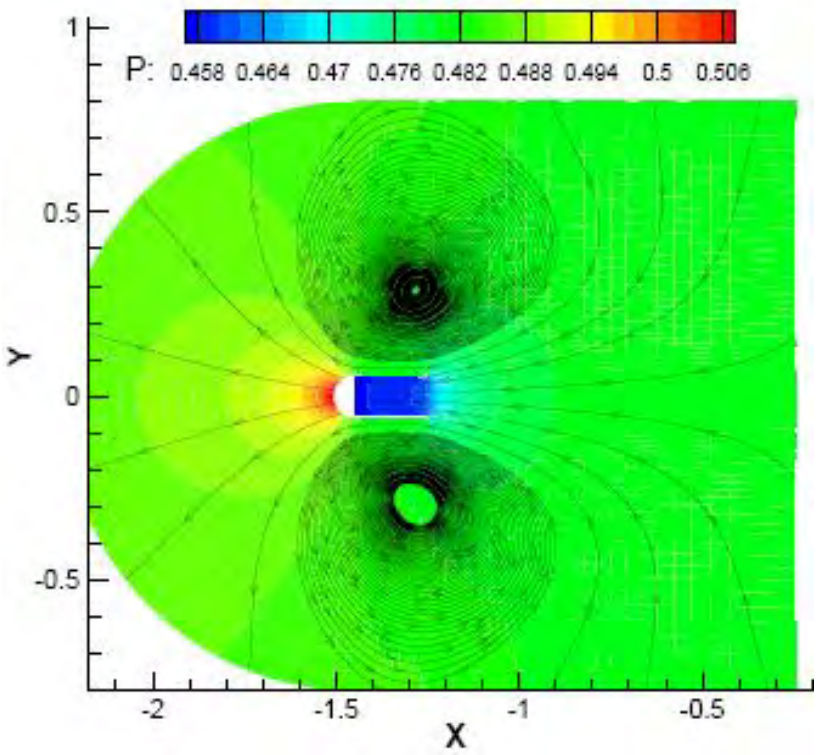
The jet-like flow field



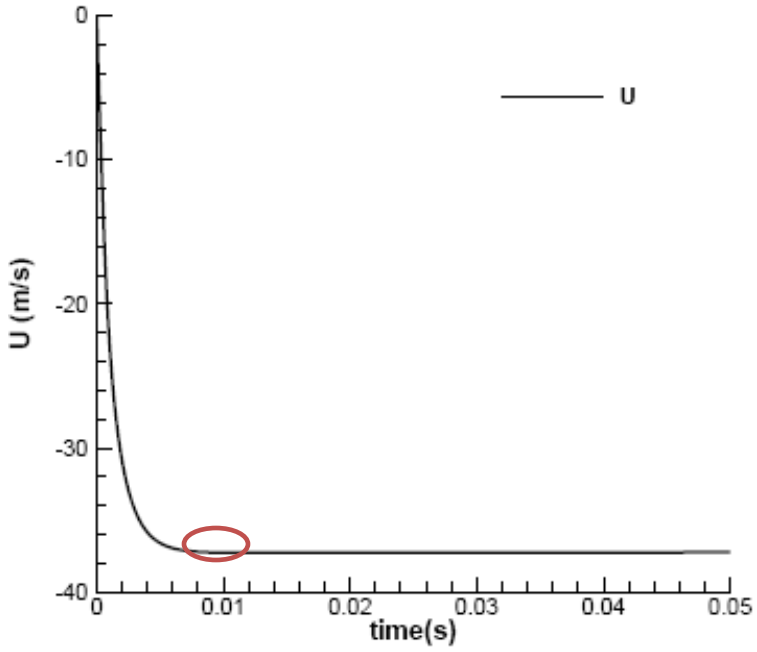


The flow field during deceleration stage

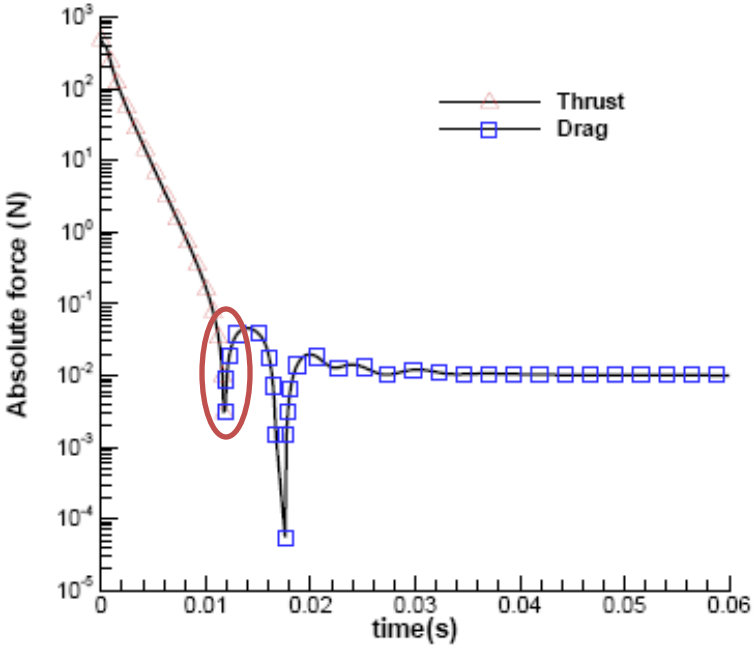




Velocity of the nozzle

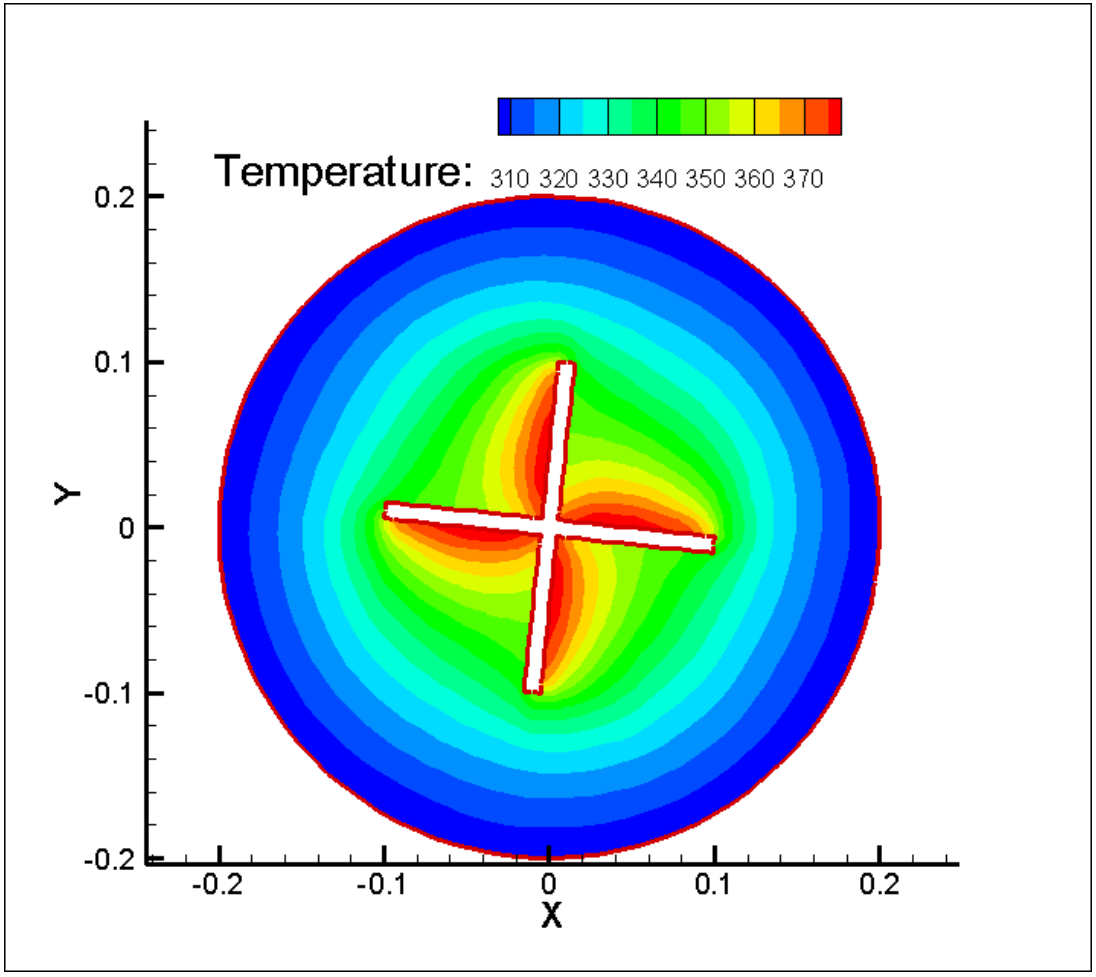


Force exerted on the nozzle



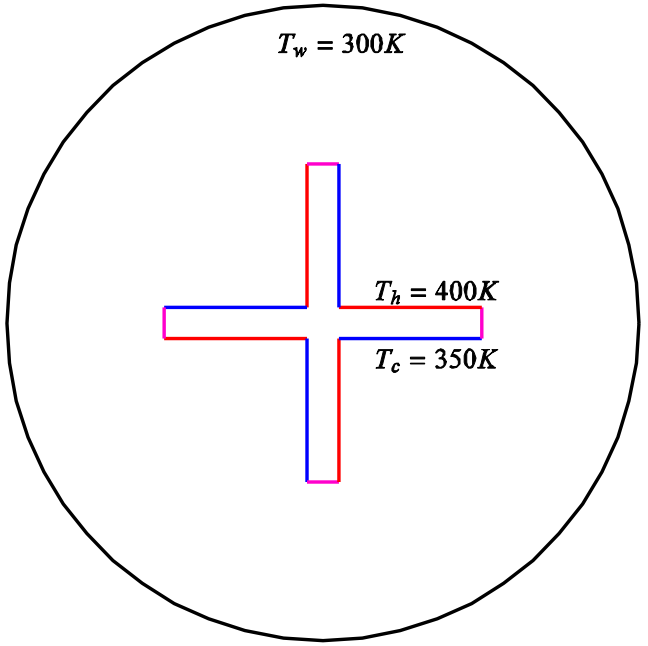
The red circles indicate the jet-like stage

Crookes radiometer



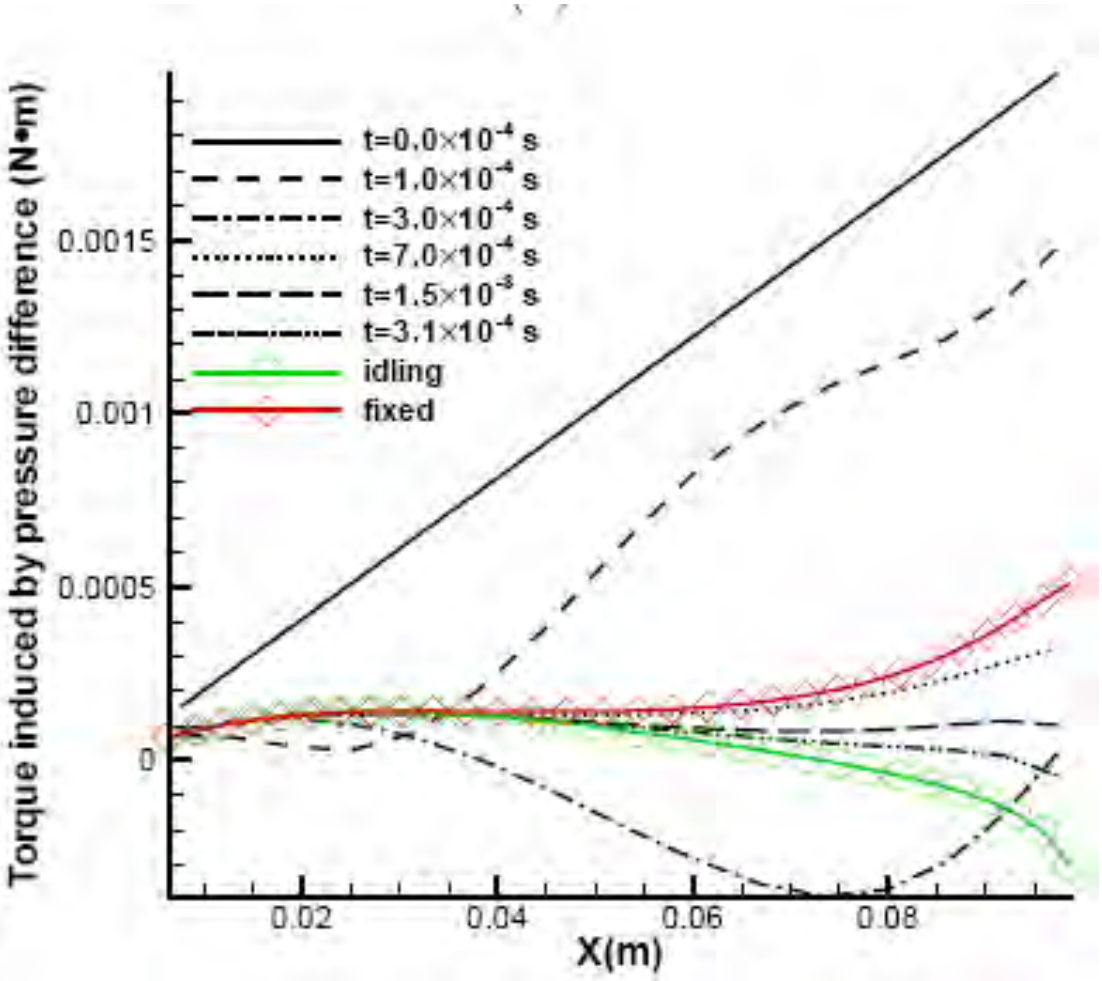
The origin of radiometric force in the Crookes radiometer

- Type
  - Pressure
  - Shear stress
- Location
  - Long arm
  - Lateral side (tip)



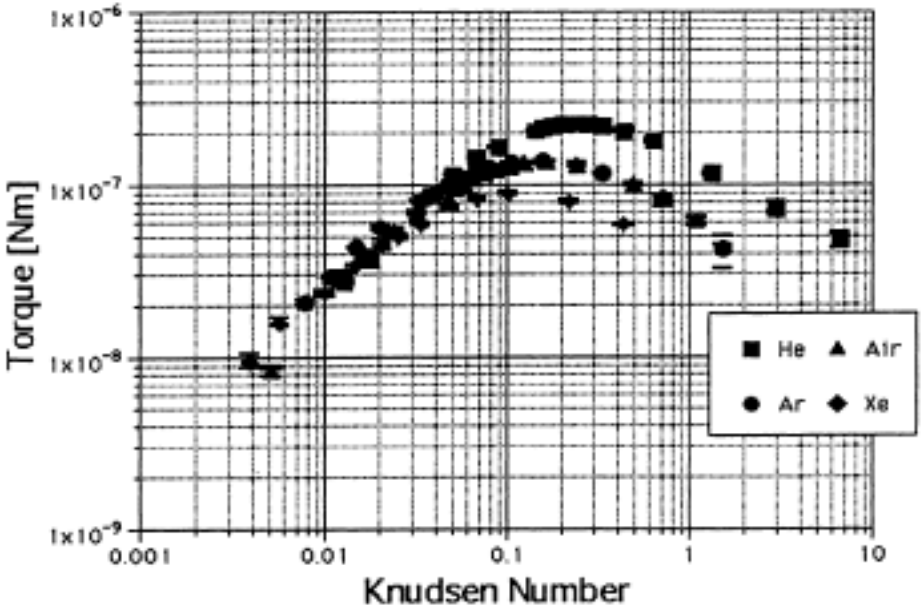
	$M_{p,l}$	$M_{s,l}$	$M_{p,t}$	$M_{s,t}$	M_{total}
Fixed	1.830×10^{-5}	-1.172×10^{-6}	-1.568×10^{-7}	-1.074×10^{-6}	1.590×10^{-5}
Idling	3.738×10^{-6}	-1.009×10^{-6}	-1.648×10^{-7}	-2.560×10^{-6}	4.262×10^{-9}

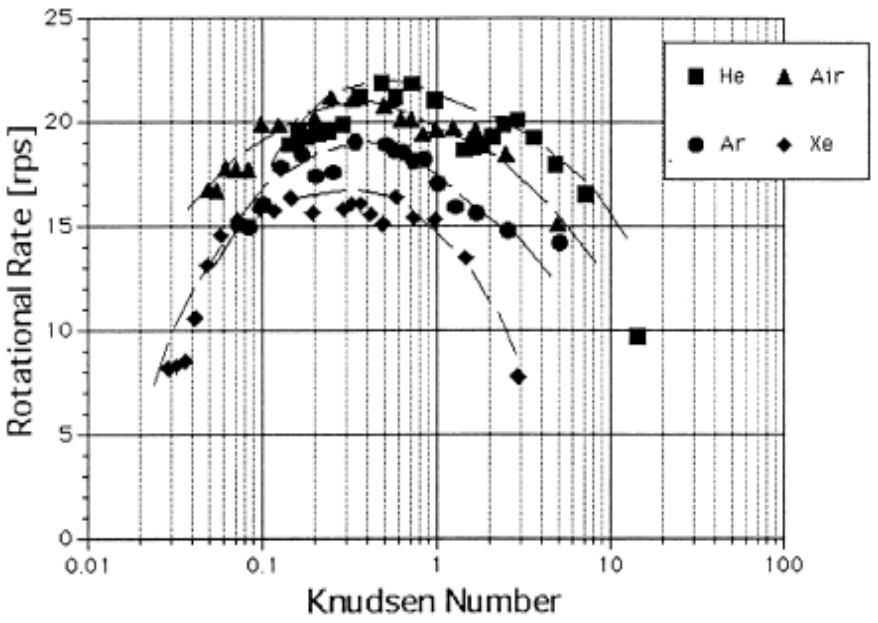
The pressure torque distribution along the long arm for Kn = 0.1



Peak shift

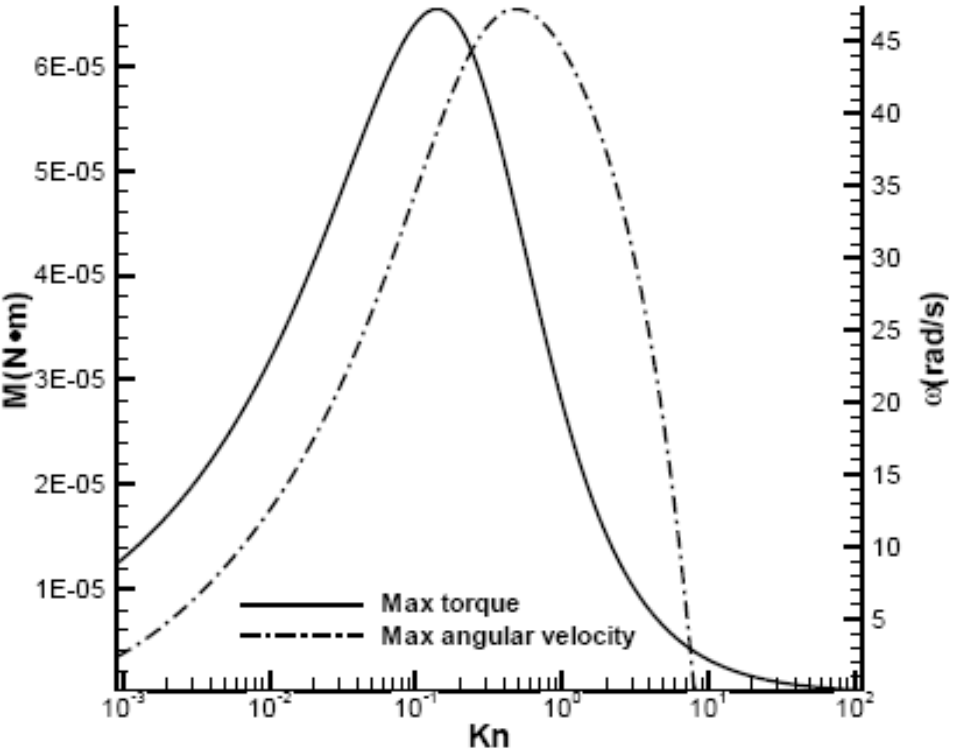
- The maximum of radiometric force and the maximum of the rotary velocity appear at different Knudsen number (Ota, 2001)



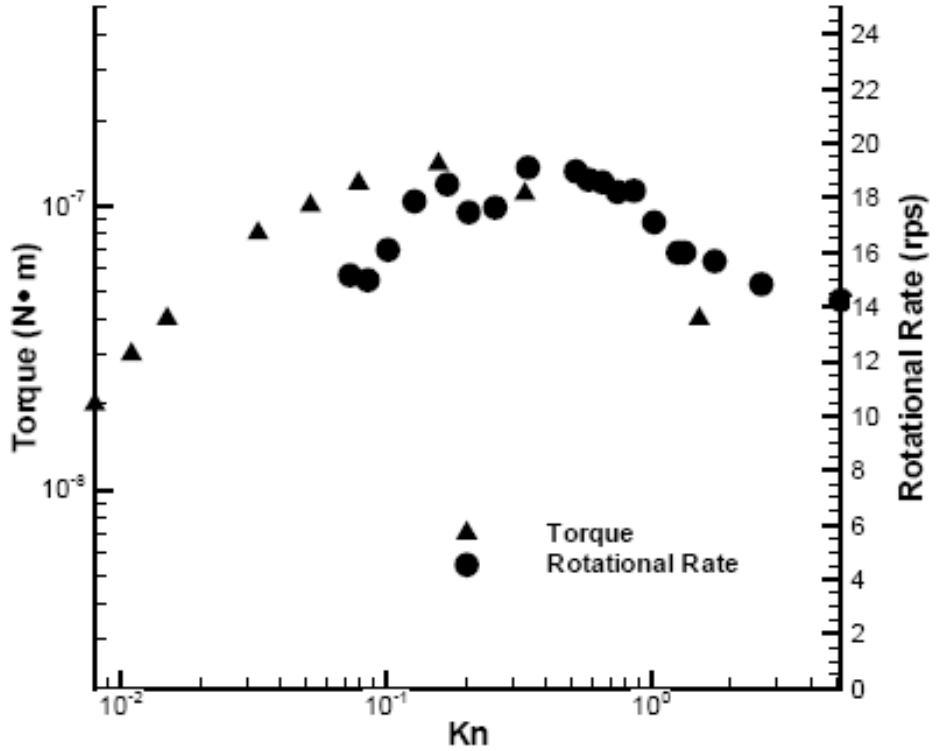


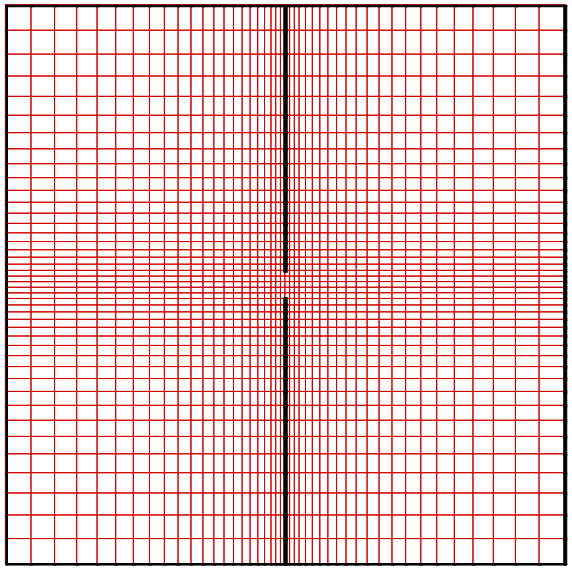
Peak shift reproduced by the semi-rational formula

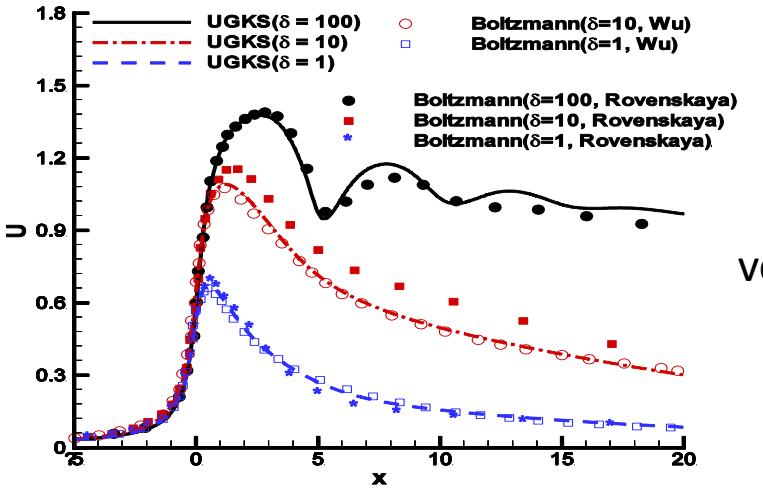
Present study



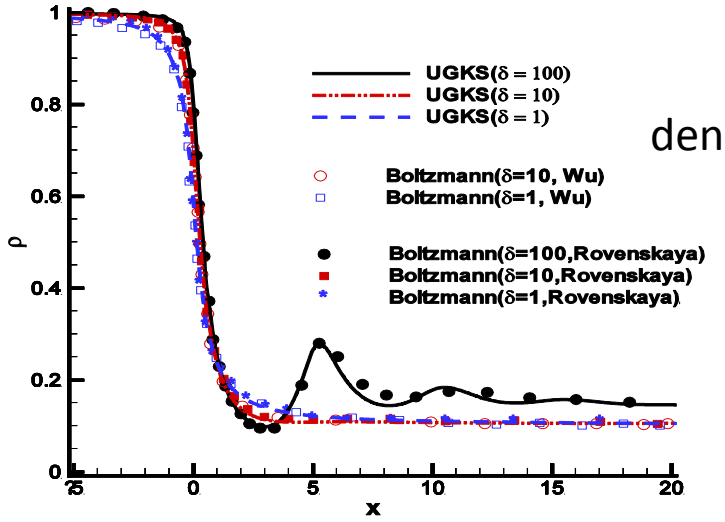
Ota



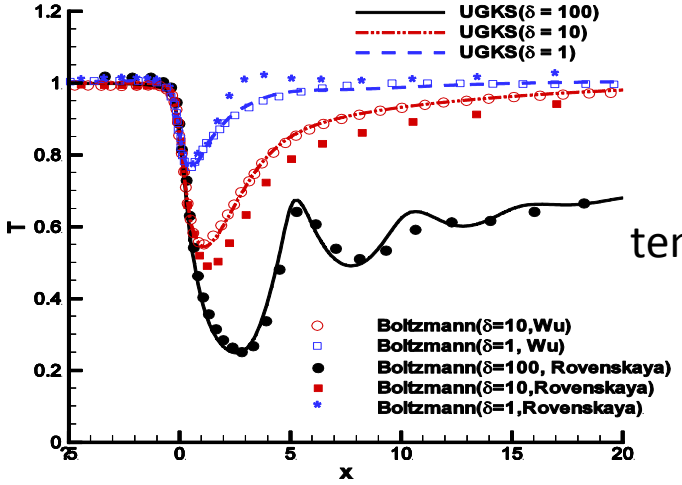




velocity



density

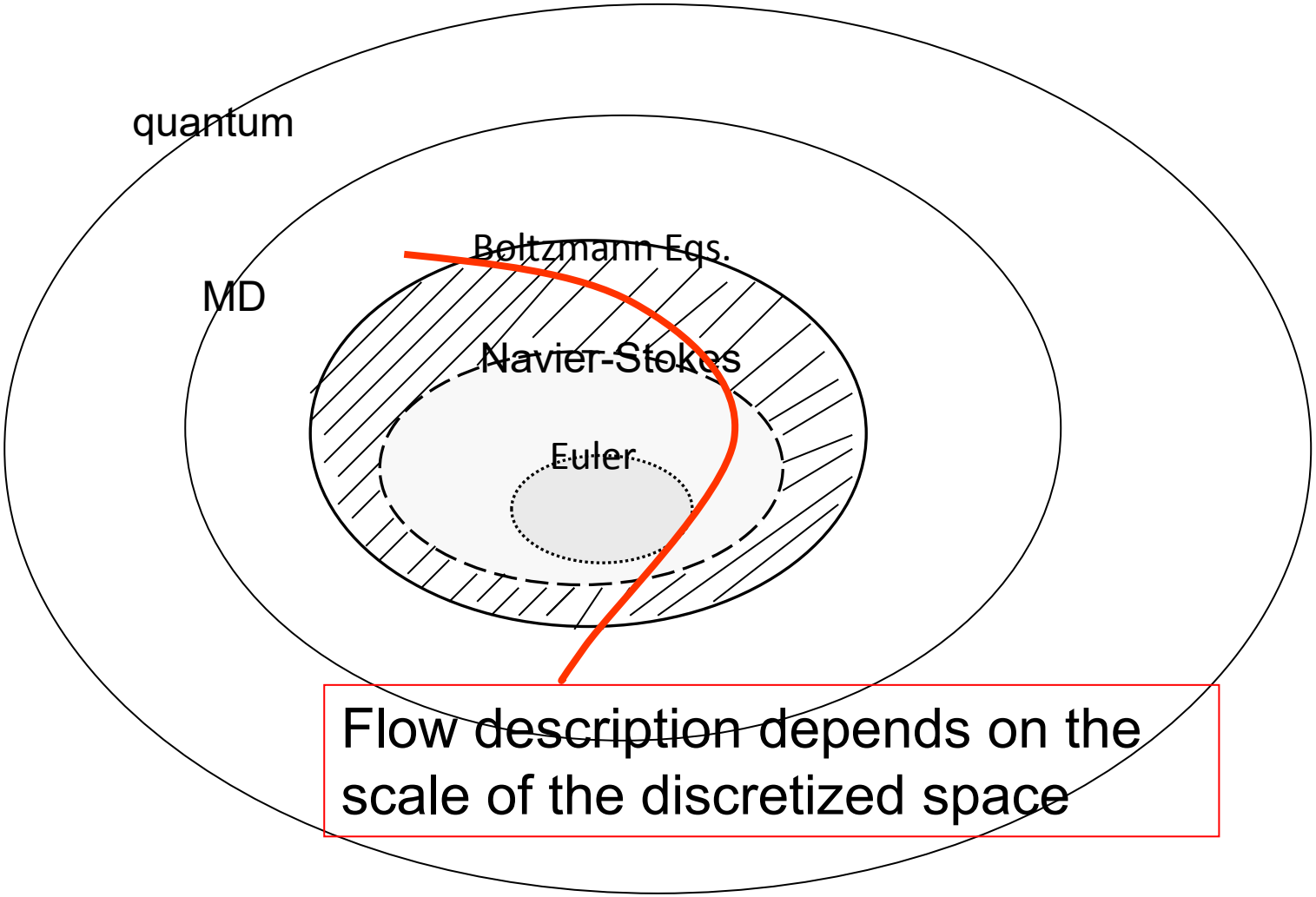


temperature

[1] Olga I. Rovenskaya a, Alexey Ph. Polikarpov b, Irina A. Graur, “Comparison of the numerical solutions of the full Boltzmann and S-model kinetic equations for gas flow through a slit”, Computers and Fluids, in press (2012).

[2] Lei Wu, Craig White, Thomas J. Scanlon, Jason M. Reese and Yonghao Zhang, “ Deterministic numerical solutions of the space-inhomogeneous Boltzmann equation using the fast spectral method”, to appear in Journal of Computational Physics (2013).

Physical modeling in different scales



From Boltzmann to NS, there should have a continuous spectrum of governing equations between them

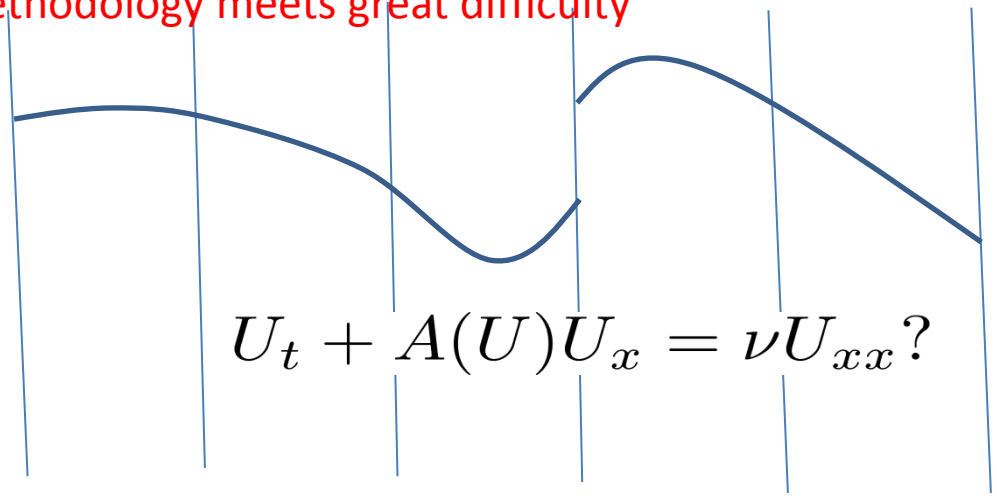
The integral solution provides a multi-scale dynamic modeling:

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

Hydrodynamic scale

Kinetic scale

Traditional CFD methodology meets great difficulty



$$U_t + A(U)U_x = \nu U_{xx}?$$

Numerical Principles

All PDEs have their own valid scales:

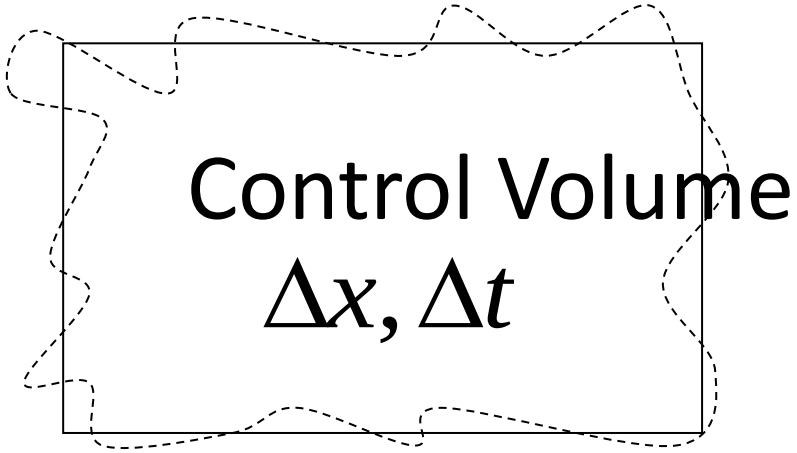
Boltzmann: mean free path, NS: dissipative structures, Euler: convective wave structures,…

Numerical PDE: A direct discretization of PDE is problematic because the cell size can be hardly matched with the PDE's modeling scale. Then, truncation error, modified equations, …, appear in the hope to get a "reliable" scheme.

Direct modeling in discretized space (including effect of cell size resolution in the description of physical flows):

PDE-based modeling: is to use PDE's evolution solution to design the numerical scheme, and this solution is not limited to PDE's modeling scale*, i.e., the evolution solution of the kinetic model is valid when time* $t \gg \tau$*. Certainly, particle-based modeling is fine as well, such as DSMC, but it is difficult to develop a scheme across multiple scales.*

PDE-based Modeling



Fundamental 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

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

The above physical process covers the whole spectrum from free molecular transport to NS solutions.

Conclusion

- Similar to the DSMC method, the unified gas-kinetic scheme (UGKS) is a PDE-based *direct physical modeling* with the update of both macroscopic and microscopic flow variables.
- The un-splitting treatment (transport + collision) of molecules passing through a cell interface plays an important role to capture both *hydrodynamic* and *kinetic scale flow physics.*
- The use of *adaptive particle velocity space* will make the equation based simulation method be competitive to DSMC.
- For low speed micro-flows, the unified gas-kinetic scheme (UGKS) is a reliable and efficient method in comparison with any other method.