Confirmation of Non-classical Laws in Nonequilibrium Gases and their Application to Verification of DSMC

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Verification and Validation (V & V) in rarefied and micro gas flows

V & V; an important issue in all of disciplines
- AIAA Guide for the Verification and Validation of CFD Committee on Standards (1998); Others (ASME)

Verification: The process of determining that a (computational) model implementation accurately represents the developer's conceptual (mathematical) description of the model and the solution to the model. Code Veri.; Calculation Veri.

Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

Why V & V? and common practice in CFD

Reliability becomes critical when laboratory level research enters into the (mature) real world (application) problem.

V & V are complicated and subtle: aerodynamics
drag: CFD dispersion 0.0021, experimental dispersion 0.0004 (goal 0.0001)
lift: CFD dispersion 0.01, goal 0.005
→ V & V depend on what we are examining!
Overall multi-faceted agreement is the most difficult.

Common CFD practice:

- Make sure correct numerical framework (ex. conservative)
- (Grid) convergence study (stable solution)
- Benchmark problems (or exact analytic solutions)

Why V & V in rarefied and micro gas flows are difficult?

- Too many computational models (governing equation, boundary condition)
  Cf. Only one in case of near local equilibrium:
  Linear uncoupled NSF + no-slip (or slip)
- DSMC is not immune since it is also highly subject to the boundary condition and post-processing methods employed.
- Lack of experimental data (how to measure exotic properties such as temperature jump?)
- Lack of theories (guide)

- no consensus what the proper master kinetic equations would be for diatomic gases
- no rigorous gas-surface molecular interaction theory

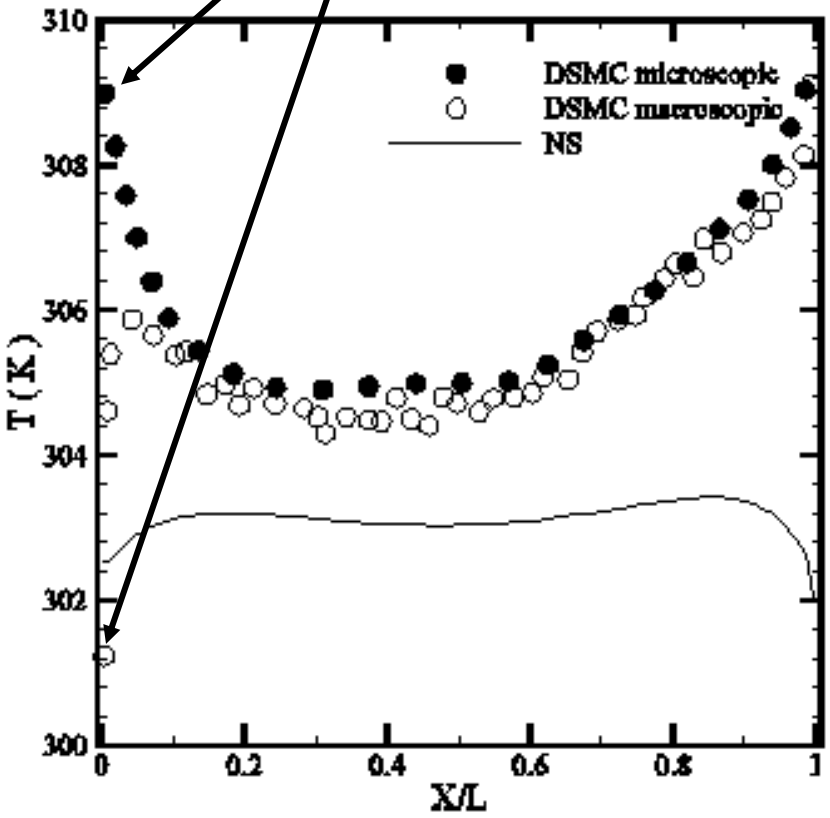
Microscopic sampling vs macroscopic (courtesy of Dr. Roohi)

Direct microscopic sampling of the molecular properties of particles that strike the wall surface

vs

macroscopic approach that accounts for all molecules in the adjacent cell

Which one should be used for the comparison with experimental or other results?



Lid-driven cavity gas flow

Scope in present study:
Verification

Comparison of DSMC with a continuum counterpart (in the level of constitutive physical laws)

Self-consistency of DSMC solutions

Continuum vs molecular

Continuum approach

Chapman-Enskog: Burnett

Moment method: Grad (1949), Eu (1992), R-13 (2005)

(constitutive equations taking into account the microscopic nature of gas molecules)

Top-down

$$\rho \frac{D}{Dt}\begin{bmatrix} 1/\rho \\ \mathbf{u} \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} -\mathbf{u} \\ p\mathbf{I} + \boldsymbol{\Pi} \\ \left(p\mathbf{I} + \boldsymbol{\Pi}\right) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \mathbf{0}$$

shear stress tensor

heat flux vector

$$p = \rho RT : \text{EOS}$$

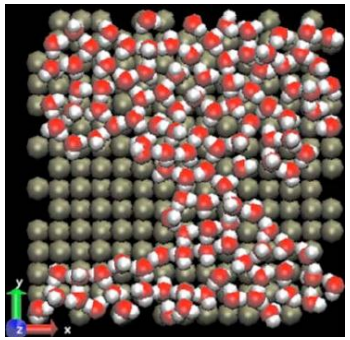
Molecular approach

DSMC

Linearized Boltzmann equation

Lattice-Boltzmann method

Bottom-up



A continuum model: moment method

Boltzmann equation

collision integral

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\mathbf{a}\cdot\nabla_v\right)f(t,\mathbf{r};\mathbf{v})=C[f,f_2]$$

$f(t,\mathbf{r};\mathbf{v})$

$\mathbf{a}$: force

Differentiating the statistical definition

$\rho\mathbf{u}\equiv\langle m\mathbf{v}f(t,\mathbf{r};\mathbf{v})\rangle$

with time

and *then combining*

with the Boltzmann equation

$$\rho=\langle mf(t,\mathbf{r};\mathbf{v})\rangle$$

$$\langle\cdots\rangle=\iiint\cdots dv_x dv_y dv_z$$

Moment equation

$$\rho\frac{D\mathbf{u}}{Dt}+\nabla\cdot(p\mathbf{I}+\boldsymbol{\Pi})=\rho\mathbf{a}$$

$$(\rho,\mathbf{u},T,\boldsymbol{\Pi},\mathbf{Q},\cdots)(t,\mathbf{r})$$

Algebraic (non-classical) constitutive relations

$$\frac{\partial \boldsymbol{\Pi}}{\partial t} + \mathbf{u}\cdot\nabla\boldsymbol{\Pi} = \boxed{-\nabla\cdot\boldsymbol{\psi}^{(\Pi)}} - 2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} + \boxed{\boldsymbol{\Lambda}^{(\Pi)}}$$

Original Grad closure $\left\langle mcccf\right\rangle = \frac{2}{5}\left(\left\langle\frac{1}{2}mc^2\mathbf{c}f\right\rangle_i\delta_{jk} + \left\langle\frac{1}{2}mc^2\mathbf{c}f\right\rangle_j\delta_{ik} + \left\langle\frac{1}{2}mc^2\mathbf{c}f\right\rangle_k\delta_{ij}\right)$

Relaxation approx. $\boldsymbol{\Lambda}^{(\Pi)} \approx -\frac{\boldsymbol{\Pi}}{p/\eta} \Leftarrow f = f^{(0)}\left[1 + \frac{1}{2}\hat{\boldsymbol{\Pi}}:\left[\hat{\mathbf{c}}\hat{\mathbf{c}}\right]^{(2)} - \hat{\mathbf{Q}}\cdot\hat{\mathbf{c}}\left(1-\frac{1}{5}\hat{c}^2\right) + \text{small}\right]$

$$\cancel{\frac{\partial \boldsymbol{\Pi}}{\partial t}} + \mathbf{u}\cdot\cancel{\nabla\boldsymbol{\Pi}} = -\frac{2}{5}\left[\nabla\mathbf{Q}\right]^{(2)} - 2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} - \frac{\boldsymbol{\Pi}}{\eta/p}1$$

steady

no convective in velocity-shear $u\cancel{\frac{\partial}{\partial x}} + \cancel{v}\frac{\partial}{\partial y}$

yielding partial differential type

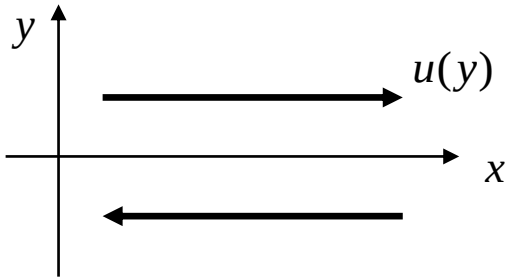
New closure $\left|\nabla\cdot\boldsymbol{\psi}^{(\Pi)}\right| < 2\left|\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}\right|$ and $\boldsymbol{\Lambda}^{(\Pi)} = -\frac{\boldsymbol{\Pi}}{p/\eta}q(\boldsymbol{\Pi},\mathbf{Q},\cdots)$

$$\cancel{\frac{\partial \boldsymbol{\Pi}}{\partial t}} + \mathbf{u}\cdot\cancel{\nabla\boldsymbol{\Pi}} = \cancel{\text{small}} \boxed{-2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} - \frac{\boldsymbol{\Pi}}{\eta/p}q(\boldsymbol{\Pi},\mathbf{Q},\cdots)}$$

yielding algebraic type

Navier-Fourier

Classical Relations



Nonlinear Coupled

Non-classical Relations

$$\Pi_{xy} \leftarrow \Pi_{xy_{NSF}} = -\eta \frac{\partial u}{\partial y}$$

$$\Pi_{yy} \leftarrow \Pi_{yy_{NSF}} = 0$$

$$Q_y \leftarrow Q_{y_{NSF}} = -k \frac{\partial T}{\partial y}$$

$$Q_x \leftarrow Q_{x_{NSF}} = 0$$

$$\Pi_{xy} \leftarrow \frac{3}{3 + 2\left(\Pi_{xy_{NSF}} / p\right)^2} \Pi_{xy_{NSF}}$$

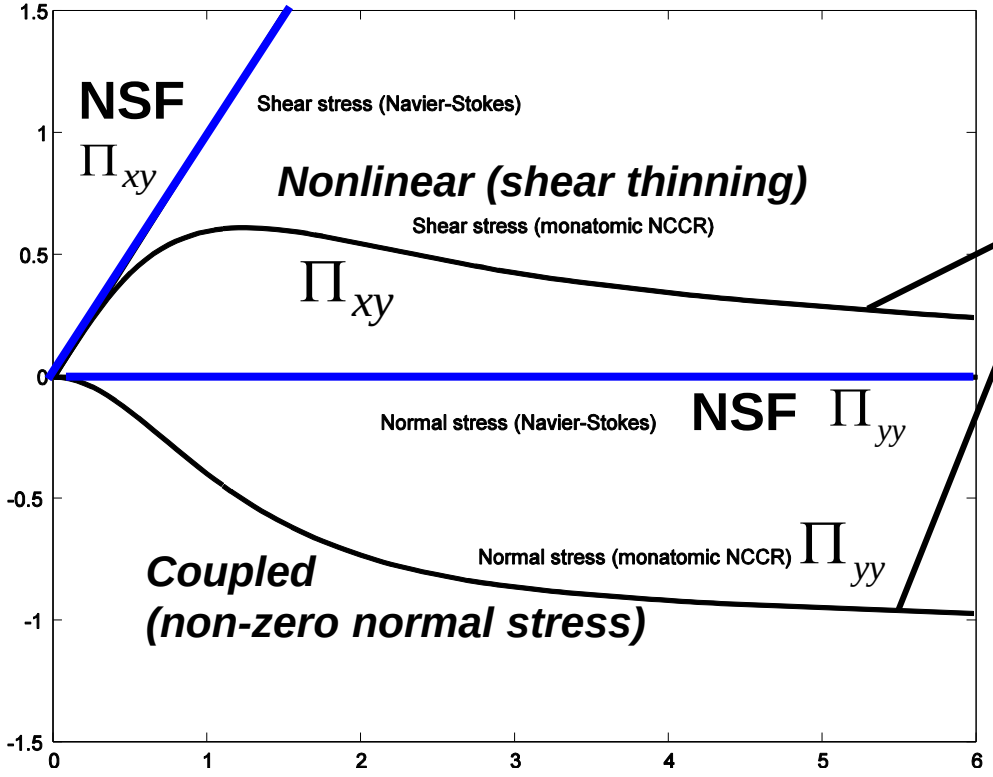
$$\left(\frac{\Pi_{xy}}{p}\right)^2 = -\frac{3}{2}\left(1 + \frac{\Pi_{yy}}{p}\right)\frac{\Pi_{yy}}{p}$$

$$Q_y \leftarrow \left(1 + \frac{\Pi_{yy}}{p}\right) Q_{y_{NSF}}$$

$$\frac{Q_x}{Q_y} = \left(1 + \frac{1}{\mathrm{Pr}}\right)\left(\frac{\Pi_{yy}}{p + \Pi_{yy}}\right)$$

Non-classical stress constraint in velocity shear

$\Pi_{yy,\,xy} \,/\, p$



$$\left(\frac{\Pi_{xy}}{p}\right)^2 = -\frac{3}{2}\left(1+\frac{\Pi_{yy}}{p}\right)\frac{\Pi_{yy}}{p}$$

kinematic stress constraint

$$-\eta\frac{du}{dy}\Big/ p$$

Benchmark problems in rarefied and micro gases

Compression

1-D shock structure (pure 1-D)

Expansion

Free-expansion

Velocity shear

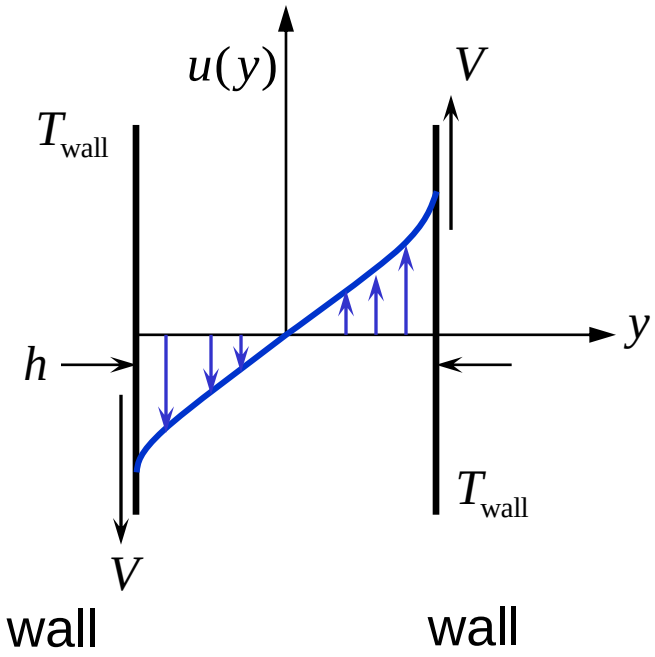
Couette (pure 1D; planar, cylindrical; boundary-driven)

Thermal transpiration (boundary-driven)

Force-driven Poiseuille (pure 1-D)

Pressure-driven Poiseuille

Gaseous Couette flow



$$M \equiv \frac{V}{\sqrt{\gamma R T_{\text{wall}}}}$$

$$\text{Kn} \equiv \sqrt{\frac{\pi}{2}} \frac{\eta_{\text{wall}} \sqrt{R T_{\text{wall}}}}{p(0) h}$$

Exact consequence of Boltmann equation

$$\frac{d}{dy} \begin{bmatrix} \Pi_{xy} \\ p + \Pi_{yy} \\ \Pi_{xy} u + Q_y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\Downarrow$$

Π_{xy} constant in y axis

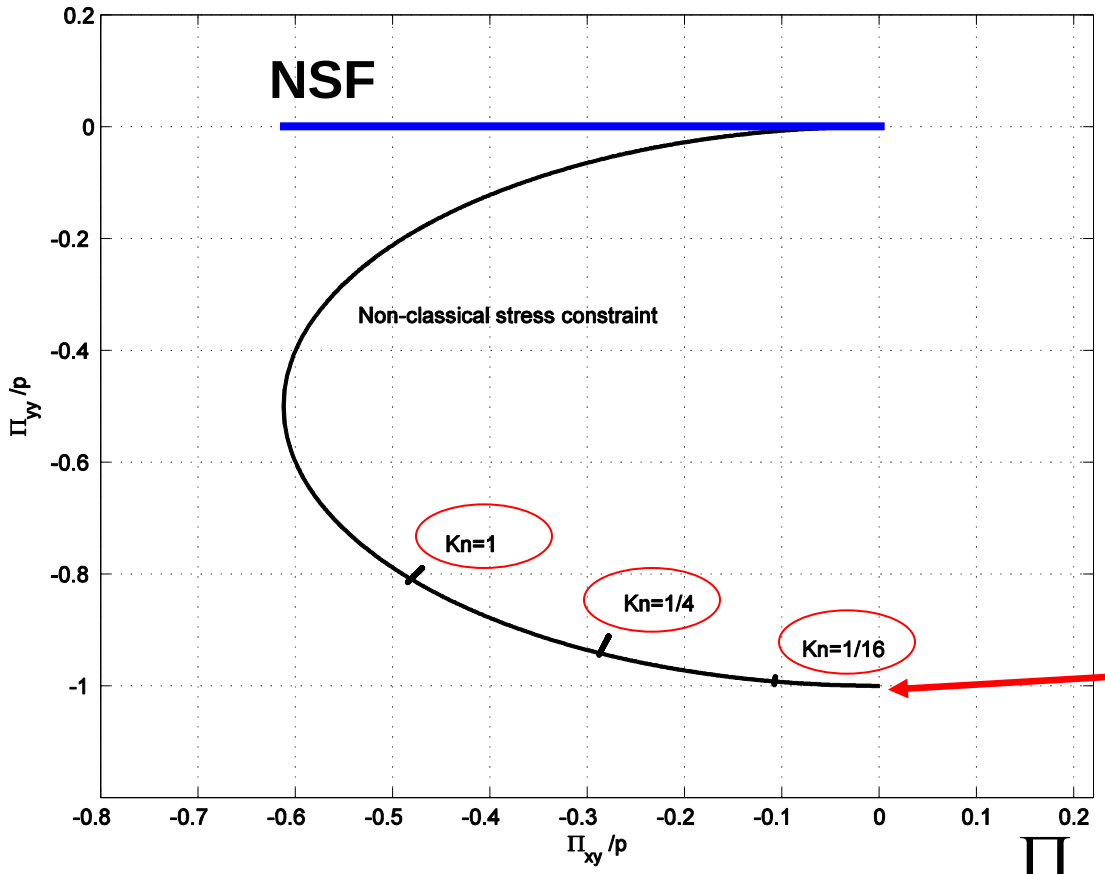
$(p + \Pi_{yy})$ constant in y axis

p constant if Π_{yy} is constant

(probably true due to flow symmetry)

Comparison of DSMC with non-classical relations

Π_{yy}/p



Π_{xy}/p

M=2.0 case

Kn=1/16,1/4,1.0

Diffusive wall

100,000 molecules

Stress constraint in elliptic form

$$\left(\frac{\Pi_{xy}}{p}\right)^2 = -\frac{3}{2}\left(1+\frac{\Pi_{yy}}{p}\right)\frac{\Pi_{yy}}{p}$$

"Diatomic gases are from Mars (hyperbolic world), monatomic gases are from Venus (elliptic world)."

Self-consistency in DSMC solutions

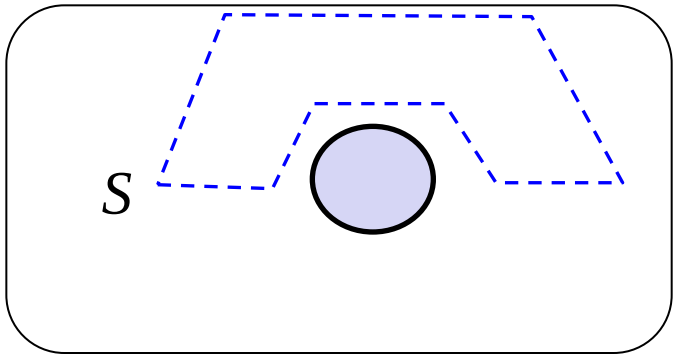
Key observation: **The conservation laws must be satisfied irrespective of computational models.** (*Comp. Fluids* 2011)

They are satisfied in cell level in case of conservative CFD codes like FLUENT.

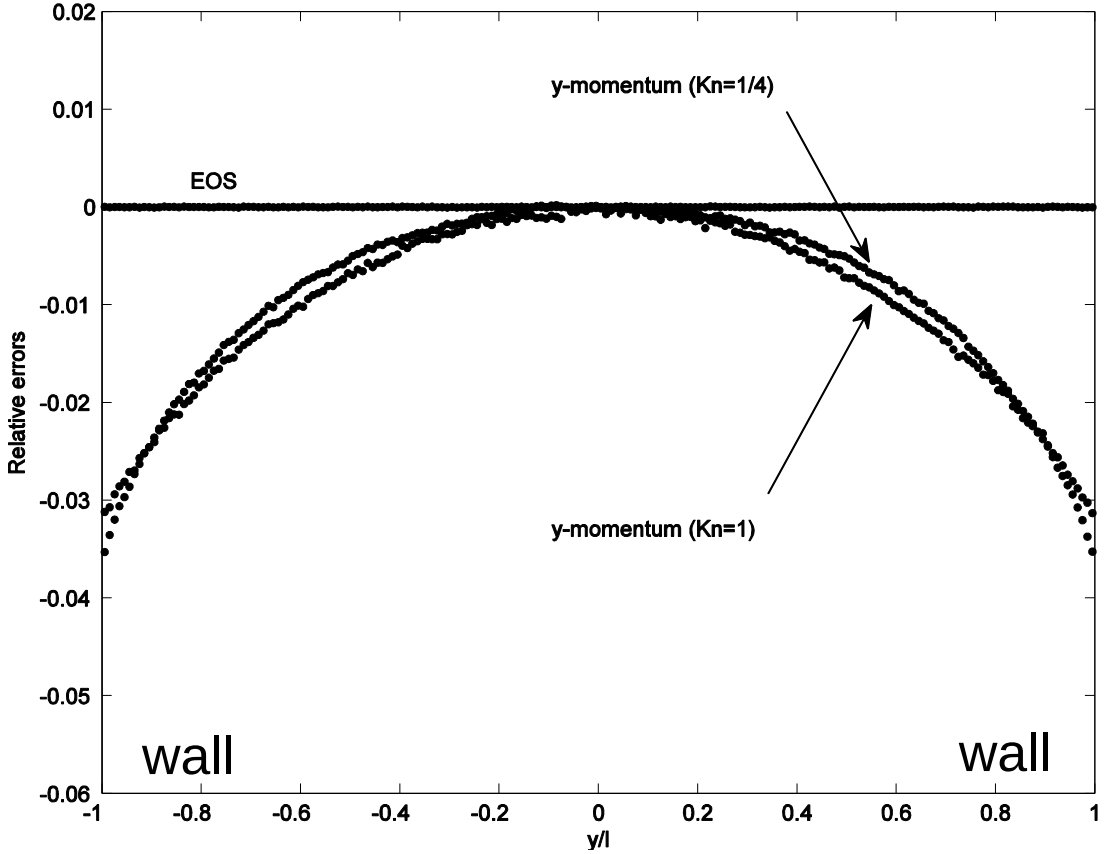
The relative internal error of numerical solutions for one-dimensional gas flow can be easily checked. (Straightforward in 2-D and 3-D cases as well)

$$\oint_S \mathbf{F}\cdot\mathbf{n}dS = 0 \quad \text{or} \quad \nabla\cdot\mathbf{F} = 0$$

S presenting the bounding surface of the control volume



Self-consistency in DSMC solutions (1-D Couette with solid wall)



$$\nabla \cdot \mathbf{F} = 0$$

$$\text{error}_{x-momentum} \equiv \Pi^*_{xy} - \left[\Pi^*_{xy}\right]_{y=0}$$

$$\text{error}_{y-momentum} \equiv p^* + \Pi^*_{yy} - 1 - \left[\Pi^*_{yy}\right]_{y=0}$$

$$\text{error}_{energy} \equiv \Pi^*_{xy}u^* + Q^*_y - \left[\Pi^*_{xy}u^* + Q^*_y\right]_{y=0}$$

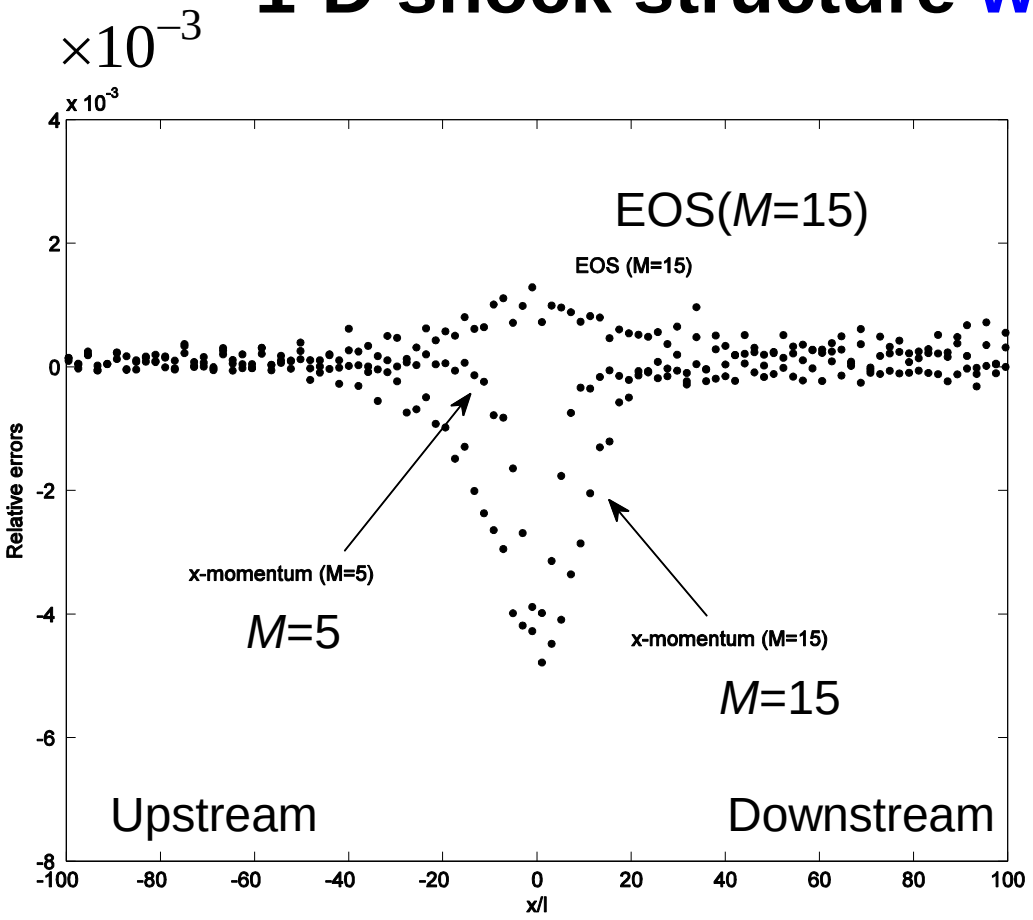
$$\text{error}_{EOS} \equiv p^* - \rho^* T^*$$

*: non-dimensionalized by values at center

The y-momentum error of the DSMC increases from the center to the solid wall.
Origin of error: the pressure

The pressure is the most critical quantity affected by the boundary condition, implying its careful treatment.

1-D shock structure without solid wall



$$\nabla \cdot \mathbf{F} = 0$$

$$\text{error}_{mass} \equiv \rho^* u^* - 1$$

$$\text{error}_{x-momentum} \equiv \left[\gamma M_1^2 (\rho^* u^* - 1) + p^* - 1 + \Pi_{xx}^* \right] \Big/ (1 + \gamma M_1^2)$$

$$\text{error}_{energy} \equiv \left[\begin{array}{l} \dfrac{\gamma}{\gamma - 1}(p^* u^* - 1) + \\ \dfrac{1}{2}\gamma M_1^2 (\rho^* u^{*3} - 1) + \Pi_{xx}^* u^* + Q_x^* \end{array} \right] \Big/ \left(\frac{\gamma}{\gamma - 1} + \frac{1}{2}\gamma M_1^2 \right)$$

$$\text{error}_{EOS} \equiv p^* - \rho^* T^*$$

*: Non-dimensionalized by upstream values

The x-momentum error is largest at the shock structure region, but its relative magnitude is very small:

Order of $O(10^{-3})$

The case not involving with wall boundary condition shows the accurate representation of conservation laws and EOS.

Concluding remarks

- V & V becoming critical when a technology moves into mature stage
- Monatomic gases from Venus (elliptic stress constraint world)
- Need of paying attention to the pressure (flowfield and surface) results in DSMC
- Need of further experimental investigation on the whole flowfields, including diatomic gases. (For example, in pressure-driven microchannel flow, cross-stream pressure distribution beyond a reduced quantity such as the mass flow rate.)