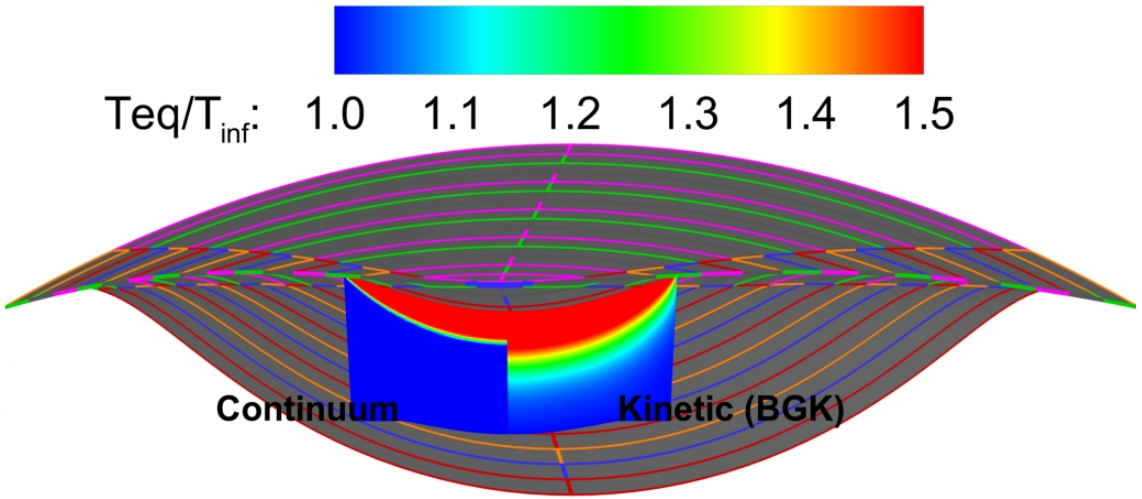
Kinetic Models and Gas-Kinetic Schemes with Rotational Degrees of Freedom for Hybrid Continuum/Kinetic Boltzmann Methods



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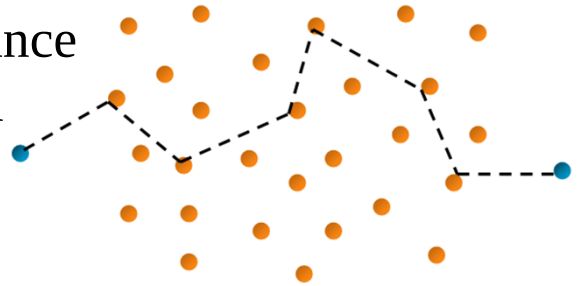
Introduction (1)

- Hypersonic flows often involve flow fields having continuum and rarefied regions
- Knudsen number: $Kn = \frac{mean\ free\ path}{scale}$ $\xrightarrow{\text{locally}}$ $\frac{\lambda}{Q}\left|\frac{dQ}{dl}\right|$

The mean free path is the distance travelled by a particle between successive collisions



- In a rarefied flow, the effect of intermolecular collisions is not sufficient to drive the fluid local toward local thermal equilibrium
  - over time scale of interest all particle degrees of freedom are in equilibrium with each other

Introduction (2)

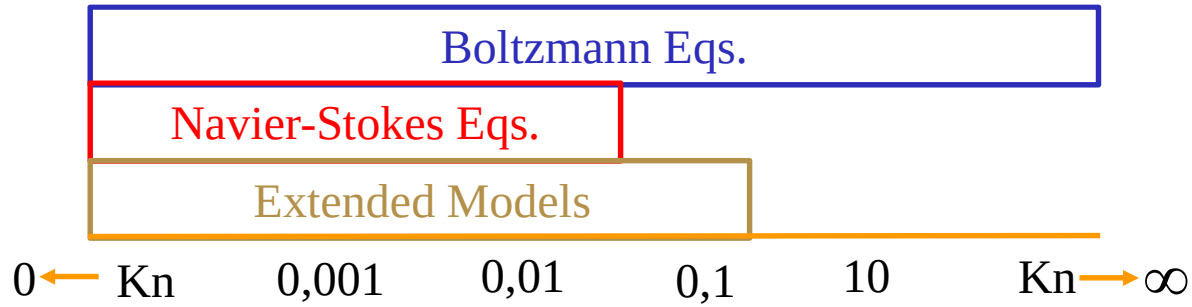
- The Botzmann Equation (BTE) describes the behaviour of a gas by mean of a distribution function, $f(\boldsymbol{x},\boldsymbol{V},t)$ representing the probability of particles with position $\boldsymbol{x}$ and velocity $\boldsymbol{V}$ at time t

$$\frac{\partial(nf)}{\partial t} + \mathbf{V}\cdot\nabla(nf) = \triangle[Q(f)]$$

$$\rho = \int_{-\infty}^{+\infty}\!\!\int\!\!\int nmf\,d\mathbf{c}\,d\xi \qquad \rho\mathbf{u} = \int_{-\infty}^{+\infty}\!\!\int\!\!\int nm\mathbf{c}f\,d\mathbf{c}\,d\xi \qquad \rho e_{tot} = \int_{-\infty}^{+\infty}\!\!\int\!\!\int \tfrac{1}{2}nm\,(\mathbf{c}^2+\xi^2)\,f\,d\mathbf{c}\,d\xi$$

Maxwellian

$$f_m = \frac{\rho}{(2\pi RT)^{3/2}}\exp\left(-\frac{c'^2}{2RT}\right)$$



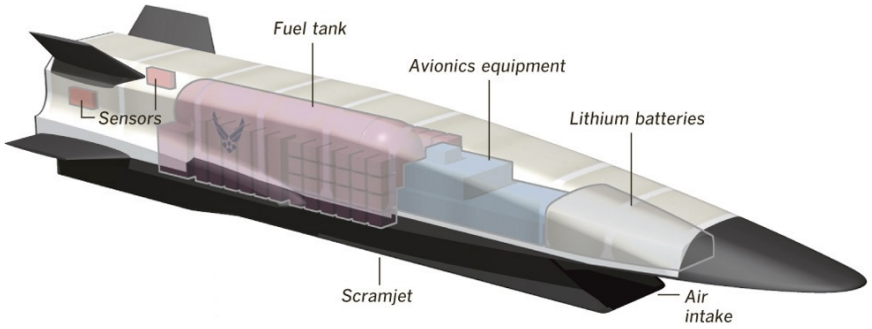
- For Kn $\longrightarrow$ 0, $f = f_m$ and, employing the Chapman-Enskog expansion, the Navier-Stokes Equations (NS) can be obtained as hydrodynamic limit of the BTE

$$\left[\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j}\right] = \rho f_{vol,\,i} - \frac{\partial p}{\partial x_i} + \mu\frac{\partial^2 u_i}{\partial x_j \partial x_j} + (\lambda' + \mu)\frac{\partial}{\partial x_i}\left[\frac{\partial u_j}{\partial x_j}\right]$$

Motivation

Partially rarefied flow: continuum flow with locally rarefied regions

- NS based computational fluid dynamics methods can simulate gas flows with Kn number below a certain limit
- BTE based methods are more expensive and become unfeasible at low Kn numbers $f(x, y, z, u, v, w; t) \longrightarrow$ more degrees of freedom
- Hybrid techniques reduces the use of Kinetic / DSMC approach where they are strictly necessary, leaving the simulation in the rest of the domain to a continuum solver



Moreover a general implementation able to cope with complex 3D geometries of aerospace interest is not common in the literature

Mathematical Models

Continuum Regime

Navier-Stokes Equations

Rarefied Regime

Boltzmann Equation

Direct Simulation Monte Carlo (DSMC)

[1]

- Statistical
- Scattering Error and expensive at intermediate Kn
- Well established for highly rarefied flows

Kinetic Boltzmann Equation

Discrete Velocity Method (DVM)

[2], [3]

Relaxation term: $\frac{F - M(F)}{\tau}$

- Deterministic
- Simplified model
- Less CPU time expensive at intermediate Kn

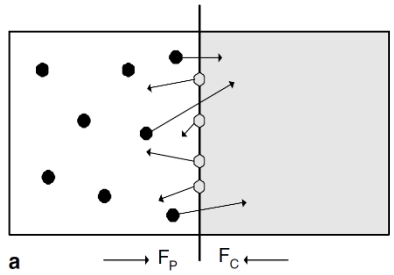
[1] Bird G.A., 1994. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. *Oxford University Press*.

[2] Bhatnagar P.L., Gross E.P and Krook M., 1954. A Model for Collisional Processes in Gases. *Phys. Rev.*, 94:511-525

[3] Shakhov E. M., 1968. Generalization of the Krook Kinetic Relaxation Equation. *Fluid Dynamics*, 3:p95-96

Coupling Techniques

Coupling by Fluxes [1], [2]

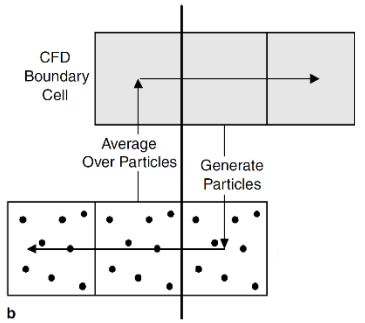


Coupling at equation level

by mean of a weight function [3]:

$$W(x,t)$$

State Based Coupling [4]



DSMC: state based mandatory for lower scattering error

DVM: various techniques have been used and there is not a common choice

[1] Le Tallec P. and Mallinger F., 1997. Coupling Boltzmann and Navier-Stokes Equation by Half Fluxes. *Journal of Computational Physics*, 136:51–67.

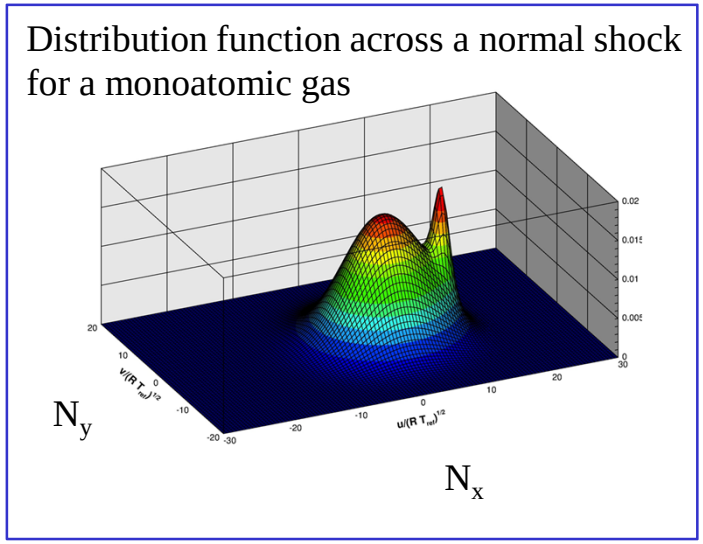
[2] Steijl R. and Barakos G., 2010. Coupled Navier-Stokes-Molecular dynamics simulations using a multi--physics flow simulation framework. International Journal for Numerical Methods in Fluids, 62:1081-1106

[3] Degond P., Shi Jin and Mieussens L., 2005. A smooth transition model between kinetic and hydrodynamic equations. *Journal of Computational Physics*, 209:665–694

[4] Schwartzentruber T.E. and Boyd I.D., 2006. A hybrid particle-continuum method applied to shock waves. *Journal of Computational Physics*, 215:402–416.

The MϕC Kinetic Solver

- Built on the Multi-Physics Code (MϕC) presented in [1]
- Discrete Velocity Method (DVM) for kinetic model equations
- A discretised velocity space $(N_x \cdot N_y \cdot N_z)$ has to be defined at each point in the physical space



- $N_x \cdot N_y \cdot N_z$ values per cell has to be updated each time step
- $N_x \cdot N_y \cdot N_z$ numerical fluxes per cell to be evaluated

[1] Steijl R. and Barakos, G., 2012. Computational Fluid dynamics of Partially Rarefied Flows with Coupled Kinetic Boltzmann/Navier-Stokes Methods. *ECCOMAS 2012*, 10-14 September, Vienna, Austria 2012

Shakhov Kinetic Model

- Kinetic models describes approximately the molecular collisions by means of a relaxation process such that moments up to a certain order are respected
- The Shakhov Model [1] considers only translational non-equilibirum, then is limited to monoatomic gases

$$\frac{\partial F}{\partial t} + \mathbf{c}\frac{\partial F}{\partial \mathbf{x}} = \frac{F^S - F}{\tau} \qquad \underline{\text{Maxwellian}} \quad F_M(T) = \frac{\rho}{(\pi T)^{3/2}} \exp\left(-\frac{c'^2}{T}\right)$$

$$F^S = F_M(T)\left[1 + \frac{8}{15}\frac{q_i^t}{p}\frac{c'_i}{T}\left(\frac{c'^2}{T} - \frac{5}{2}\right)\right] \qquad \underline{\text{Collision Time}} \quad \tau = \frac{\mu}{p}$$

$$\rho = \int_{-\infty}^{+\infty} F d\mathbf{c} \qquad \rho u_i = \int_{-\infty}^{+\infty} c_i F d\mathbf{c} \qquad \frac{3}{2}\rho T + \rho u_x^2 = \int_{-\infty}^{+\infty} c^2 F d\mathbf{c}$$

[1] Shakhov E., 1968. Generalization of the Krook Kinetic Relaxation Equation. *Mekhanika Zhidkosti i Gaza*, 3(5):142–145.

Rykov Kinetic Model (1)

- The Rykov Model [1] considers also rotational non-equilibirum
- Considering the rotational degrees of freedom fully excited the model can be reduced

$$\begin{cases} \frac{\partial F_0}{\partial t} + \mathbf{c}\frac{\partial F_0}{\partial \mathbf{x}} = \frac{F_0^{eq} - F_0}{\tau} \\ \frac{\partial F_1}{\partial t} + \mathbf{c}\frac{\partial F_1}{\partial \mathbf{x}} = \frac{F_1^{eq} - F_1}{\tau} \end{cases}$$

the rotational degrees of freedom contribution is included in the distribution functions definition

$$F_0 = \int_{-\infty}^{+\infty} F\, d\xi \qquad F_1 = \int_{-\infty}^{+\infty} \xi^2 F\, d\xi$$

$$\rho = \int_{-\infty}^{+\infty} F_0 d\mathbf{c} \qquad \rho u_i = \int_{-\infty}^{+\infty} c_i F_0 d\mathbf{c} \qquad \frac{3}{2}\rho T_t + \rho u_x^2 = \int_{-\infty}^{+\infty} c^2 F_0 d\mathbf{c} \qquad \rho T_r = \int_{-\infty}^{+\infty} F_1 d\mathbf{c}$$

[1] Rykov, V., 1975. A Model Kinetic Equation for a Gas with Rotational Degrees of Freedom. *Fluid Dynamics*, 10(6):pp. 959–966.

Rykov Kinetic Model (2)

$$F_0^{eq} = \frac{1}{Z_r} F_0^r + \left(1 - \frac{1}{Z_r}\right) F_0^t$$

$$F_1^{eq} = \frac{1}{Z_r} F_1^r + \left(1 - \frac{1}{Z_r}\right) F_1^t$$

Collision number

$$Z_r = \frac{\tau_r}{\tau} > 1$$

$$F_0^r = F_M(T)\left[1 + \frac{8}{15}\omega_0 \frac{q_i^t}{p}\frac{c'_i}{T}\left(\frac{c'^2}{T} - \frac{5}{2}\right)\right]$$

$$F_0^t = F_M(T_t)\left[1 + \frac{8}{15}\frac{q_i^t}{p_t}\frac{c'_i}{T_t}\left(\frac{c'^2}{T_t} - \frac{5}{2}\right)\right]$$

$$F_1^r = TF_M(T)\left[1 + \frac{8}{15}\omega_0 \frac{q_i^t}{p}\frac{c'_i}{T}\left(\frac{c'^2}{T} - \frac{5}{2}\right) + 4\omega_1(1-\delta)\frac{q_i^r c'_i}{pT}\right]$$

$$F_1^t = T_r F_M(T_t)\left[1 + \frac{8}{15}\frac{q_i^t}{p_t}\frac{c'_i}{T_t}\left(\frac{c'^2}{T_t} - \frac{5}{2}\right) + 4(1-\delta)\frac{q_i^r c'_i}{p_t T_r}\right]$$

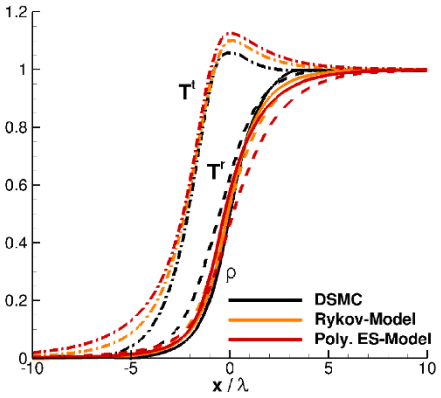
$$F_M(T) = \frac{\rho}{(\pi T)^{3/2}} \exp\left(-\frac{c'^2}{T}\right)$$

- A variable collision number can be considered and the expression obtained from molecular dynamics in [1] is employed in the current work

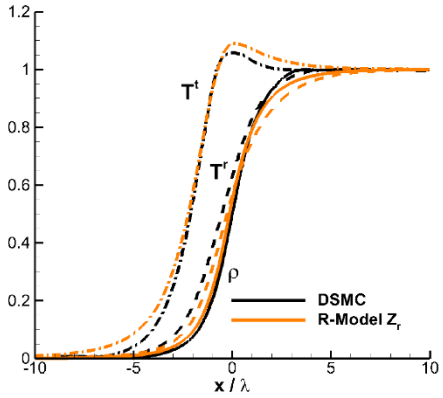
$$Z_r = \left[a_1 \left(\frac{T_t}{1K}\right)^{1/4} + a_2 \left(\frac{T_t}{1K}\right)^{-1/4} - a_3 \left(\frac{T_t}{1K} - 1000\right)\right]\left[1 - b\left(1 - \frac{T_r}{T_t}\right)\right]$$

[1] Valentini, P., Zhang, C. and Schwartzentruber, T., 2012. Molecular Dynamics Simulation of Rotational Relaxation in Nitrogen: Implications forcRotational Collision Number Models. *Physics of Fluids*, 24:106101:1–23.

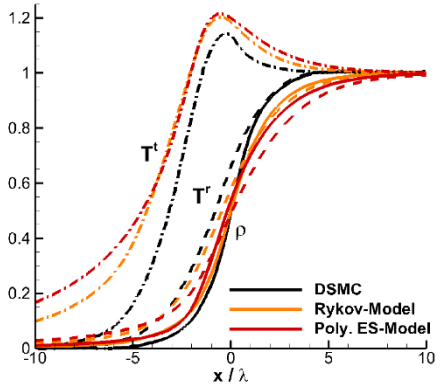
Rykov Kinetic Model Results (1)



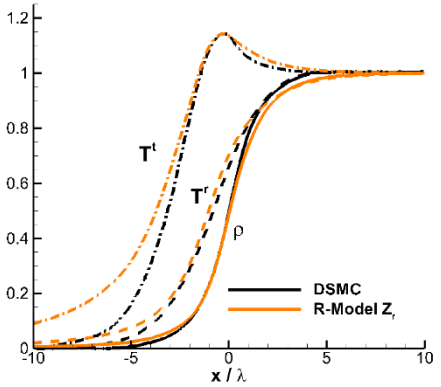
(a) M= 2.8



(b) M= 2.8



(a) M= 10



(b) M= 10

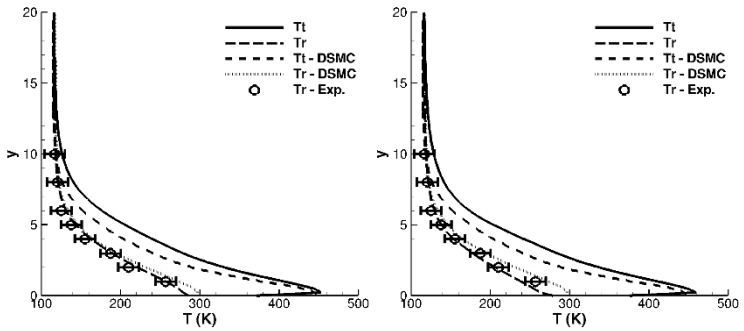
- Compared with the polyatomic ES Model [1] with respect to the DSMC results reported in [2] for normal shocks
- The Rykov Model achieves a slightly better agreement with the DSMC results than the polyatomic ES model
- Agreement that can be further improved employing a variable collision number
- The ES Model at the moment does not include variation of the collision number

[1] Andries, P., LeTallec, P., Perlat, J.-P., and Perthame, B., 2000. The Gaussian-BGK Model of Boltzmann Equation with Small Prandtl Number. *European Journal of Mechanics - B/Fluids*, 19:813–830.

[2] Alsmeyer, H., 1976. Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorption of an Electron Beam. *Journal of Fluid Mechanics*, 74(3):497–513.

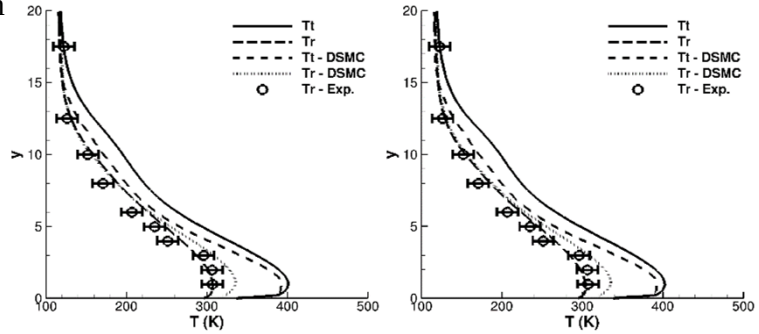
Rykov Kinetic Model Results (2)

X = 5 mm

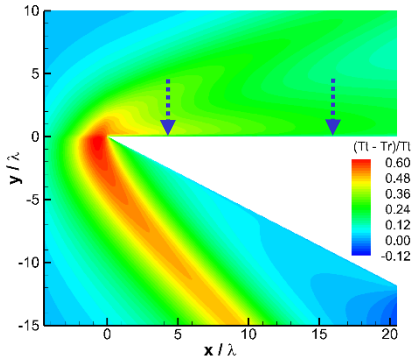


(a) Rykov model with variable Z_r (b) ES model

X = 20 mm



(a) Rykov model with variable Z_r (b) ES model



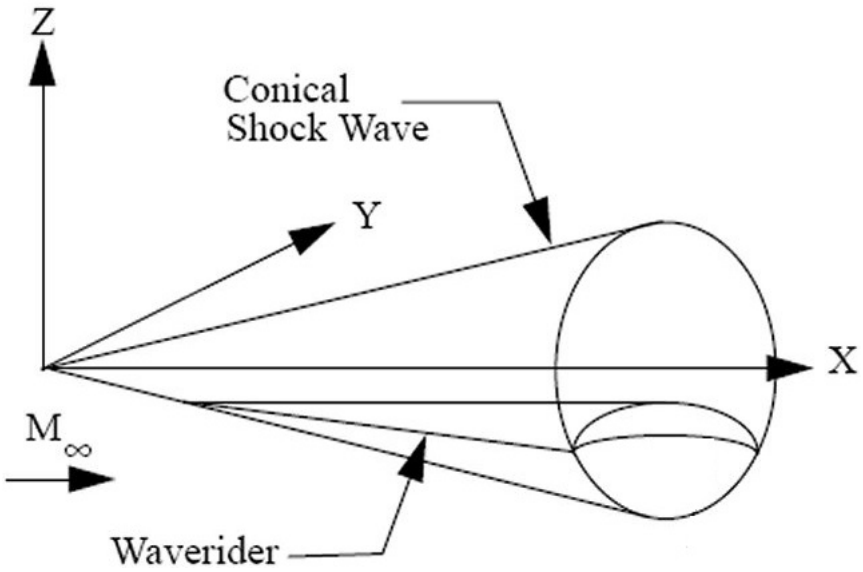
- Experiment presented in [1] for a rarefied flow around a flat plate
- The ES model slightly under-predicts the rotational temperature near the wall, leading also to a higher temperature gradient at the wall
- Both models predict a higher translational temperature in the thermal layer

For a monoatomic gas the Rykov and the polyatomic ES models reduce to the Shakhov model and the monoatomic ES model and in [2] a comparison shown that the Shakhov model predicts more accurate solutions than the ES model.

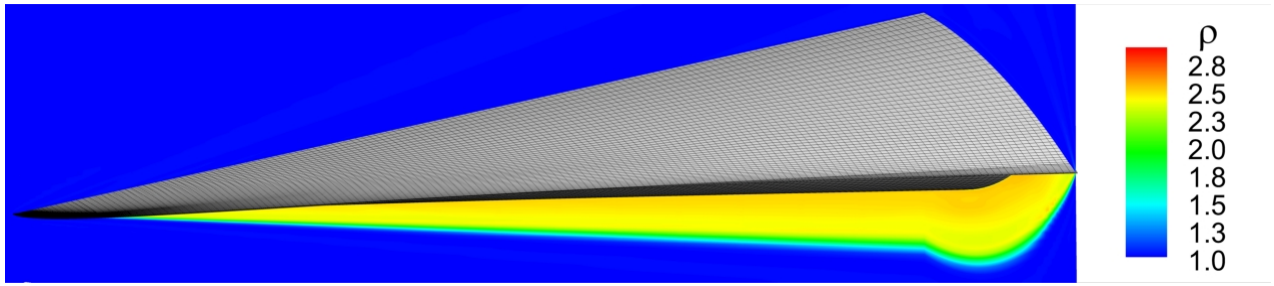
[1] Tsuboi, N. and Matsumoto, Y., 2005. Experimental and Numerical Study of Hypersonic Rarefied Gas Flow over Flat Plates. *AIAA Journal*, 43(6):1243–1255.
[2] Chen, S., Xu, K., 2013. A Comparison and Unification of Ellipsoidal Statistical and Shakhov Models.

Waverider Test Case (1)

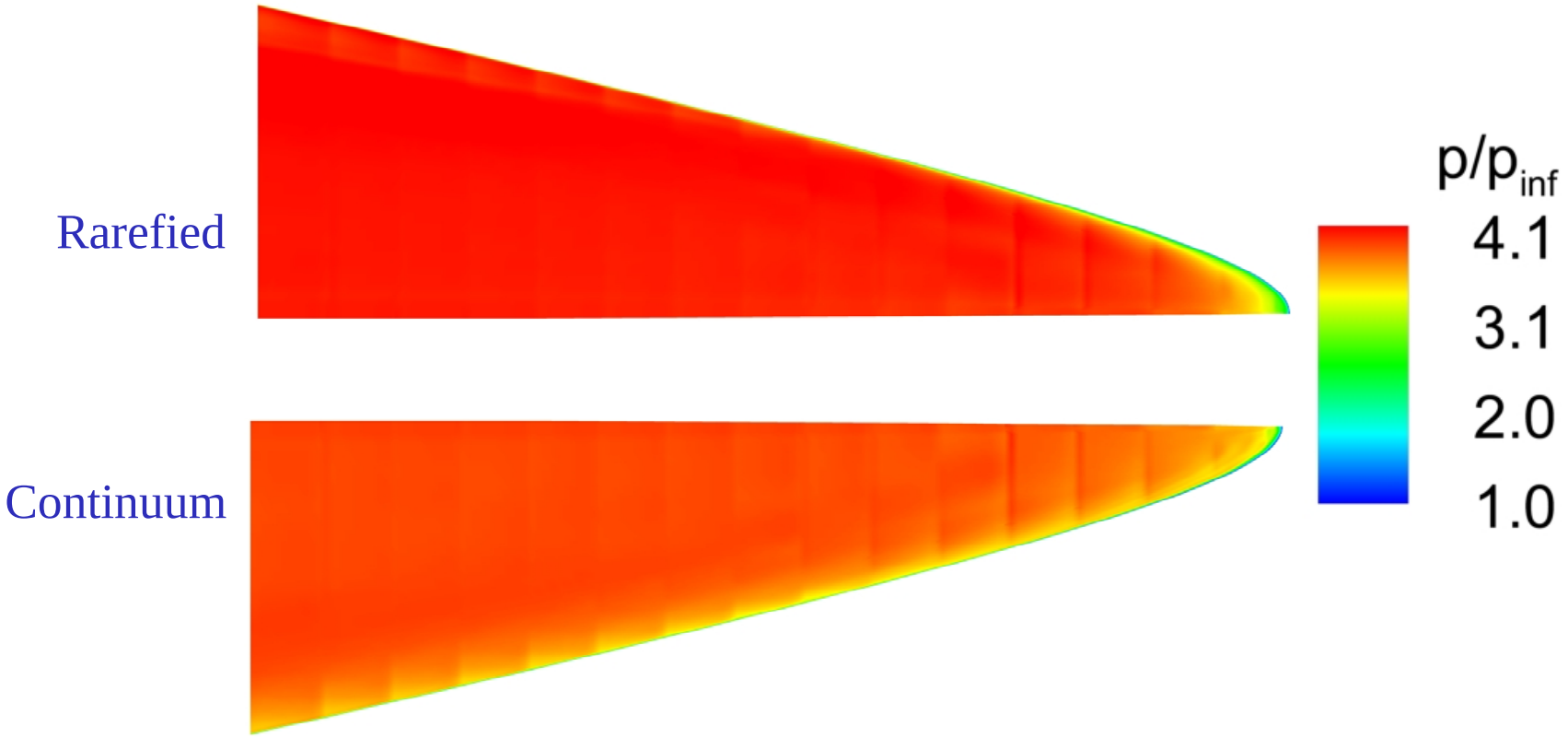
- A waverider is a shape designed from a known hypersonic, typically conical, flow field



- The waverider is designed such that the shock is attached along the outer leading edge



Waverider Test Case (2)



- *0,5* milion kinetic cells
- *12x12x12* velocity space

→ almost *192* GB of RAM required

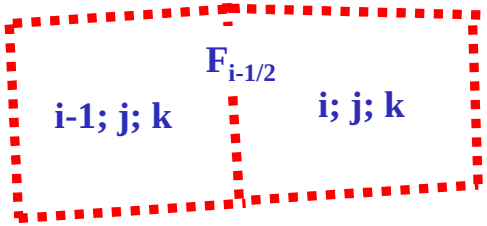
Gas-Kinetic Schemes (1)

- First examples in [1] and [2], in contrast to the commonly used ROE or AUSM fluxes, GKS reconstructs a local kinetic problem around the cell interfaces to calculate the numerical fluxes in the Finite Volume method
- The fluxes include both Euler and viscous contributions but expensive
- A recent sucessfull scheme is the Unified Gas-Kinetic Scheme (UGKS) [3]
- The UGKS is able to predict continuum and slightly rarefied flows
- A similar approach has been used in the present work to define a Gas-Kinetic scheme for near-continuum flows
- This, in the context of this project, will allow an extension of the domain where the continuum solver can be employed, reducing the domain where the memory expensive discrete velocity method is needed

[1] Pullin DI. 1980. Direct simulation methods for compressible inviscid ideal gas flow. *Journal of Computational Physics*. 34:231.
[2] Mandal JC, Deshpande SM. 1994. Kinetic flux vector splitting for Euler equations. *Computers & Fluids*. 23:447.
[3] Xu K. and Huang J.-C., 2010. A Unified Gas-Kinetic Scheme for Continuum and Rarefied Flows. *Journal of Computational Physics*, 229:7747–7764.

Gas-Kinetic Schemes (2)

Integrating the kinetic model equation in a control volume



$$F|_i^{n+1} = F|_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} \left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) dt + \frac{\Delta t}{2}\left(\frac{F_M|_i^{n+1} - F|_i^{n+1}}{\tau^{n+1}} + \frac{F_M|_i^n - F|_i^n}{\tau^n}\right)$$

and taking the moments $\hat{\boldsymbol{\Psi}} = (1,\ c_x,\ \mathbf{c}^2)^T$ (monoatomic) / $\hat{\boldsymbol{\Psi}} = (1,\ c_x,\ \mathbf{c}^2+\xi^2,\ \xi^2)^T$ (diatomic)

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{-\infty}^{+\infty} \hat{\boldsymbol{\Psi}}\left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2}\right) d\mathbf{c}dtd\xi + \int_{t^n}^{t^{n+1}}\int_{-\infty}^{+\infty} \hat{\boldsymbol{\Psi}}\frac{F_M|^n - F|^n}{\tau^n} d\mathbf{c}d\xi$$

the update of the macroscopic variables can be obtained, where the following compatibility conditions can be used

$$\int_{-\infty}^{+\infty} \hat{\boldsymbol{\Psi}}\frac{F_M|^n - F|^n}{\tau^n} d\mathbf{c} \leftrightarrow \begin{cases} (0,\ 0,\ 0)^T & \text{(monoatomic)} \\ (0,\ 0,\ 0,\ s)^T & \text{(diatomic)} \end{cases}$$

Gas-Kinetic Schemes (3)

- General solution of the kinetic model

$$F(x_{i+1/2},t,c_x|_m) = \frac{1}{\tau}\int_{t^n}^{t} F_{eq}(t',c_x|_m, x_{i+1/2}-c_x|_m(t-t'))\exp\left(-\frac{t-t'}{\tau}\right)dt' +$$

$$+\exp\left(-\frac{t}{\tau}\right)\boxed{F^0(t^n,\mathbf{c}|_m, x_{i+1/2}-c_x|_m(t-t^n))}$$

- UGKS limit for a well-resolved flow [1]

$$F = F_{eq} - \tau\left(\frac{\partial F_{eq}}{\partial t} + \mathbf{c}\frac{\partial F_{eq}}{\partial \mathbf{x}}\right) + t\frac{\partial F_{eq}}{\partial t}$$

in the UGKS a non-equilibrium F^0 is given by the Chapman-Enskog expansion

for which a higher order model extension, that modifies the collision time, is available

$$\tau^* = \frac{\tau}{1+\tau(D^2F_{eq}/DF_{eq})}$$

Obtained substituting the C.-E. expansion with τ^* in the kinetic model equation

[1] Xu K. and Josyula E., 2006. Continuum Formulation for Non-equilibrium Shock Structure Calculation. *Communications in Computational Physics*, 1(3):425–450.

Shakhov Gas-Kinetic Scheme

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}} \left([c_x F]|_{i-1/2} - [c_x F]|_{i+1/2} \right) d\mathbf{c}dt$$

$$F = F^S - \tau \left(\frac{\partial F_0^S}{\partial t} + c_x \frac{\partial F^S}{\partial x} \right) + t \frac{\partial F^S}{\partial t}$$

- The Maxwellian and Shakhov correction derivatives have been defined analytically

$$\frac{\partial F^S}{\partial \alpha} = F^S \left(\frac{1}{F_M} \frac{\partial F_M}{\partial \alpha} + \frac{1}{\Phi} \frac{\partial \Phi}{\partial \alpha} \right)$$

$$\Phi^S = \frac{8}{15} \frac{q_x^t c'_x}{\rho T^2} \left(\frac{c'^2}{T} - \frac{5}{2} \right)$$

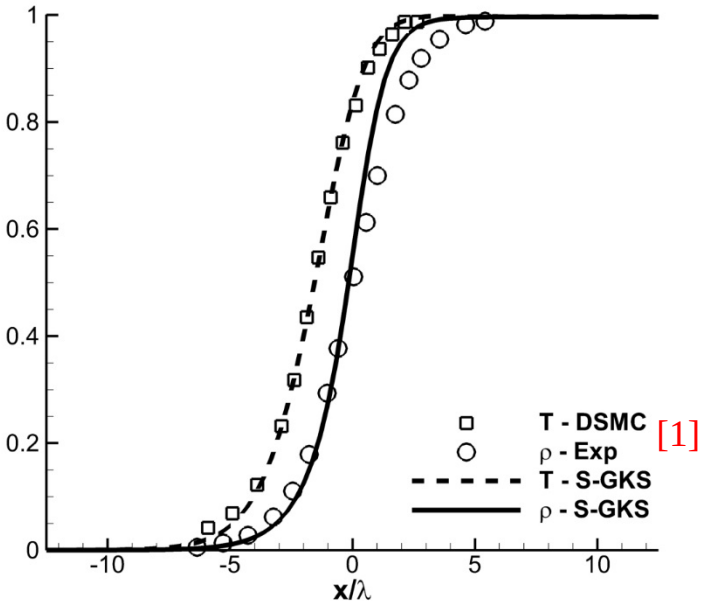
- From the compatibility conditions we have the time derivative of the macro-variables

$$\frac{\partial \mathbf{W}}{\partial t} = - \int_{-\infty}^{+\infty} \hat{\mathbf{\Psi}} c_x \frac{\partial F^S}{\partial x} d\mathbf{c}$$

- The time derivatives for the heat flux can be obtained by taking the relative moment of the model equation
- The macroscopic variables spatial derivatives can be reconstructed by means of a discretisation approach

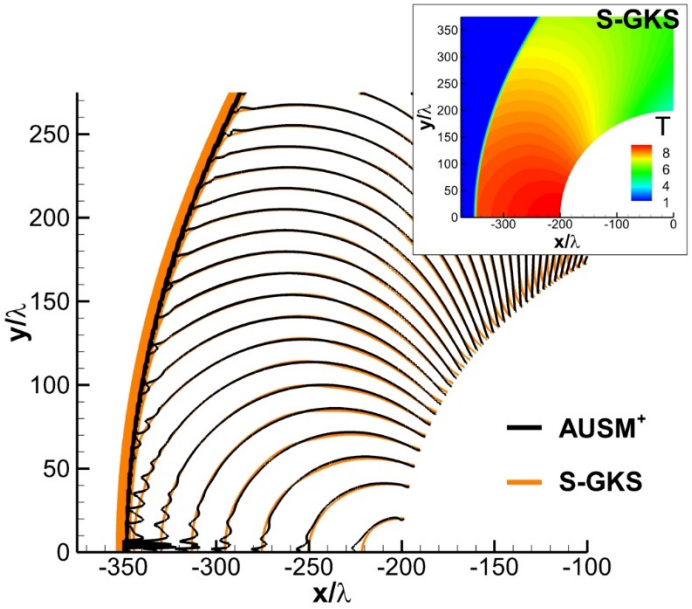
S-GKS Preliminary Results (1)

Mach 2.05 Shock



[1]

Mach 5 Cylinder

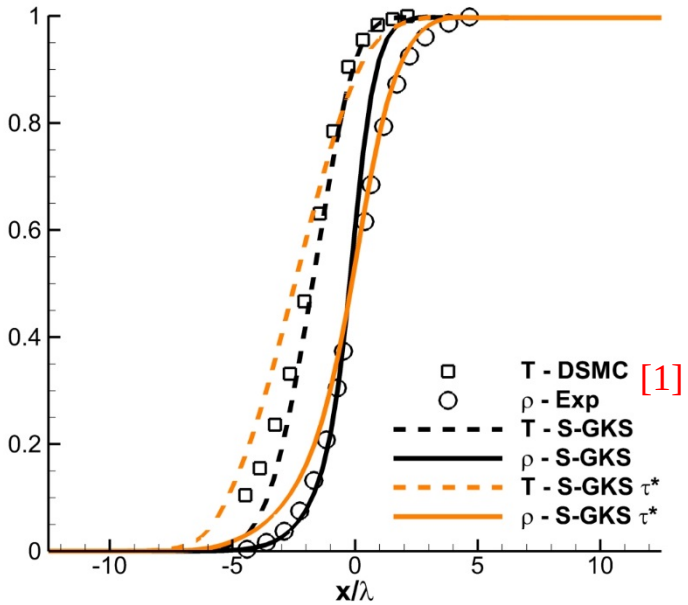


- The Gas-Kinetic Scheme is able to resolve the shock structure …
- … and presents less anomalies than a commonly employed AUSM$^+$

[1] Alsmeyer, H., 1976. Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorption of an Electron Beam. *Journal of Fluid Mechanics*, 74(3):497–513.

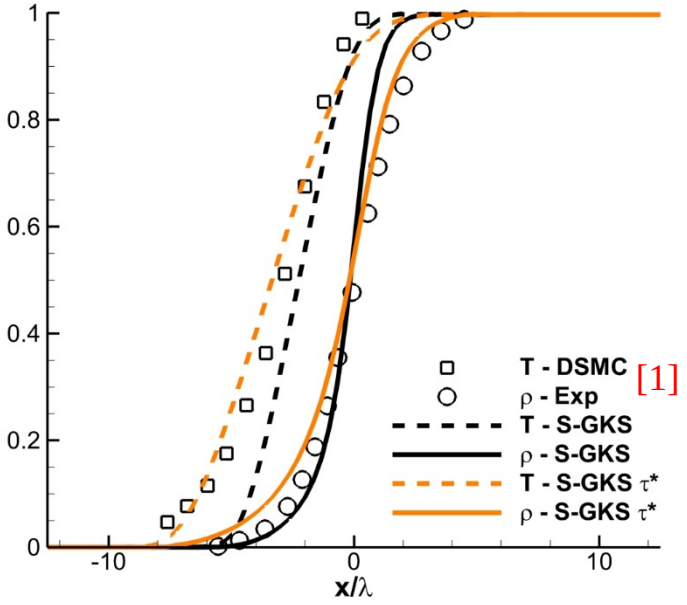
S-GKS Preliminary Results (2)

Mach 3.8 Shock



[1]

Mach 9 Shock



[1]

- However, due to the continuum formulation, it predicts a steeper shock
- A better shock thickness prediction can be obtained introducing τ^*

[1] Alsmeyer, H., 1976. Density Profiles in Argon and Nitrogen Shock Waves Measured by the Absorption of an Electron Beam. *Journal of Fluid Mechanics*, 74(3):497–513.

S-GKS Preliminary Performance Analysis

Computational Time

	GKS	GKS-τ*	DVM
2D	0.02	0.06	0.17
3D	0.65	1.37	4.0

seconds per iteration

Mach 3.8 normal shock test case (~3000 cells)

All test have been done in the same conditions on a 4 core Intel® Xeon®

- The S-GKS is around 70% faster than the DVM

Memory Usage

The memory cost reduction is significant, in fact:

- $N_x \cdot N_y \cdot N_z$ values to store per physical cell per time step needed for the DMV and the full UGKS
- 5 values to store per physical cell per time step needed for the S-GKS

Rykov Gas-Kinetic Scheme

- Similar approach to the monoatomic case but now 2 functions need to be reconstructed

$$\mathbf{W}_i^{n+1} = \mathbf{W}_i^n + \frac{1}{\Delta x}\sum_m \int_{t^n}^{t^{n+1}} \hat{\mathbf{\Psi}}_0 \left([c_x|_m F_0]|_{i-1/2} - [c_x|_m F_0]|_{i+1/2} \right) dt +$$

$$+ \frac{1}{\Delta x}\sum_m \int_{t^n}^{t^{n+1}} \hat{\mathbf{\Psi}}_1 \left([c_x|_m F_1]|_{i-1/2} - [c_x|_m F_1]|_{i+1/2} \right) dt + \frac{\Delta t}{2}\left(\mathbf{S}_i^{n+1} + \mathbf{S}_i^n \right)$$

$$\hat{\mathbf{\Psi}}_0 = (1,\ c_x,\ \mathbf{c}^2,\ 0)^T \qquad \hat{\mathbf{\Psi}}_1 = (0,\ 0,\ 1,\ 1)^T$$

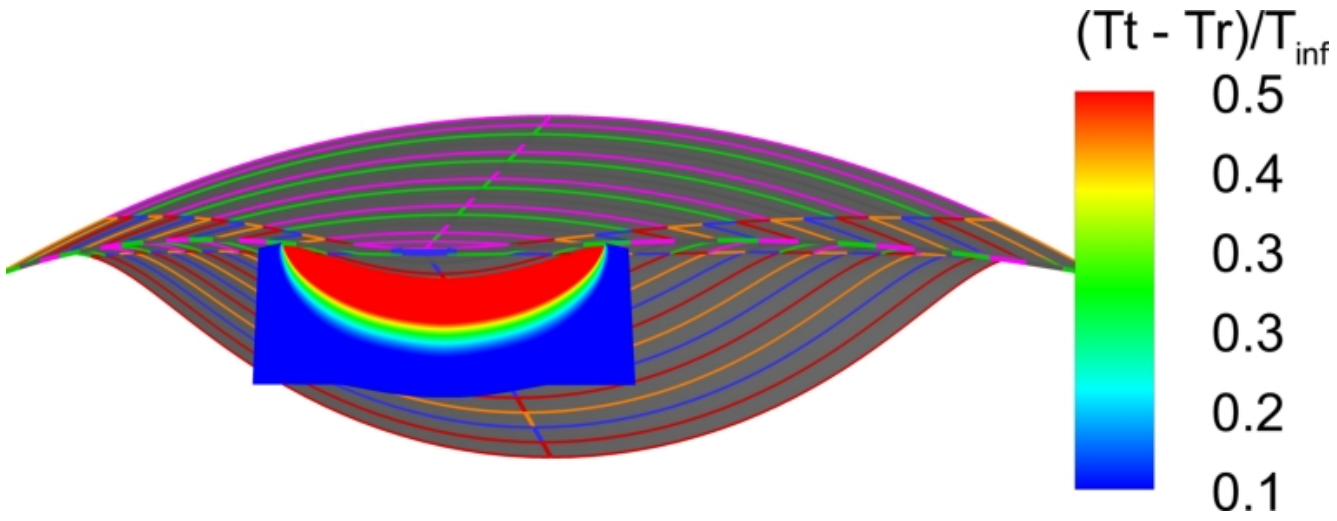
$$F_0 = F_0^{eq} - \tau\left(\frac{\partial F_0^{eq}}{\partial t} + c_x\frac{\partial F_0^{eq}}{\partial x}\right) + t\frac{\partial F_0^{eq}}{\partial t} \qquad F_1 = F_1^{eq} - \tau\left(\frac{\partial F_1^{eq}}{\partial t} + c_x\frac{\partial F_1^{eq}}{\partial x}\right) + t\frac{\partial F_1^{eq}}{\partial t}$$

$$\frac{\partial F_0^{eq}}{\partial \alpha} = \frac{1}{Z_r}\frac{\partial F_0^r}{\partial \alpha} + \left(1 - \frac{1}{Z_r}\right)\frac{\partial F_0^t}{\partial \alpha} \qquad \frac{\partial F_1^{eq}}{\partial \alpha} = \frac{1}{Z_r}\frac{\partial F_1^r}{\partial \alpha} + \left(1 - \frac{1}{Z_r}\right)\frac{\partial F_1^t}{\partial \alpha}$$

- The Maxwellian and correction derivatives have been defined analytically

Future Work

- Implementation and development of the diatomic extension of the Gas-Kinetic Scheme
- Assessment of the Gas-Kinetic Scheme in the context of Hybrid simulations
- Coupling Technique to exchange information between the Kinetic Model and the Gas-Kinetic Scheme
- Complex test case of aerospace interest: Waveriders



Thank you