DE LA RECHERCHE À L'INDUSTRIE

Models and Numerical method for the simulation of rarefied flows in atmospheric reentry applications

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Outline of the talk

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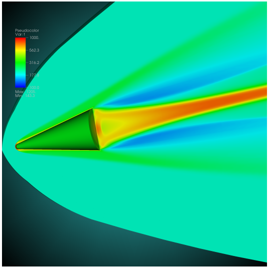
1. Aerodynamics in rarefied regime
   - Atmospheric re-entry
   - Various Regimes during re-entry
   - Rarefied regime
2. Physical model
3. Advanced modelling for rarefied atmosphere
4. Numerical method
5. Conclusions and future work

Atmospheric re-entry context

- Flow around spacecraft
- High speed flow, High Mach number : hypersonic conditions
- Sphere-cone configuration
- Quantities of interest : heat flux on the boundary and aerodynamic coefficients

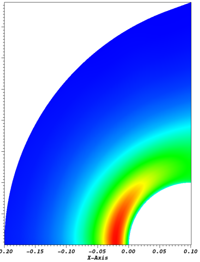


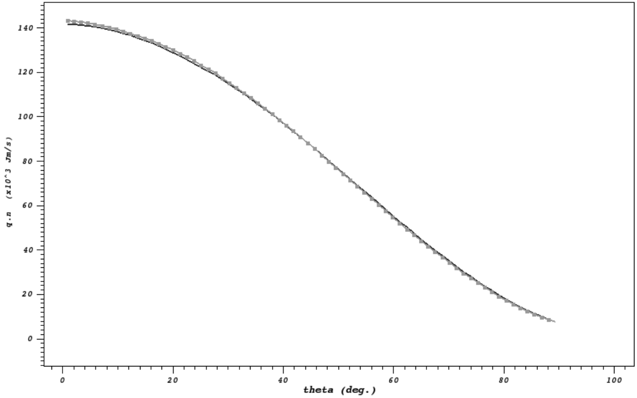
Looking for **steady state solution** :

time scale of the relaxation $\ll$ time scale of the trajectory

Example of heat flux

Heat flux computed on a classical sphere-cone geometry radius of the sphere 0.1m, at 90 km altitude, Mach 20.

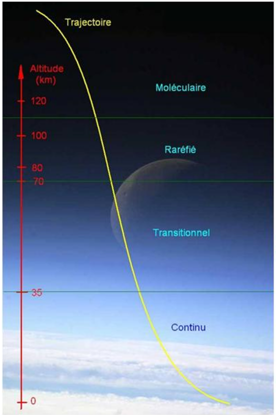




Temperature

Heat Flux

Knudsen number $Kn = \frac{\lambda}{L}\left(\frac{\text{mean free path}}{\text{characteristic length}}\right)$



Free molecular zone ($Kn > 10$)

Kinetic theory

Navier-Stokes ($Kn < 0.1$)

- Between 120 and 60 km : rarefied atmosphere
- High values of the Knudsen number (between 0.1 and 10) -> Navier-Stokes is no more valid
- Use of the Kinetic theory of gases, with Boltzmann equation

For theses altitudes (120 to 60 km) : use of the model by **B**hatnagar **G**ross **K**rook[1] (BGK).

- Relaxation toward the Maxwellian equilibrium.
- A kinetic code at CEA-CESTA solve BGK model in 2D planar, 2D axisymetric and 3D.
- Computation on TERA100 (supercomputer of the CEA-DAM).

1. P.L. Bathnagar, E.P. Gross, M. Krook, A model for collision processes in gases. Physical Review, Vol 94, Né 3 (511-525), 1954

Outline of the talk

Kinetic theory of gases

In kinetic theory we describe the probability density function

$$f \equiv f(t, \mathbf{x}, \mathbf{v})$$

with time t, space $\mathbf{x} \in \mathbb{R}^{\mathbf{3}}$ and speed $\mathbf{v} \in \mathbb{R}^{\mathbf{3}}$.
The density function is solution of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f)$$

- Left hand side of the equation : transport of the particles of the gas
- $Q(f, f)$: collisions between particles

Boundary conditions :

- upstream flow
- on the wall of the spacecraft : diffusive condition (at wall temperature), specular or mixed (Maxwell condition with accommodation coefficient).

The BGK model

In the context of atmospheric re-entry, between 120 and 60 km, flows are at transitional state.

Use of the Bathnagar, Gross, and Krook (BGK) model : a relaxation of f toward Maxwellian equilibrium.

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\tau}(\mathcal{M}(f) - f)$$

with

- The Gaussian function (Maxwellian) $\mathcal{M}(f) = \frac{\rho}{(2\pi RT)^{3/2}} e^{\frac{-|\mathbf{v}-\mathbf{u}|^2}{2RT}}$
- $\tau = \tau(t, \mathbf{x})$ relaxation rate

Physical parameter of the BGK model

The relaxation rate of the BGK model is determined from the characteristics of the gas :

$$\tau = \frac{\mu}{\rho\, R\, T} = \frac{1}{\rho\, R\, T}\mu_{ref}\left(\frac{T}{T_{ref}}\right)^{\omega}$$

For air flow[2] : $\omega = 0.77$, $T_{ref} = 273K$, $\mu_{ref} = 1.719\, 10^{-5}\, N.s.m^{-2}$

Only one scale in BGK model (relaxation rate), not able to describe flows like air with Prandtl number different of 1.

2. G.A. Bird, Molecular gas dynamics and the direct simulation of gas flows, Oxford Science Publications, 1994

Properties of BGK

- Conservation of mass, momentum and kinetic energy, entropy decrease (H theorem).
- Integrating of the density function along $\mathbf{v}$ variable gives relation between f and macroscopic quantities :

$$\begin{pmatrix} \rho \\ \rho\mathbf{u} \\ E \end{pmatrix} = \int_{\mathbf{v}} \begin{pmatrix} f(t,\mathbf{x},\mathbf{v}) \\ \mathbf{v}\, f(t,\mathbf{x},\mathbf{v}) \\ \frac{1}{2}\,|\mathbf{v}|^2\, f(t,\mathbf{x},\mathbf{v}) \end{pmatrix} d\mathbf{v}$$

  Asymptotic limit of BGK model when $Kn \to 0$ (around 60 km) :

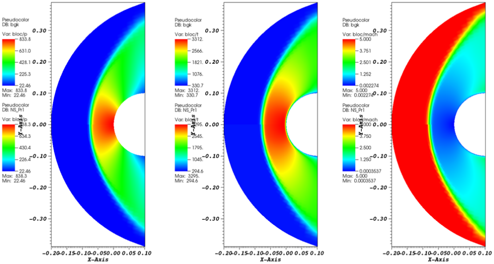
  $(\rho,\ \rho\mathbf{u},\ E)$ solutions of Navier-Stokes equations.

- Possible comparison between solutions of BGK model and Navier-Stokes equations.

BGK vs Navier-Stokes ($Pr = 1$)

Academic test case (flow around sphere of 0.1 m)
Mach number 5, 60 km of altitude
above : BGK solution
under : Navier-Stokes solution (Prandtl = 1)

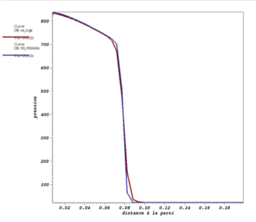
Pressure Temperature Mach



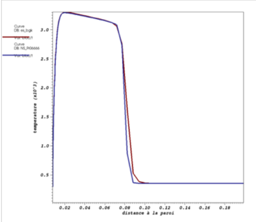
BGK vs Navier-Stokes ($Pr = 1$)

Good agreement between macroscopic quantities (1D section) and wall heat flux

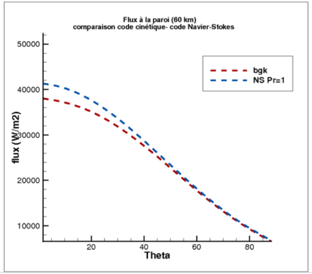
Pressure



Temperature



Pressure and Temperature normal to the wall



Wall heat flux

Drawback of the BGK model

- BGK model is dedicated to monoatomic gases. As air is a polyatomic gas, an extension of BGK model for polyatomic was done [3].
  - f is described with additional variable I (internal energy), and degree of freedom δ ($\delta = 2$ for diatomic).
  - Reduced distribution technique : description of $\tilde{f} = \int_I f(t, \mathbf{x}, \mathbf{v}, I)\, dI$ and $\tilde{g} = \int_I I^{2/\delta} f(t, \mathbf{x}, \mathbf{v}, I)\, dI$
  - $\tilde{f}$ and $\tilde{g}$ are solutions of BGK equations

- Prandtl number problematic : with BGK model, Prandtl number is 1. But for air, Prandtl is equal to 0.71.
  The ES-BGK model [4] is proposed and was implemented in the CEA-CESTA kinetic code.

3. B. Dubroca, L. Mieussens, A conservative and entropic discrete-velocity model for rarefied polyatomic gases, ESAIM-Proceedings Vol. 10 - CEMRACS 1999, 127-139 (2001).
4. P. Andries, P. Le Tallec, J.P. Perlat, and B. Perthame. The Gaussian BGK model of Boltzmann equation with small Prandtl numbers. European Journal of Mechanics : B Fluids, 813-830, 2000.

Outline of the talk

idea : replace the Maxwellian $\mathcal{M}$ by a anisotropic Gaussian $\mathcal{G}$

BGK model

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\tau}(\mathcal{M}(\rho, \mathbf{u}, T) - f)$$

with $\mathcal{M}(\rho, \mathbf{u}, T) = \frac{\rho}{(2\pi RT)^{3/2}} e^{\frac{-|\mathbf{v}-\mathbf{u}|^2}{2RT}}$

ES-BGK Model

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\tau}(\mathcal{G}(\rho, \mathbf{u}, \mathcal{T}) - f)$$

with $\mathcal{G}(\rho, \mathbf{u}, \mathcal{T}) =$

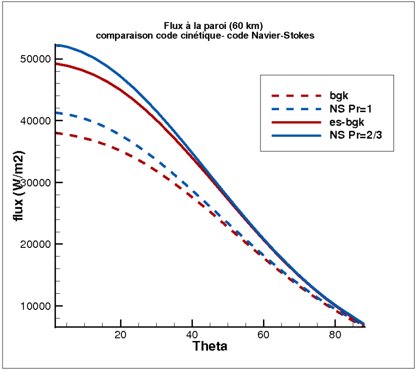
$$\frac{\rho}{\sqrt{det(2\pi\mathcal{T})}} e^{\frac{-(\mathbf{v}-\mathbf{u})\mathcal{T}^{-1}(\mathbf{v}-\mathbf{u})}{2}}.$$

Tensor of temperature $\mathcal{T} = \mathcal{T}(\nu, \theta)$; one can obtain the Prandtl number by Chapman-Enskog expansion : $\tau = \frac{\mu}{Pr\,\rho\,R\,T}$ with $Pr = \frac{1}{1-(1-\theta)\nu}$.

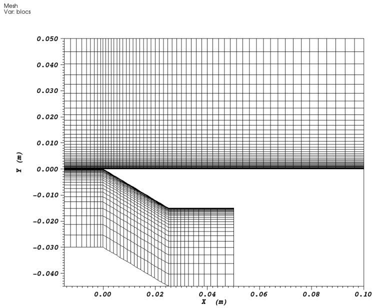
With well chosen parameters, one can retrieve Prandtl number for monoatomic gas, i.e. $\frac{2}{3}(\nu = -0.5, \theta = 0)$ and polyatomic gas $\frac{5}{7}(\nu = -0.5, \theta = 1/5)$.

ES-BGK vs Navier-Stokes ($Pr = 2/3$)

Good agreement on macroscopic quantities (1D section) and on heat flux for monoatomic gas with ES-BGK model (Prandtl=2/3)



Validation on flow around flat plate [5] (experiment and numerical simulation) [6]



5. Experimental and Numerical Study of Hypersonic Rarefied Gas Flow over Flat Plates, Tsuboi,Matsumoto, AIAA JOURNAL Vol. 43, No. 6, June 2005

6. intern ship of M. Capelli (student from Enseirb-Matmeca)

Description of chemical reactions

Work done by L. Desvillettes, F. Charles, S. Brull and L. Mieussens

Modelling of chemical reactions :

- chemical species : N_2, 0_2, N, O, NO ;
- N_2 and 0_2 major species, computed by BGK equation with source terms due to chemical reactions ;
- N, O et NO, minor species, considered as macroscopic quantities ;
- Simple and easy to implement model.

On this subject :

- **post-doctoral contract** at CEA-CESTA (2015) : we are looking for candidates, don't hesitate to apply !

Outline of the talk

The BGK discrete model : deterministic method

Use of a deterministic method instead of a stochastic one (DSMC for example).
Determination of f in each point in space $\mathbf{x}$ and speed $\mathbf{v} \in \mathbb{R}^3$ (unbounded domain !).
BGK discrete velocity model :

$$\frac{\partial f_k}{\partial t} + \mathbf{v}_k \cdot \nabla_{\mathbf{x}} f_k = \frac{1}{\tau} \left(\mathcal{E}_{\mathcal{V}}(\mathbf{v}_k) - f_k \right), \text{ pour tout } \mathbf{v}_k \in \mathcal{V}$$

with $\mathcal{E}_{\mathcal{V}}$ an approximation[7] of the Maxwellian $\mathcal{M}(f)$.
Using a Finite Volume method for the space discretization, one can obtain, for $\delta f^n = f^{n+1} - f^n$

$$\left(\frac{I}{\Delta t} + Q^n + R^n\right)\delta f^n = S^n$$

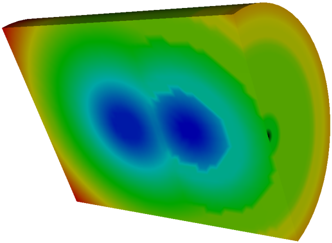
7. L. Mieussens, Convergence of a discrete-velocity model for the Boltzmann-BGK equation, Computers Math. Applic., 41(1-2), 83-96 (2001)

Improvement : Locally refined discrete velocity grids

Locally refined velocity grid[8] in order to decrease computation time.
Methodology :

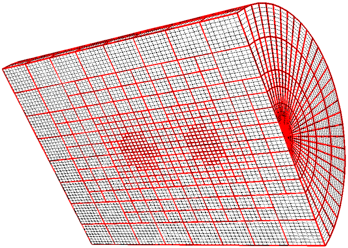
- Definition of a support function $\phi(\mathbf{v}) = c\sqrt{R\,T(\mathbf{x})}$ where $\mathbf{x}$ is such than $\mathbf{u}(\mathbf{x}) = \mathbf{v}$, with $\mathbf{u}$ and T obtained by a pre-computation (with Navier-Stokes model) or estimation (with Rankine-Hugoniot relation).
- Use it for the refinement of the velocity grid

Gain in computation time and memory between 7 (in 2D) and 30 (in 3D),
same results in wall heat flux computation.

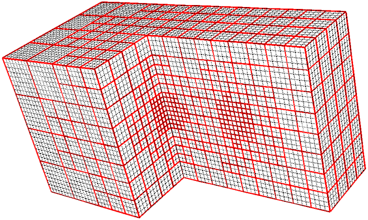


8. C. Baranger, J. Claudel, N. Hérouard, L. Mieussens, Locally refined discrete velocity grids for stationary rarefied flow simulations , J. Comput. Phys., 257(15), 572-593 (2014)

Examples of refined velocity grids



Refined velocity grids in 2D axi
(66495 nodes vs 6900 nodes)



Refined velocity grid in 3D
(65536 nodes vs 2 956 nodes)

Outline of the talk

Conclusions

- Re-entry in rarefied regime was described by the BGK model, but improved with the ES-BGK model ;
- Since 2010, many achievements were obtained regarding physical model and numerical realisations.
- Numerical resolution of BGK and ES-BGK model : deterministic scheme was used in the CEA-CESTA kinetic code ;

Future work

- Ph.D.Thesis of Nicolas Hérouard on asymptotic preserving schemes (2011-2014)
  - Discontinuous Galerkin method in 1D configuration for linearised BGK model ;
  - Boundary conditions and order of the scheme ;
- New model with chemical reactions
- A modified Fokker Planck equation for rarefied gas dynamics (J. Mathiaud)
- Collaboration will come with a laboratory of Orléans ICARE(with a wind tunnel 'MarHy' dedicated to hypersonic rarefied regime) : high Mach experiment in rarefied regime (Mach 5 with air, Mach 20 with nitrogen).
- New **post-doctoral position** will be available in 2015 (founded by LabEx CPU Bordeaux) on study of the overlap zone in altitude between kinetic model and Navier-Stokes description : we are looking for candidates, don't hesitate to apply !