ВЦ РАН

Dorodnicyn Computing Center
Russian Academy of Sciences

A deterministic method of solving the full Boltzmann equation for 1D flows

Sergey Zabelok

Workshop on Non-equilibrium Flow Phenomena in Honor of Mikhail Ivanov’s 70th Birthday

June 15-18, 2015, Novosibirsk, Russia

Motivation

Simulations for rarefied gas

- DSMC
- Direct Solution of the Boltzmann equation (discrete velocity approach)
  - Full Boltzmann integral
    - ✓ Deterministic methods (Aristov, Zabelok, Ohwada, Varghese, Malkov et. al., Aleksandr Alekseenko & Josyula)
    - ✓ Monte-Carlo and Korobov methods (Tcheremissine, Aristov, UFS)
  - Model collision integral
    - BGK, S-model, R-model, ES-model (Titarev, UFS)
  - Linearized Boltzmann integral
  - …

Motivation

Simulations for rarefied gas

- DSMC
- Direct Solution of the Boltzmann equation (discrete velocity approach)
  - Full Boltzmann integral
    - ✓ Deterministic methods (Aristov, Zabelok, Ohwada, Varghese, Malkov et. al., Aleksandr Alekseenko & Josyula)
    - ✓ Monte-Carlo and Korobov methods (Tcheremissine, Aristov, UFS)
  - Model collision integral
    - BGK, S-model, R-model, ES-model (Titarev, UFS)
  - Linearized Boltzmann integral
  - …

ВЦ РАН

Motivation

- Many deterministic methods for computation of full collision integral in the Boltzmann equation have been constructed recently.
  - T. Ohwada, *Phys. Fluids A* **5** , 217 (1993)
  - V.V. Aristov, S.A. Zabelok, *Comp. Math. Math. Phys.* **42**, 406–418 (2002)
  - A. Alekseenko, E. Josyula, *J. Comp. Phys.* **272**, 170–188 (2014).
  - E. A. Malkov, Ye. A. Bondar, A. A. Kokhanchik, S. O. Poleshkin, M. S. Ivanov *Shock Waves* **25** (2015)
- All methods are extremely time consuming
- The purpose of the present work is to construct a deterministic method which will speedup 1D computations by using the axial symmetry for the distribution function

Boltzmann equation

A monoatomic gas without inner degrees of freedom and external forces is considered.

$$\frac{\partial f}{\partial t} + (\boldsymbol{\xi} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}) f = I(f, f)$$

The collision integral is

$$I(f, f) = \int [f(\boldsymbol{\xi}') f({\boldsymbol{\xi}'}_1) - f(\boldsymbol{\xi}) f(\boldsymbol{\xi}_1)]\, g\, \sigma(g, \boldsymbol{s})\, d\boldsymbol{s}\, d\boldsymbol{\xi}_1$$

$$\boldsymbol{g} = \boldsymbol{\xi} - \boldsymbol{\xi}_1, \boldsymbol{\xi}' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} + \frac{1}{2} g \boldsymbol{s}, \boldsymbol{\xi}' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} - \frac{1}{2} g \boldsymbol{s},$$

$$\boldsymbol{s} = \left\{p, \sqrt{1 - p^2} \cos \varepsilon, \sqrt{1 - p^2} \sin \varepsilon \right\}$$

ВЦ РАН

A deterministic approach (3D velocity space)

- The velocity space is considered to be finite and divided into a number of cells
- The distribution function is supposed to be constant inside each cell and is represented as a linear combination of basis functions:

$$f(t,\boldsymbol{r},\boldsymbol{\xi}) = \sum_{i=1}^{N} f_i(t,\boldsymbol{r})e_i(\boldsymbol{\xi})$$

- The collision integral (for fixed $t,\boldsymbol{r}$) is approximated using the above formula

$$I(f,f)(\boldsymbol{\xi}) = \\ = \int \left[\sum_{l=1}^{N} f_l e_l(\boldsymbol{\xi}') \sum_{m=1}^{N} f_m e_m(\boldsymbol{\xi}'_1) - \sum_{i=1}^{N} f_i e_i(\boldsymbol{\xi}) \sum_{k=1}^{N} f_k e_k(\boldsymbol{\xi}_1) \right] g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, d\boldsymbol{\xi}_1$$

A deterministic approach (3D velocity space)

- Consider a velocity point of cell with number *i*: $\boldsymbol{\xi} = \boldsymbol{\xi}_i$

$$I(\boldsymbol{\xi}_i) == \sum_{l=1}^{N} \sum_{m=1}^{N} f_m\, f_l \int e_m(\boldsymbol{\xi}'_1) e_l(\boldsymbol{\xi}')\, g\, \sigma(g, \boldsymbol{s})\, d\boldsymbol{s}\, d\boldsymbol{\xi}_1 \Bigg|_{\xi=\xi_i}$$

$$- f_i \sum_{k=1}^{N} f_k \int e_k(\boldsymbol{\xi}_1) g\, \sigma(g, \boldsymbol{s})\, d\boldsymbol{s}\, d\boldsymbol{\xi}_1 \Bigg|_{\xi=\xi_i}$$

- The integrals in the above formula can be taken numerically, which results in the following formula:

$$I(\boldsymbol{\xi}_i) = \sum_{l=1}^{N} \sum_{m=1}^{N} A_{ilm} f_m\, f_l - f_i \sum_{k=1}^{N} b_{ik} f_k$$

A deterministic approach (3D velocity space)

➢Conservation laws are satisfied with the use of conservative correction:

$$I(\boldsymbol{\xi}_i) = \sum_{l=1}^{N}\sum_{m=1}^{N} A_{ilm} f_m f_l - f_i\, P_i(\boldsymbol{\xi}_i) \sum_{k=1}^{N} b_{ik} f_k$$

$$P_i(\boldsymbol{\xi}_i) = 1 + a_0 + \boldsymbol{a}_1 \cdot \boldsymbol{\xi}_i + a_2(\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_i)$$

2 scalars a_0 and a_2 and 3D vector $\boldsymbol{a}_1$ are found by multiplying collision integral by collision invariants $\psi_\alpha = 1$, $\boldsymbol{\xi}_i$, $(\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_i)$:

$$\sum_{k=1}^{N} I(\boldsymbol{\xi}_i)\, \psi_\alpha = 0$$

A deterministic approach (3D velocity space)

- The collision integral is presented in a simple form.
- The number of arithmetic operations is proportional to $N^{8/3}$.
- For regular Cartesian mesh the number of unique values of A_{ilm} is proportional to $N^{5/3}$.
- For model of hard spheres analytic integration over collision parameters can be done.
- The method can be easily and **effectively** implemented for multiprocessor and/or GPU computers.

1D in physical space problems

ВЦ РАН

- The distribution function depends only on 2 velocity components (axial symmetry).
- The collision integral depends on the same 2D velocities

Collision integral for axial symmetry in velocity space

The collision integral

$$I(f,f) = \int [f(\boldsymbol{\xi}')f(\boldsymbol{\xi}'_1) - f(\boldsymbol{\xi})f(\boldsymbol{\xi}_1)]\, g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, d\boldsymbol{\xi}_1$$

is written in cylindrical coordinates

$$\xi_x = \eta_x,\ \xi_y = \eta_r \cos\eta_\varphi, \xi_z = \eta_r \sin\eta_\varphi\,.$$

In these coordinates collision integral is written as follows

$$I(f,f)\left(\eta_x,\eta_r,\eta_\varphi\right) = \int [f(\boldsymbol{\eta}')f(\boldsymbol{\eta}'_1) - f(\boldsymbol{\eta})f(\boldsymbol{\eta}_1)]\, g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, \eta_{r1} d\boldsymbol{\eta}_1$$

Collision integral for axial symmetry in velocity space

$$I(f,f)(\eta_x,\eta_r,\eta_\varphi) = \int [f(\boldsymbol{\eta}')f(\boldsymbol{\eta}'_1) - f(\boldsymbol{\eta})f(\boldsymbol{\eta}_1)]\, g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, \eta_{r1} d\boldsymbol{\eta}_1$$

As for axial symmetry both f and $I(f,f)$ do not depend on η_φ. This dependence can be removed from the above formula substituting any value for η_φ, *e.g.* $\eta_\varphi = 0$. Introducing 2-dimensional vector

$$\boldsymbol{\zeta} = \{\eta_x, \eta_r\}$$

the collision integral is written as follows

$$I(f,f)(\boldsymbol{\zeta}) = \int [f(\boldsymbol{\zeta}')f(\boldsymbol{\zeta}'_1) - f(\boldsymbol{\zeta})f(\boldsymbol{\zeta}_1)]\, g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, \zeta_{r1}\, d\eta_{\varphi 1}\, d\boldsymbol{\zeta}_1.$$

In this formula $\eta_{\varphi 1}$ plays the role of collision parameter.

ВЦ РАН

Deterministic approach, the same as for general case

- The velocity space is considered to be finite and divided into a number of cells
- The distribution function is supposed to be constant inside each cell and is represented as a linear combination of basis functions:

$$f(t,\boldsymbol{r},\boldsymbol{\zeta}) = \sum_{i=1}^{N} f_i(t,\boldsymbol{r}) e_i(\boldsymbol{\zeta})$$

- The collision integral (for fixed $t, \boldsymbol{r}$) is approximated using the above formula

$$I(f,f)(\boldsymbol{\zeta}) = \\ = \int \left[\sum_{l=1}^{N} f_l e_l(\boldsymbol{\zeta}') \sum_{m=1}^{N} f_m e_m(\boldsymbol{\zeta}'_1) - \sum_{i=1}^{N} f_i e_i(\boldsymbol{\zeta}) \sum_{k=1}^{N} f_k e_k(\boldsymbol{\zeta}_1) \right] g\, \sigma(g,\boldsymbol{s})\, d\boldsymbol{s}\, \zeta_{r1}\, d\eta_{\varphi 1}\, d\boldsymbol{\zeta}_1$$

Deterministic approach, the same as for general case

- Consider a velocity point of cell with number *i*: $\boldsymbol{\zeta} = \boldsymbol{\zeta}_i$

$$I(\boldsymbol{\zeta}_i) == \sum_{l=1}^{N} \sum_{m=1}^{N} f_m f_l \int e_m(\boldsymbol{\zeta}'_1) e_l(\boldsymbol{\zeta}')\, g\, \sigma(g, \boldsymbol{s})\, d\boldsymbol{s}\, \zeta_{r1}\, d\eta_{\varphi 1} d\boldsymbol{\zeta}_1 \Big|_{\zeta=\zeta_i}$$

$$- f_i \sum_{k=1}^{N} f_k \int e_k(\boldsymbol{\zeta}_1) g\, \sigma(g, \boldsymbol{s})\, d\boldsymbol{s}\, \zeta_{r1}\, d\eta_{\varphi 1}\, d\boldsymbol{\zeta}_1 \Big|_{\zeta=\zeta_i}$$

- The integrals in the above formula can be taken numerically, which results in the following formula:

$$I(\boldsymbol{\xi}_i) = \sum_{l=1}^{N} \sum_{m=1}^{N} A_{ilm} f_m f_l - f_i \sum_{k=1}^{N} b_{ik} f_k$$

ВЦ РАН

Deterministic approach, the same as for general case

➢Conservation laws are satisfied with the use of conservative correction:

$$I(\boldsymbol{\zeta}_i) = \sum_{l=1}^{N}\sum_{m=1}^{N} A_{ilm} f_m\, f_l - f_i\, P_i(\boldsymbol{\zeta}_i) \sum_{k=1}^{N} b_{ik} f_k$$

$$P_i(\boldsymbol{\zeta}_i) = 1 + a_0 + \boldsymbol{a}_1 \cdot \boldsymbol{\zeta}_i + a_2(\boldsymbol{\zeta}_i \cdot \boldsymbol{\zeta}_i)$$

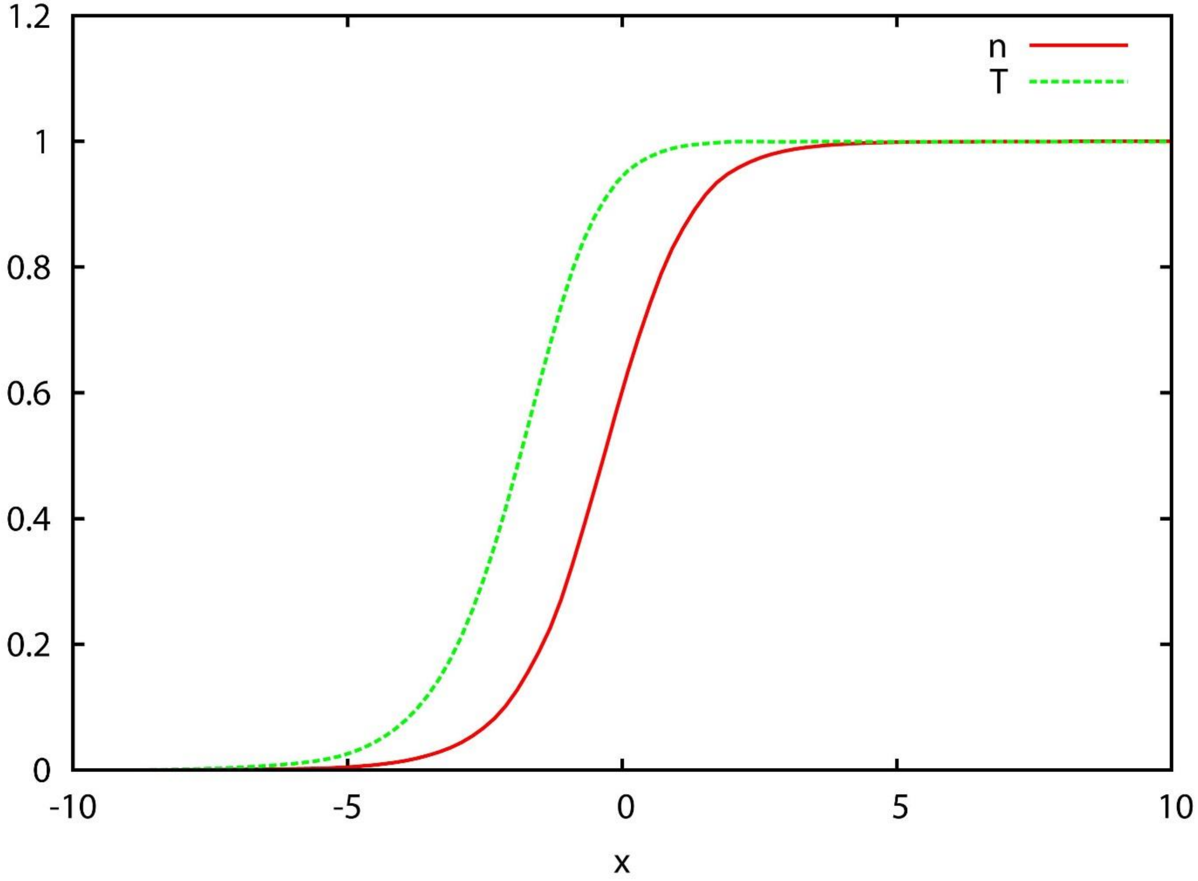
2 scalars a_0 and a_2 and 2D vector $\boldsymbol{a}_1$ are found from the linear system obtained by multiplying collision integral by collision invariants $\psi_\alpha = 1, \boldsymbol{\zeta}_i, (\boldsymbol{\zeta}_i \cdot \boldsymbol{\zeta}_i)$:

$$\sum_{k=1}^{N} I(\boldsymbol{\zeta}_i)\, \psi_\alpha = 0$$

The properties of the deterministic collision integral for 2d velocity space

- The collision integral is presented in a simple form.
- The number of arithmetic operations is proportional to N^3.
- For regular Cartesian mesh the number of unique values of A_{ilm} is proportional to $N^{5/2}$.
- More computations are necessary to calculate the values of A_{ilm}
- The method can be easily and **effectively** implemented for multiprocessor and/or GPU computers.

Numerical simulation, 1D shock wave problem, M=3



Conclusion

- A simple deterministic method for approximation Boltzmann collision integral is constructed for 2D velocity distribution function using piecewise constant approximation of the distribution function in finite velocity mesh.
- Conservation laws are maintained with the use of conservative correction
- M=3 shock wave problem is solved
- Future development will include
  - Various collision potentials and models
  - GPU implementation
  - Higher Mach number problems computations

Acknowledgements

This work was supported by Russian Foundation for Basic Research (grant 15-07-02986)

ВЦ РАН

Acknowledgements

Thank you for your attention!