Exploring Direct Simulation Monte-Carlo Techniques for Science Applications

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Students' Motivation

Students background in mathematical statistics, theory of probability, and molecular physics helps them in simulating real physical phenomena in gases and plasmas using Direct Simulation Monte-Carlo (DSMC) methods. The introduction of these methods to students and results of their exploration projects focusing on various practical applications are reviewed in this presentation.

The DSMC Methodology and Applications

The DSMC techniques were introduced by Prof. G. A. Bird [1-3] and successfully used for 60+ years in various practical applications:

- Rarefied-gas dynamics, molecular physics, thermodynamics, and aeronautics
- Nano-scale technologies in medicine, chemistry.

Samples of computer programs (written in Java, C, FORTRAN, and other languages) can be found in [1-4]. These codes were modified by students and used in their projects.

The validity of Monte-Carlo simulations was examined in the following case studies:

- The role of sample sizes in probabilistic analysis
- Values of "well-known" twofold integrals
- Values of the error function
- Surfaces and volumes of simple-shape bodies.

Students' Mini-case Studies:

- Molecular collisions [5]
- Estimations of gas transport coefficients [5]
- Structures of shock waves [1, 2, 4, 5-7]
- Aerodynamics of simple-shape probes [6, 8].

NOTE: All these cases cannot be solved by applying analytical or numerical approaches in solving ordinary and/or partial differential equations that are simply not applicable for studying these molecular phenomena.

Examples of Aerodynamic Projects

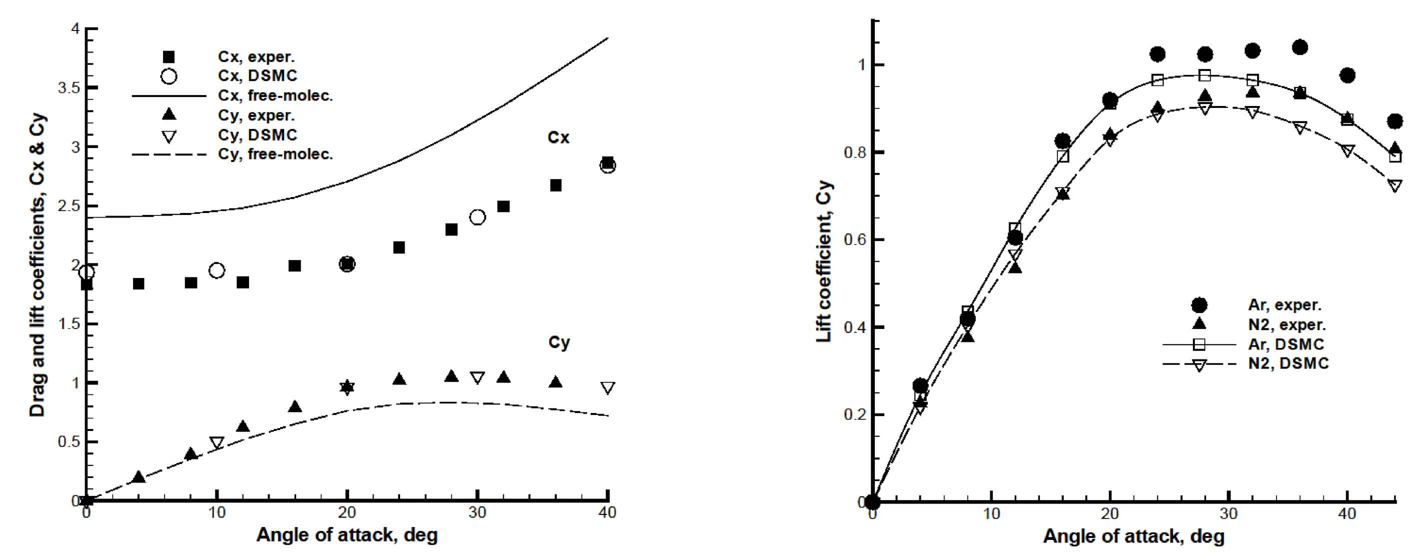

Fig. 1 *Left*: Drag and lift coefficients c_x, c_y for a wedge ($2\theta = 40$ deg) in He at Reynolds number $Re_0 = 4$ and $M_\infty = 11.8$. *Right*: Lift coefficient c_y of the wedge at $Re_0 = 3$ in Ar and N2.

Findings:

- The transitional-regime lift is bigger than the free-molecular lift value by a factor of 1.25.
- Data for different molecular gases γ indicates a significant difference (10%) in the values of lift coefficients c_y.

Aerodynamics of Rotating Cylinder (Inverse Magnus Effect)

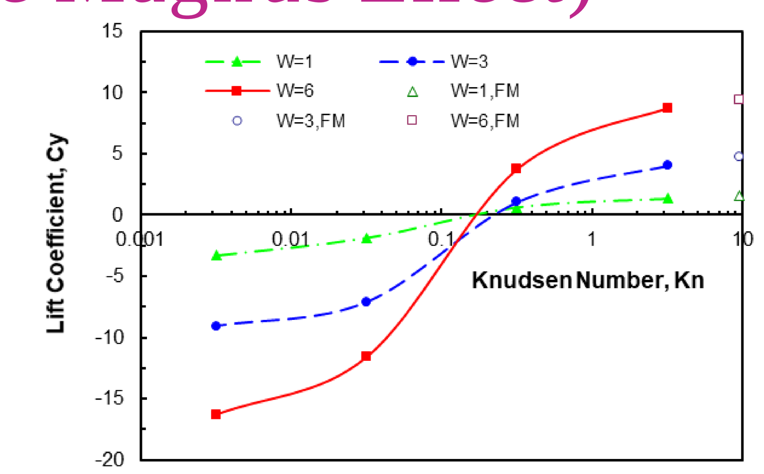

Fig. 2 Lift coefficient C_y of a spinning cylinder vs. Knudsen number $Kn_{\infty,D}$ at Mach number M_∞ = 0.15 and different spin rates W in argon.

Examples of Gas-expanding Projects:

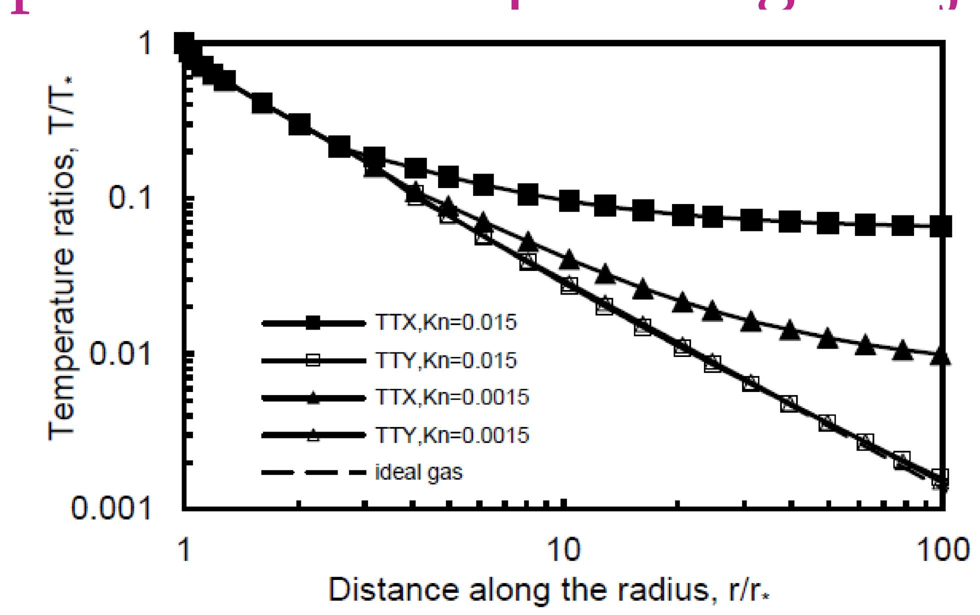

Fig. 3 Parallel (*TTX*) and transverse (*TTY*) temperature distributions in expansion of argon into vacuum at $Kn_* = 0.015$ and 0.0015.

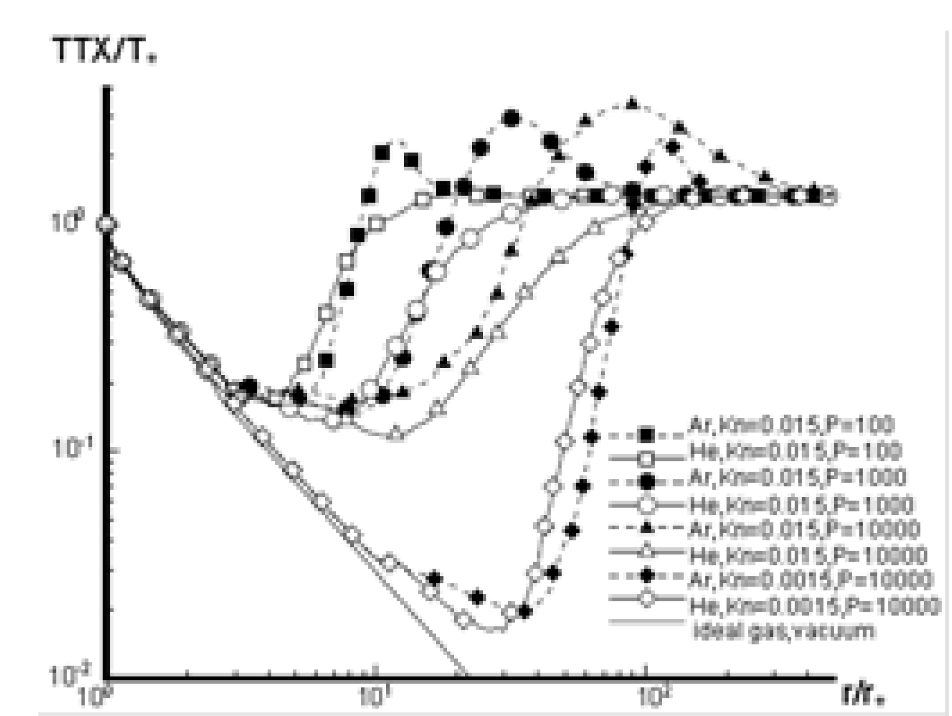

Fig. 4 Parallel temperatures *TTX* of species in spherical expanding flow of Ar-He mixture at different Knudsen numbers Kn_* and pressure ratios P.

REFERENCES: [1] G. A. Bird. Molecular Gas Dynamics. Clarendon, Oxford, England, 1976.
[2] G. A. Bird. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford, 1994.
[3] G. A. Bird. The DSMC Method, CreateSpace Independent Publishing Corp., Oxford, 2013.
[4] M. S. Ivanov et al. Computational tools for rarefied aerodynamics. Rarefied Gas Dynamics, 1994
[5] V. Riabov. Journal of Thermophysics and Heat Transfer, 14(3):404-411, 2000.
[6] V. Riabov. Journal of Spacecraft and Rockets, 35(4):424-433, 1998.
[7] V. Riabov. Journal of Thermophysics and Heat Transfer, 17(4):526-533, 2003.
[8] J. N. Moss. DSMC Simulations of Ballute Aerothermodynamics. AIAA Paper 2005-4949.

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