AAE 590D: MOLECULAR GAS DYNAMICS
FALL 2010

> If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on the the next generations of creatures, what statement would contain the most information in the fewest words? I believe it is the *atomic hypothesis* that *all things are made of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.*
>
> Richard Feynman, Six Easy Pieces
> Ch. 1 Atoms in Motion

The course is about microscopic approach to understanding the behavior of a gas which states that all substances are composed of a large number of very small particles (molecules or atoms). The observable properties of gas are the consequence of the actions of the molecules making up the gas. We will cover gas dynamic phenomena that require the molecular description such as the structure of shock wave, high-altitude aerodynamics and expansions into vacuum, velocity slip and aerodynamic forces in nano/microsystems.

Objectives include developing abilities to:
1) Calculate basic gas properties such as temperature, pressure, flow velocity, gas stresses and fluxes from the molecular velocity distribution function.
2) Identify gas flow regimes (continuum, slip, transitional, free molecular) and applicable governing equations.
3) Apply equilibrium fluxes to solve simple free-molecular flow problems.
4) Setup and conduct direct simulation Monte Carlo modeling for simple rarefied flow problems.

Day & Time: M, W 3:00 - 4:15 pm **Room:** Physics 201
Course page: http://web.ics.purdue.edu/~alexeenk/590d
Additional material on Blackboard Vista

Instructor: A. A. Alexeenko (U-lek-se'-en-ko).
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Office Hours: M, W 4:30 – 5:30 or by appointment

Textbooks:
1) G.A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford Science Publications, 2nd Rev. Edition, 1994 [Reprint 2004]. On reserve in Engineering library.
2) Y. Sone, *Molecular Gas Dynamics: Theory, Techniques, and Applications.* Birkhauser, 2006. Available electronically through Purdue libraries.
Additional Texts:
3) T. Gombosi, *Gas Kinetic Theory.* Cambridge UP, 1994.
4) W.G. Vincenti, C.H.Kruger, *Introduction to Physical Gas Dynamics.* Krieger, 1965 [Reprint 2002]
5) E.H. Kennard, *Kinetic Theory of Gases*. McGraw-Hill, 1938.

Grading: Homework 40% Midterm 30 % Course Project 30%

Exam: Middterm exam the week of October 6 – 10. Closed books, open notes.

Course Projects: Project proposal due before October break; progress report due first week of November. Project presentations during the last week of classes. Teams of up to two. Select a problem that is interesting to you and requires application of molecular gas dynamics.

Outline

Chapter 1: Introductory concepts of kinetic theory of gases. Pressure and temperature, peculiar and flow velocity. Stresses and fluxes. Mean free path and collision dynamics.
Chapter 2: Boltzmann equation. Assumptions. Derivation. Collision models.
Chapter 3: Solution of Boltzmann equation

- 3.1: Exact solutions for selected problems. Shock wave. Heat transfer. Couette flow.
- 3.2: Numerical methods for BE and applications. Basics of the DSMC method. Basics of discrete velocity method. Examples.

Tentative Schedule

Week	Topics
1	**Chapter 1:** Molecular hypothesis. Elementary gas kinetic theory. Pressure and temperature.
2	Molecular collisions and scattering. Binary collision dynamics. Collision frequency and mean free path.
3	**Chapter 2:** Velocity distribution function. The Boltzmann Equation: assumptions, derivation, non-dimensional form
4	Summational invariants. H-theorem and equilibrium. Maxwell velocity distribution function, experimental verification. Boltzmann H-function and entropy.
5	Moment transfer equation. Conservation equations. Connection between BE and Euler, Navier-Stokes equations.
6	Transport properties: viscosity, thermal conductivity, diffusivity. Knudsen layer, velocity slip and temperature jump.
7	**Midterm I**
8	**Chapter 3:** Overview of numerical methods of rarefied gas dynamics. Intermolecular potentials and molecular models. **Project proposals due.**
9	Introduction to DSMC. Review of relevant probability and statistics.
10	Pseudo random number generators. Inverse-cumulative and acceptance-rejection sampling.
11	DSMC algorithms.
12	Collisional schemes, models for internal energy relaxation and chemical reactions. Gas-surface interaction. **Progress reports due.**
13	Discrete ordinate method. Quadratures. Numerical solution of linearized Boltzmann, BGK/ES model kinetic equations.
14	Free molecular flows: expansion into vacuum, low-pressure damping in MEMS.
15	Slip and transitional flows: Couette and Poiseuille problems.
16	Thermal transpiration. Applications to microflows. Thruster exhaust plumes, satellite contamination.
Finals	**Project presentations**