# ASEN 6061 MOLECULAR GAS DYNAMICS and DSMC Fall 2022



Instructor: Professor Chris Roseman & Professor Brian M. Argrow

Office: TBD, (for office hours)

Office Hours: Tuesday 12:45-2:00pm (in-person & virtual)

Wednesday 10:00am-12:00pm (virtual)

Contact: Include "ASEN 6061" in subject line

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Course website: http://canvas.colorado.edu

Distance Students/Lecture Recordings: This class will use classroom capture to record lectures and those will be posted to the website

**Applications:** High-Knudsen-number modeling and simulation for physics-based, gas-surface interaction; on-orbit satellite drag and trajectory analysis; high-speed atmospheric entry; weakly-ionized and reacting rarefied flows; flow in miniature and MEMS devices...

#### Learning Goals

- Learn fundamentals of kinetic theory, the basis for the molecular description of a dilute gas.
- Learn the foundations, implementation, and applications of the Direct Simulation Monte Carlo (DSMC) method for modeling rarefied-gas flows

## Learning Outcomes

- Understanding of basic kinetic theory and molecular models
- Understanding of the appropriate applications and limitations of kinetic theory and DSMC
- Ability to obtain and verify simple one-dimensional and two-dimensional DSMC results using a custom DSMC code and an open source state-of-the-art code

**Course Overview:** Description of the composition and flow of gases on a microscopic level to examine the behavior of the molecules that make up a macroscopic flow system. Thermodynamic properties, transport phenomena, and the governing Boltzmann Equation are derived from molecular collision dynamics and the kinetic theory. Kinetic theory and DSMC are introduced in project-based assignments and in-class discussion.

**Prerequisites:** Familiarity with compressible flows and thermodynamics, with some differential equations and tensor notation. Simple programming and numerical methods using programming languages such as C++, MATLAB, Mathematica, or Python.

## **Course Outline:**

- 1. Kinetic Theory
- 2. Binary Elastic Collisions
- 3. Basic Kinetic Theory
- 4. Equilibrium Gas Properties
- 5. Inelastic Collisions and Surface Interactions
- 6. Collisionless (Free-Molecular) Flow
- 7. Transition Regime Flows
- 8. DSMC Topics



**Text:** Boyd & Schwartzentruber, Nonequilibrium Gas Dynamics and Molecular Simulation, Cambridge, 2017. Online (need to be on UCB internet):

https://www.cambridge.org/core/books/nonequilibrium-gas-dynamics-and-molecularsimulation/E317E76AA03C6C2C0A78A67EAB122C30

Additional References:

G. A. Bird, **Molecular Gas Dynamics and the Direct Simulation of Gas Flows**, Oxford, 1994. Online:

https://app.knovel.com/web/toc.v/cid:kpMGDDSGF3/viewerType:toc//root\_slug:molecular-gasdynamics

Bird, G. A., **The DSMC Method**, **Version 1.1**, 2013, ISBN 9781492112907 (https://www.createspace.com/3689652).

Vincenti and Kruger, Introduction to Physical Gas Dynamics, Wiley, 1965; Krieger, 1986.

Grading:	PROJECTS		
	Project 1 – Test Particle Monte Carlo Code Project 2 – Direct Simulation Monte Carlo Code Project 3 – SPARTA Simulation Study		20% 25% 20%
	HOMEWORK, UNIT QUIZZES	15%	

### **Classroom Behavior**

Both students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote or online. Those who fail to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, political affiliation or political philosophy. For more information, see the classroom behavior policy, the Student Code of Conduct, and the Office of Institutional Equity and Compliance.

#### **Requirements for COVID-19**

As a matter of public health and safety, all members of the CU Boulder community and all visitors to campus must follow university, department and building requirements and all public health orders in place to reduce the risk of spreading infectious disease. CU Boulder currently requires COVID-19 vaccination and boosters for all faculty, staff and students. Students, faculty and staff must upload proof of vaccination and boosters or file for an exemption based on medical, ethical or moral grounds through the MyCUHealth portal.

The CU Boulder campus is currently mask-optional. However, if public health conditions change and masks are again required in classrooms, students who fail to adhere to masking requirements will be asked to leave class, and students who do not leave class when asked or who refuse to comply with these requirements will be referred to Student Conduct and Conflict Resolution. For more information, see the policy on classroom behavior and the Student Code of Conduct. If you require accommodation because a disability prevents you from fulfilling these safety measures, please follow the steps in the "Accommodation for Disabilities" statement on this syllabus.

If you feel ill and think you might have COVID-19, if you have tested positive for COVID-19, or if you are unvaccinated or partially vaccinated and have been in close contact with someone who has COVID-19, you should stay home and follow the further guidance of the Public Health Office (contacttracing@colorado.edu). If you are fully vaccinated and have been in close contact with someone who has COVID-19, you do not need to stay home; rather, you should self-monitor for symptoms and follow the further guidance of the Public Health Office (contacttracing@colorado.edu). {Faculty: insert your procedure here for students to alert you about absence due to illness or quarantine. Because of FERPA student privacy laws, do not require students to state the nature of their illness when alerting you. Do not require "doctor's notes" for classes missed due to illness; campus health services no longer provide "doctor's notes" or appointment verifications.}

## Accommodation for Disabilities

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the <u>Disability Services website</u>. Contact Disability Services at 303-492-8671 or <u>dsinfo@colorado.edu</u> for further assistance. If you have a temporary medical condition, see <u>Temporary Medical Conditions</u> on the Disability Services website.

### **Preferred Student Names and Pronouns**

CU Boulder recognizes that students' legal information doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns are listed on instructors' class rosters. In the absence of such updates, the name that appears on the class roster is the student's legal name.

#### Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the <u>Honor Code</u>. Violations of the Honor Code may include, but are not limited to: plagiarism, cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution (honor@colorado.edu); 303-492-5550). Students found responsible for violating the <u>Honor Code</u> will be assigned resolution outcomes from the Student Conduct & Conflict Resolution as well as be subject to academic sanctions from the faculty member. Additional information regarding the Honor Code academic integrity policy can be found on the <u>Honor Code website</u>.

#### Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, protected-class discrimination and harassment, and related retaliation by or against members of our community on- and off-campus. These behaviors harm individuals and our community. The Office of Institutional Equity and Compliance (OIEC) addresses these policies, and individuals who believe they have been subjected to misconduct can contact OIEC at 303-492-2127 or email cureport@colorado.edu. Information about university policies, reporting options, and support resources can be found on the <u>OIEC website</u>.

Please know that faculty and graduate instructors have a responsibility to inform OIEC when they are made aware of any issues related to these policies regardless of when or where they occurred to ensure that individuals impacted receive information about their rights, support resources, and resolution options. To learn more about reporting and support options for a variety of concerns, visit <u>Don't Ignore It</u>.

## **Religious Holidays**

Campus policy regarding religious observances requires that faculty make every effort to deal reasonably and fairly with all students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. Contact Prof. Roseman if you need any accommodations due to religious observances as soon as possible. See the campus policy regarding religious observances for full details.