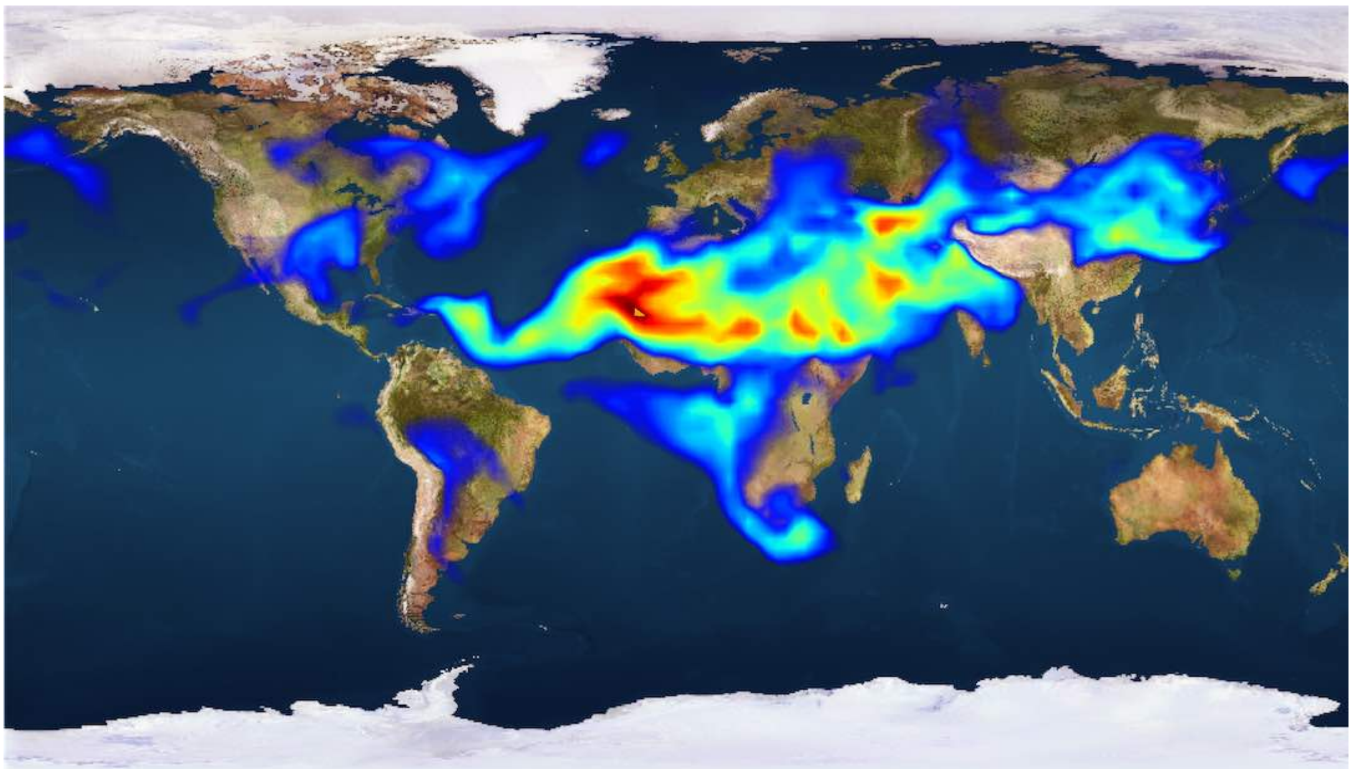
DEPT. OF EARTH & ENVIRONMENTAL SCIENCES, UNIVERSITY OF ROCHESTER

Fundamentals of Atmospheric Modeling

EES 234/434



Instantaneous snapshot of GEOS-Chem ^{222}Rn simulation.

Spring 2021

Syllabus

Last Updated: January 24, 2021

Contents

1 Overview

Course Location: Online
Course Time: Tu/Th 2:00 PM-3:15 PM Eastern

Recitation Location: Online
Recitation Time: Fr 2:00 PM-3:15 PM Eastern

Instructor: Prof. Lee T. Murray
Personal Pronouns: he/his/him
E-mail: lee.murray@rochester.edu
Office Hours: One hour after each synchronous live lecture, or by e-mail appointment

1.1 Description

Global atmospheric models are critical research and policy tools used to understand and predict the weather, climate change, and air pollution. This course provides an applied introduction to the physics, chemistry, and numerical methods underlying simulations of the spatial and temporal evolution of mass, energy, and momentum in planetary atmospheres. Topics include: finite-differencing the equations of atmospheric dynamics, radiative transfer models, numerical methods for solving systems of chemical ordinary differential equations, parameterization of small-scale processes, surface exchanges, inverse modeling, and model evaluation techniques. Assignments focus on the implementation and application of simple models by students; no prior experience with scientific programming will be assumed. Students will also gain experience using state-of-the-science models of atmospheric chemistry and/or climate in a final project of their choosing.

1.2 Pre-requisites

Required, unless granted permission by instructor:

- MTH 165 (Linear Algebra with Differential Equations) or equivalent
- PHY 121 (Mechanics) or equivalent
- CHM 131-132 (Intro. College Chemistry) or equivalent
- EES 105 (Intro. to Climate Change) or 218 (Atmospheric Chemistry) or 236 (Atmospheric Physics) or equivalent

Recommended, but not required:

- PHY 255 (Intro. to Fluid Dynamics)

1.3 Main Learning Goals

By the end of the course, students will:

- Understand the fundamental equations that govern the evolution of mass, energy and momentum in planetary atmospheres
- Learn the numerical methods used to solve these equations as efficiently and accurately as possible
- Understand the limitations of today's computers, models, and numerical methods with respect to simulating the atmosphere
- Gain practice and confidence in basic programming and graphical plotting using the R programming language
- Gain experience running and interpreting output from the same models used by today's scientists to inform air quality, weather forecasting and climate change science and policy

2 Readings

2.1 Required

Book

Brasseur, G. P., and D. J. Jacob (2017), *Modeling of Atmospheric Chemistry*, Cambridge University Press, Cambridge, UK, doi:10.1017/9781316544754.

Wilks, D. S. (2011), *Statistical Methods in the Atmospheric Sciences*, Elsevier Science Technology, ProQuest Ebook Central, online at https://ebookcentral.proquest.com/lib/rochester/detail.action?docID=689817.

Articles and Excerpts

Miller, S. M., et al. (2013), Anthropogenic emissions of methane in the united states, *Proceedings of the National Academy of Sciences*, *110*(50), 20,018–20,022, doi:10.1073/pnas.1314392110.

2.2 Supplemental

Books

Jacobson, M. Z. (2005), *Fundamentals of Atmospheric Modeling*, 2nd ed., Cambridge University Press, Cambridge, UK, doi:10.1017/CBO9781139165389.

Stull, R. (2016), *Practical Meteorology: An Algebra-based Survey of Atmospheric Science*, 1.00b ed., Univ. of British Columbia, https://www.eoas.ubc.ca/books/Practical_Meteorology/.

ARTICLES

Brunner, D., et al. (2003), An evaluation of the performance of chemistry transport models by comparison with research aircraft observations. Part 1: Concepts and overall model performance, *Atmos Chem Phys*, *3*(5), 1609–1631, doi:10.5194/acp-3-1609-2003.

Fishman, J., et al. (2008), Remote Sensing of Tropospheric Pollution from Space, *B Am Meteorol Soc*, *89*(6), 805–821, doi:10.1175/2008BAMS2526.1.

Henze, D. K., A. Hakami, and J. H. Seinfeld (2007), Development of the adjoint of geos-chem, *Atmospheric Chemistry and Physics*, *7*(9), 2413–2433, doi:10.5194/acp-7-2413-2007.

Jolliff, J. K., J. C. Kindle, I. Shulman, B. Penta, M. A. M. Friedrichs, R. Helber, and R. A. Arnone (2009), Summary diagrams for coupled hydrodynamic-ecosystem model skill assessment, *J Marine Syst*, *76*(1-2), 64–82, doi:10.1016/j.jmarsys.2008.05.014.

Marenco, A., et al. (1998), Measurement of ozone and water vapor by Airbus in-service aircraft: The MOZAIC airborne program, an overview, *J Geophys Res*, *103*(D19), 25,631, doi:10.1029/98JD00977.

Michalak, A. M., L. Bruhwiler, and P. P. Tans (2004), A geostatistical approach to surface flux estimation of atmospheric trace gases, *Journal of Geophysical Research: Atmospheres*, *109*(D14), doi:https://doi.org/10.1029/2003JD004422.

Singh, H. B., W. H. Brune, J. H. Crawford, D. J. Jacob, and P. B. Russell (2006), Overview of the summer 2004 Intercontinental Chemical Transport Experiment–North America (INTEX-A), *J Geophys Res*, *111*(D24), D24S01, doi:10.1029/2006JD007905.

Taylor, K. E. (2001), Summarizing multiple aspects of model performance in a single diagram, *J Geophys Res Atmos*, *106*(D7), 7183–7192, doi:10.1029/2000JD900719.

Thompson, A. M. (2003), Southern Hemisphere Additional Ozonesondes (SHADOZ) 1998–2000 tropical ozone climatology 1. Comparison with Total Ozone Mapping Spectrometer (TOMS) and ground-based measurements, *J Geophys Res*, *108*(D2), 8238, doi:10.1029/2001JD000967.

Wesely, M. L. (1989), Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models, *Atmos Environ*, *23*(6), 1293–1304, doi:10.1016/0004-6981(89)90153-4.

3 Schedule

3.1 Lectures

Below is the tentative class schedule, with topics for each class, associated readings, and problem set due dates. Schedule subject to change pending course progress. If students do not attend the synchronous lecture, they are required to watch the asynchronous recording before the next synchronous lecture.

Required reading assignments in **bold** must be completed before lecture. Supplemental or alternative readings in *italics*.

Tuesday	Thursday
Feb 2nd **1** **Overview** Key Topics 1. Course description and expectations Reading • **Syllabus** **E-mail Prof. your NetID for BlueHive account**	4th **2** **History of Atmospheric Modeling** Key Topics 1. Numerical weather forecasting (NWF) 2. General circulation models (GCMs) 3. Chemical transport models (CTMs) 4. Chemistry-climate and Earth system models (CCMs/ESMs) Reading • ***Brasseur and Jacob* (2017) Ch. 1** • *Jacobson* (2005) Ch. 1
9th **3** **Atmospheric Structure** Key Topics 1. Pressure, temperature and density 2. Equation of state (Ideal Gas Law) 3. Hydrostatic Equilibrium (Barometric Law) and Hypsometric (Thickness) Equation Reading • ***Brasseur and Jacob* (2017) Ch. 2.1, 2.3, 2.4, 2.6.1** • *Jacobson* (2005) Ch. 2.1-2.4	11th **4** **Atmospheric Thermodynamics** Key Topics 1. Global energy budget 2. Adiabatic lapse rate 3. Potential temperature 4. Atmospheric stability Reading • ***Brasseur and Jacob* (2017) Ch. 2.2, 2.6.2** • *Jacobson* (2005) Ch. 2.6 **PS1 Due Feb 12 @ 23:59**
16th **5** **Moist Thermodynamics** Key Topics 1. Latent heat 2. Clausius-Clapeyron relationship 3. Moist adiabat Reading • ***Brasseur and Jacob* (2017) Ch. 2.5, 2.6.2** • *Jacobson* (2005) Ch. 2.5	18th **6** **Atmospheric Dynamics** Key Topics 1. Real and apparent (Coriolis) forces 2. Geostrophic balance 3. General circulation of the atmosphere 4. Barotropic and baroclinic atmosphere Reading • ***Brasseur and Jacob* (2017) Ch. 2.7-2.11** • *Stull* (2016) Ch. 11

<table>
<tr><th>Tuesday</th><th>Thursday</th></tr>
<tr><td>23rd 7
The Fundamental Equations: Part I
Key Topics
1. Continuity equation
2. Thermodynamic equation
3. Momentum equation
Reading
• Brasseur and Jacob (2017) Ch. 4.1, 4.5
• Jacobson (2005) Ch. 3</td><td>25th 8
The Fundamental Equations: Part II
Key Topics
1. Horizontal coordinate systems
2. Spherical coordinates
3. Cartesian coordinates
Reading
• Brasseur and Jacob (2017) Ch. 4.5
• Jacobson (2005) Ch. 4
PS2 Due Feb 26 @ 23:59</td></tr>
<tr><td>Mar 2nd 9
The Fundamental Equations: Part III
Key Topics
1. Vertical coordinate systems
2. Hydrostatic and non-hydrostatic models
3. Altitude coordinate systems
4. Pressure (sigma) coordinate systems
5. Hybrid coordinate systems
Reading
• Brasseur and Jacob (2017) Ch. 4.6
• Jacobson (2005) Ch. 5</td><td>4th 10
Numerical Methods for Advection: Part I
Key Topics
1. Operator Splitting
2. Elementary Finite Difference Methods
3. Elementary Finite Volume Methods
4. Flux-Corrected Transport
Reading
• Brasseur and Jacob (2017) Ch. 7.1-6
• Jacobson (2005) Ch. 6</td></tr>
<tr><td>9th 11
Numerical Methods for Advection: Part II
Key Topics
1. Lagrangian/Semi-Lagrangian Methods
2. Spectral, Finite Element, and Spectral Element Methods
3. Numerical Fixers and Filters
Reading
• Brasseur and Jacob (2017) Ch. 7.7-11
• Jacobson (2005) Ch. 6</td><td>11th 12
Radiative Transfer Models
Key Topics
1. Radiative transfer equation
2. Absorption and scattering by gases and particles
3. Optical depth
Reading
• Brasseur and Jacob (2017) Ch. 5.1-5.2
• Jacobson (2005) Ch. 9
PS3 Due Mar 12 @ 23:59</td></tr>
<tr><td>16th 13
Radiative Transfer Models
Key Topics
1. Radiative transfer equation
2. Absorption and scattering by gases and particles
3. Optical depth
Reading
• Brasseur and Jacob (2017) Ch. 5.1-5.2
• Jacobson (2005) Ch. 9</td><td>18th 14
Atmospheric Chemistry: Gas-Phase Overview
Key Topics
1. Odd oxygen and HO_x radicals
2. Reactive nitrogen
3. Volatile organic compounds and carbon monoxide
4. Ozone and OH production and loss
Reading
• Brasseur and Jacob (2017) Ch. 3.1-3.8
• Jacobson (2005) Ch. 10.1, 11</td></tr>
</table>

TUESDAY	THURSDAY
23rd **15** **Atmospheric Chemistry: Condensed-Phase Overview** Key Topics 1. Aerosol size distributions 2. Chemical composition 3. Mixing state, hygroscopicity, and activation 4. Optical properties Reading • ***Brasseur and Jacob* (2017) Ch. 3.9** • *Jacobson* (2005) Ch. 13 **Final Project Topic Due via Email to Prof.**	25th **16** **Formulation of Chemical Rates** Key Topics 1. Photolysis 2. Gas-phase chemical kinetics 3. Multiphase and heterogeneous chemistry Reading • ***Brasseur and Jacob* (2017) Ch. 5.3-5.5** • *Jacobson* (2005) Ch. 10.2-6 **PS4 Due Mar 26 @ 23:59**
30th **Study Break**	Apr 1st **17** **Numerical Integration of Chemical Systems** Key Topics 1. General Considerations 2. Explicit Chemical Solvers 3. Implicit Chemical Solvers Reading • ***Brasseur and Jacob* (2017) Ch. 6** • *Jacobson* (2005) Ch. 12
6th **18** **Cloud Thermodynamics & Dynamics** Key Topics 1. Vertical Momentum Equation in a Cloud 2. Convective Available Potential Energy (CAPE) 3. Cumulus Parameterizations 4. Cloud Microphysics 5. Wet Deposition Reading • ***Brasseur and Jacob* (2017) Ch. 8.8-8.9** • *Jacobson* (2005) Ch. 18.1-8	8th **19** **Surface Processes: Planetary Boundary Layer** Key Topics 1. Turbulent fluxes 2. Surface friction height 3. Eddy diffusion Reading • ***Brasseur and Jacob* (2017) Ch. 8.7** • *Jacobson* (2005) Ch. 8 **PS5 Due Apr 09 @ 23:59**
13th **20** **Surface Processes: Air-Surface Exchange** Key Topics 1. Emissions 2. Dry deposition 3. Two-way fluxes Reading • ***Brasseur and Jacob* (2017) Ch. 9** • *Jacobson* (2005) Ch. 20 • *Wesely* (1989)	15th **21** **Inverse Modeling & Data Assimilation: Part I** Key Topics 1. Bayes' Theorem 2. Inverse problem for scalars Reading • ***Brasseur and Jacob* (2017) Ch. 11.1-11.3**

TUESDAY	THURSDAY
20th **22** **Inverse Modeling & Data Assimilation: Part II** Key Topics 1. Inverse problem for vectors 2. Error-covariance matrices 3. Jacobian matrix 4. Averaging kernel matrix Reading • ***Brasseur and Jacob* (2017) Ch. 11.4-11.5**	22nd **23** **Inverse Modeling & Data Assimilation: Part III** Key Topics 1. Adjoint Methods 2. Geostatistical Inverse Methods Reading • ***Brasseur and Jacob* (2017) Ch. 11.4.4** • ***Miller et al.* (2013)** • *Michalak et al.* (2004) • *Henze et al.* (2007) **PS6 Due Apr 23 @ 23:59**
27th **24** **Inverse Modeling & Data Assimilation: Part IV** Key Topics 1. Kalman Filter ("3-D VAR") 2. Data Assimilation ("4-D VAR") 3. Observing System Simulation Experiments (OSSEs) Reading • ***Brasseur and Jacob* (2017) Ch. 11.6-11.9**	29th **25** **Atmospheric Observations & Model Evaluation: Part I** Key Topics 1. Interpreting model output 2. Determining statistical significance 3. Techniques for simplifying complex output (EOF, Spectral Analyses) Reading • ***Wilks* (2011) Ch 9, Ch. 12**
May 4th **26** **Atmospheric Observations & Model Evaluation: Part II** Key Topics 1. *In situ* observations 2. Remote sensing 3. Characterization of errors Reading • ***Brasseur and Jacob* (2017) Ch. 10.1-10.3** • *Marenco et al.* (1998) • *Thompson* (2003) • *Singh et al.* (2006) • *Fishman et al.* (2008)	6th **27** **Atmospheric Observations & Model Evaluation: Part III** Key Topics 1. General considerations for model evaluation 2. Using models to interpret observations Reading • ***Brasseur and Jacob* (2017) Ch. 10.4-10.7** • *Taylor* (2001) • *Brunner et al.* (2003) • *Jolliff et al.* (2009) **PS7 Due May 07 @ 23:59**
11th **Exam Period** **Final Project Presentation During Exam Slot**	13th **Exam Period** **Final Project Report Due on Sat May 15 @ 23:59**

3.2 Recitation

In addition to lecture, we will meet every Friday from 2-3 PM for a recitation in which we will work on the Problem Sets, Coding Exercises and our Final Projects together as a group. Recitation is not required, but it is strongly encouraged.

4 Grading

Your final grade will be calculated with the following breakdown

Quizzes:	5 %
Participation:	5 %
Problem Sets:	40 %
Final Project Report:	40 %
Final Project Presentation:	10 %
Total:	100 %

4.1 Quizzes

At the end of each class, there will be a short quiz in Blackboard on the main concepts covered by the reading / lecture. Students must complete the quiz before the next synchronous live lecture.

4.2 Participation

The participation score will reflect the following activities:

- Asking and answering questions about course content and coding in the online "Ask a Question" forum in Blackboard.
- General participation: e.g., by asking or answering questions during lecture and recitation, and/or by asking questions during office hours.

4.3 Final Project and Presentation

All students will perform a term project, generate a final report, and present a summary to the class in lieu of a final exam. Following consultation with Prof. Murray, students will select a portion of either the GEOS-Chem CTM, the GISS ModelE GCM or the NCAR WRF NWF model that they find interesting. They will examine and alter the underlying model code and parameters, and perform sensitivity simulations to examine the impact of these changes on the simulated atmosphere. The project will culminate in a written report containing the following content:

- A plain English description of the model component and how it works, which may incorporate “pseudo-code”
- A description of any limitations of the method as presently implemented
- A description of alternative methods found in the scientific literature for the component, with a discussion of their pros and cons
- An analysis of changes in the simulated atmosphere with sensitivity experiment performed by the student, including plots, with a discussion of the underlying physical, chemical and/or numerical reasons.

EES 234 reports will be required to be at least 10 pages in length. EES 434 reports will be required to be at least 20 pages. All page counts include figures and references. All text must use 10-pt font with

1.5-line spacing.

All text **must** be written following the Style Guide and Reference Format of the American Geophysical Union.

EES 434 enrollees are encouraged to work with Prof. Murray to identify a scientific question relevant to their research for their analysis. Expectations for the analysis and external literature review will be higher for EES 434.

All students are strongly encouraged to submit a rough draft of their reports at least a week before they are due for feedback.

Students will be required to present a 15-minute presentation of their final project to their classmates, followed by 5 minutes of questions from the audience. Presentations will occur during the final exam time slot. Students are encouraged to share their slides with Prof. Murray in advance for feedback.

Rubrics for the grading of the Final Report and Presentation are available for viewing in Blackboard.

5 Computers

Students will require access to a personal computer for this course.

Simulations for the final project will need to be performed on UR's high-performance computing (HPC) system, named "BlueHive," maintained by the Center for Integrated Research Computing (CIRC).

Students who do not already have an account on BlueHive should provide Prof. Murray with their NetIDs, and CIRC will establish new accounts that will expire at the end of the semester.

Students will need to install VPN on their personal computers and set up Duo 2FA in order to access BlueHive; **this must be done while on the campus network**. Be sure to read and follow the use policies for the system, which is shared by many members of the university for their research activities.

Students may do their homework assignment coding on BlueHive or their own personal computers.

6 Homework Policy

The aim of the problem sets is to help you learn the course concepts and gain experience with scientific programming. Working together with your classmates is thus encouraged, but **you must indicate who you worked with on your submission.** Nevertheless, problem sets and code should always be written up individually, and **all submitted code will be analyzed with a plagiarism checker** for uniqueness.

In addition to any handwritten submissions, all code used for each problem set is to be submitted digitally via e-mail to Prof. Murray by the start of class on its due date.

All assignments will be done using the R programming language (`http://www.r-project.org`), a powerful open-source and cross-platform scripting language for statistical and scientific analyses and graphics. Good code is well commented and includes liberal use of indentation, alignment, and white space to aid in readability. **All code submitted must follow Google's Style Guide for R**. Code that fails to follow the style standards will be penalized.

All assignments – unless otherwise explicitly allowed – will be limited to the use the following R base functions:

- Arithmetic Operators (`+`, `-`, `*`, `/`, `^`, `%%`, `%*%`)
- Logical Operators (`<`, `<=`, `>`, `>=`, `==`, `!=`, `!`, `|`, `&`)
- Logarithms and Exponential Functions (`exp`, `log10`, `log`)
- Trigonometric Functions (`cos`, `sin`, `tan`, `acos`, `asin`, `atan`, `atan2`, `cospi`, `sinpi`, `tanpi`)
- Control Flow Functions (`if`, `else`, `for`, `while`, `break`, `next`, `apply`)

You may check your solutions with higher-level functions (e.g., the differential equation solvers in the `deSolve` package), and are even encouraged to do so. However, the assignments are designed to teach you what is going on behind the scenes, and therefore anything you submit must be built from scratch without use of the higher-level packages except when explicitly granted permission in the assignment.

Show all work, explaining in sufficient detail how you arrived at the answer. Some questions will be easy to answer, and you may be able to do them in your head, but you must still explain how you arrived at your answer. **A correct answer with no work shown earns no credit.** A numerical answer without units is also incorrect.

Problem sets are due at the end of day indicated. After that, 10% is deducted off the possible total score for each day late. No credit is given after one week late. You will be granted four late days for use throughout the semester, which you may use at your discretion.

Problem Set 1 will be performed through `http://www.datacamp.com`. Problem Sets 2-7 will be submitted through GradeScope. GradeScope does not allow for combined problem sets and coding exercises, so you will need to upload all handwritten problems and generated figures to "Problem Set X" and the requested R scripts to "Coding Exercise X."

Students enrolled in EES 434 will have additional problems per homework assignment; these are indicated in GradeScope with the suffix "G."

7 Classroom Policies

7.1 Zoom Etiquette

Except when asking or answering questions, one's microphone should remain muted. To ask a question or volunteer to answer a question, please use the "Raise Hand"[1] feature of Zoom, in order to prevent us talking over one another. Or please feel free to type any questions into the chat box, which I will be monitoring.

Students are not required to have their video on during online lectures, especially if your Internet connection is unstable. However, I do request that you leave your video on whenever possible, as it helps me adjust my pacing by reading your faces for comprehension.[2]

7.2 Diversity and Inclusion

This classroom is an inclusive and welcoming learning environment for all students regardless of background or ability, consistent with University policy, state and federal laws and the instructor's personal beliefs. Students must respect the different experiences, identities, beliefs and values expressed by their peers, and refrain from derogatory comments about other individuals, cultures, groups, or viewpoints.

Please let me know if you have any preferred nicknames and/or pronouns that you would like me to use.

In the event you encounter any barrier(s) to full participation in this course due to the impact of a disability, please contact the Office of Disability Resources. The access coordinators in the Office of Disability Resources can meet with you to discuss the barriers you are experiencing and explain the eligibility process for establishing academic accommodations. You can reach the Office of Disability Resources at: disability@rochester.edu; (585) 276-5075; Taylor Hall; `http://www.rochester.edu/college/disability`.

7.3 Special Circumstances

Given the extraordinary circumstances of the COVID-19 pandemic, I acknowledge that students may be subject to a host of pressures and difficulties that will make learning this semester especially difficult. I encourage you to meet with me about any concern or situation that affects your ability to complete your academic work successfully.

[1] Click on "Participants" on the bottom of the screen; the "Raise Hand" option then appears in the lower right. `https://support.zoom.us/hc/en-us/articles/205566129-Raising-your-hand-in-a-webinar`

[2] Also, pets are more than welcome!

8 ACADEMIC HONESTY

All assignments and activities associated with this course must be performed in accordance with the University of Rochester's Academic Honesty Policy. A comprehensive description of the University of Rochester's Academic Honesty Policy is available at: `http://www.rochester.edu/college/honesty`. For this course, the quizzes and project need to be completed individually, but I encourage collaboration on the problem sets.

9 INITIAL MEETING

I would like to learn about your background and goals, both for this course and for the future, to help tailor the semester to those interests. You are encouraged to schedule (via e-mail) a quick 5-10 minute meeting early in the semester. The meeting is entirely optional and will not impact your participation grade.

10 FEEDBACK

I want you to get the most out of this class. Students are encouraged to offer feedback at any time about the course and my instruction to me in person, through e-mail to lee.murray@rochester.edu, or via an anonymous note placed in my departmental mailbox located in Hutchison Hall 227.