2nd Semester, AY 2020-2021

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Applied Physics 157

Module A

00 Preface

Instructor's Notes

1. This App Physics 157 Module A includes a syllabus and a weekly study guide that includes the list of readings, learning tasks, and coding exercises that you should complete over the next 4 weeks.

2. Programming is an activity where "learning by doing" is effective. Thus, code submissions should still be your own. Even if you can copy/paste from the starter code — retyping (and even rewriting it to reflect your own style) helps.

3. Engage in group discussions. Use Microsoft Teams chat, or even have impromptu meetings with your classmates online.

4. In trying out new tools, some may work wonderfully well and some may be turn out to be downright awful. Let us know right away if you encounter any issues.

Part I

Course Syllabus

01 About the Course

UP Diliman General Catalogue entry

Course code	Applied Physics 157
Course title	Computational Analysis and Modeling in Physics
Credit	4 units
Description	Computational models in physics; numerical simulations of physical systems; stochastic simulation and algorithms; image processing; multidimensional detection techniques; pattern recognition
Instructors	(Module A) May T. Lim - may@nip.upd.edu.ph (Module B) Reinabelle C. Reyes - rreyes@nip.upd.edu.ph (Module C) Maricor N. Soriano - jing@nip.upd.edu.ph

UVLe https://uvle.upd.edu.ph/course/view.php?id=15628

Microsoft Teams https://teams.microsoft.com/l/team/
19%3a5c4b55fd8cca43d8bed83390059e2d2c

02 References

1. [PfCP] S. Linge and H.P. Langtangen. Programming for Computations - Python. Springer. 2020. https://link.springer.com/content/pdf/10.1007%2F978-3-030-16877-3.pdf. License: CC-BY-4.0
2. [NumFys] NumFys: A resource for use of computational physics with Python, covering many topics in physics (Dept. of Physics, Norwegian University of Science and Technology). https://www.numfys.net License: CC-BY-NC-4.0
3. [TC] A.B. Downey. Think Complexity, 2nd ed. Green Tea Press. 2016. Chapters 6, 9. https://greenteapress.com/complexity2/thinkcomplexity2.pdf
4. [Net] M. Coscia. The Atlas for the Aspiring Network Scientist. 2021. Chapters 3, 4, 6, 9, 10, 11, and 14. https://www.networkatlas.eu
5. [LanV] R. Landau. Computational Physics videos. http://sites.science.oregonstate.edu/~landaur/Books/CPbook/eBook/Lectures/index.html
6. [LanN] R. Landau. Computational Physics Jupyter notebooks. http://sites.science.oregonstate.edu/~landaur/Books/CPbook/eBook/Notebooks/ (start

03 Mode and channels of delivery

AP157 will be conducted in a remote and asynchronous manner through the UVLe, Google Colab, and Microsoft Teams platforms.

UVLe

The AP157 UVLe page is https://uvle.upd.edu.ph/course/view.php?id=15628

Consultations via MS Teams

Ask your questions in the corresponding channel on MS Teams. We'll also have a weekly online consultation session every Wednesday, 10am. Code discussions, if any, will be uploaded in **https://github.com/maytlim/ap157**

Class discussion

You may freely discuss with me or your classmates by starting or replying to a conversation in the corresponding activity channel. All questions are welcome. Examples are problems with code, debugging questions, interpreting the text, sharing resources/tricks, etc. If you come across a nice tutorial (video or otherwise), please feel free to share them.

04 Grading system

Course requirements (for Module A)

100%	Reports (3)

Reports are one-page PDF (minimum font size = 12) write-ups where you will list down: a) top three (3) takeaways (i.e. key concepts) from that section; b) top three (3) code snippets that you think are essential to modeling/analyzing the topic; and c) top pitfalls (maximum of 3) -- you may even have struggled through them. There is no mandatory format (i.e. essay, presentation slide, ...) except the 1-page limit and the minimum font size. Do practice good design -- **https://developer.apple.com/design/tips/**. I will be checking for concept accuracy, insights, and succinctness. Some points will be deducted for poor grammar (so spell check at the minimum). Maximum score per activity is 100 points. All submissions must be your own work. In addition, you may submit a 3-minute video (shorter is better) to discuss the content of the PDF (you may use slides). This video is entirely optional.

Coding exercises. As a start, you should be able to replicate the figures in the reading materials for the week. Along the way, we gain understanding of the core concepts by asking and answering follow-up questions. The habit of performing version control should also be innate by the end of the semester.

Part II

Weekly Guide

05 Optional: Developing good programming habits

Learning tasks

By the end of this week, you must be able to:

1. Run code in Google Colaboratory and establish your remote computing workflow
2. Set up *git* to perform version control for your codes and sync to GitHub
3. Understand the need for testing code and write basic code to perform testing

Readings and resources

What is Colaboratory? https://colab.research.google.com

GitHub Cheat Sheet. https://education.github.com/git-cheat-sheet-education.pdf

[PfCP] 6.6. Testing Code, pp. 150 - 161

K. Reitz and T. Schlusser. Testing your Code. The Hitchhiker's Guide to Python. https://docs.python-guide.org/writing/tests/

M. Wouts. Jupytext. https://github.com/mwouts/jupytext

Coding exercises

Create a test for an area of a square calculator given a side length. Run this code in Google Colab.

Challenge problem: Include Jupytext in your Google Colab / GitHub pipeline.

06 Week 1: Random numbers and random walks

Learning tasks

By the end of this week, you must be able to:

1. Show the basic properties of the random walker.
2. Explain how they are related to Brownian motion, the motion of impurities in a lattice, and the large distance properties of macromolecules.
3. Use high quality, research grade, portable, (pseudo) random number generators.
4. Explain when Monte Carlo simulations are used.

Readings and resources

Videos: http://sites.science.oregonstate.edu/~landaur/Books/CPbook/eBook/Lectures/mp4Lecs/MonteCarlo_ipad.html and http://sites.science.oregonstate.edu/~landaur/Books/CPbook/eBook/Lectures/mp4Lecs/MonteCarloApps_ipad.html

[NumFys] Diffusion-limited aggregation * Self-avoiding random walk in 2D * Introduction to Brownian motion and diffusion

Coding exercises

Replicate the [NumFys] examples in Google Colab.

07 Week 2: Monte Carlo simulations

Learning tasks

By the end of this week, you should be able to:

1. Explain importance sampling and the Metropolis algorithm
2. Explain how cluster Monte Carlo algorithms work
3. Simulate the Ising model on a two dimensional rectangular lattice using the Metropolis algorithm.
4. Discuss the thermalization of the system and the effect of correlations between successive spin configurations generated during the simulation.
5. Explain how the autocorrelation function and the time scale defined by it, the autocorrelation time, play a central role in the study of the statistical independence of our measurements.
6. Determine statistical errors that take into account autocorrelations and predict the amount of resources needed for reaching a specific accuracy goal.

Readings and resources

[NumFys] * Ising model in 1D and 2D * Equilibrium Monte Carlo simulation of the 2D Ising model

E. Luijten. Introduction to Cluster Monte Carlo Algorithms. Lect. Notes Phys. 703, 13–38 (2006)

Coding exercises

Replicate the [NumFys] examples in Google Colab.

08 Monte Carlo simulations - 2D Ising model

Notes

You should be able to:

1. Simulate the Ising model on a two dimensional rectangular lattice using the Metropolis algorithm.
2. Discuss the thermalization of the system and the effect of correlations between successive spin configurations generated during the simulation.
3. Explain how the autocorrelation function and the time scale defined by it, the autocorrelation time, play a central role in the study of the statistical independence of our measurements.
4. Determine statistical errors that take into account autocorrelations and predict the amount of resources needed for reaching a specific accuracy goal.

09 Week 3: Cellular automata

Learning tasks

By the end of this week, you must be able to:

1. Define a cellular automaton.
2. Demonstrate Wolfram's 1D CA models.
3. In the context of CA, discuss determinism, randomness and universality.
4. Implement CAs.

Readings and resources

[TC] pp. 67 - 87

Coding exercises

Answer [TC] exercises 5.1 - 5.5. Use a separate Jupyter notebook for each exercise.

10 Week 3: Agent-based models

Learning tasks

By the end of this week, you must be able to:

1. Discuss the motivation for making agent-based models.
2. Implement Schelling's segregation model.
3. Run the Sugarscape model of Epstein and Axtell.
4. Define an emergent property.

Readings and resources

[TC] pp. 141 - 158

Coding exercises

Answer [TC] exercises 9.1 - 9.3. Use a separate Jupyter notebook for each exercise.

11 Week 4: Network tools

Learning tasks

By the end of this week, you must be able to:

1. Enumerate situations when a graph/network model are useful.
2. Explain how an adjacency matrix is used to represent a graph/network.
3. Use clustering, path length and degree distribution to describe networks.

Readings and resources

[Net] Chapters 3, 4, 6, 9, 10, 11, and 14

Exercises

Perform the corresponding exercises for Chapters 3, 4, 6, 9, 10, 11, and 14 at https://www.networkatlas.eu/exercise.htm.

Try out the exercises before looking at the solutions. For solutions containing codes, run in Google Colab.

Part III

Advanced Topics

12 More readings

Monte Carlo methods

Chapters 29-32 of D. MacKay. “Information Theory, Inference, and Learning Algorithms” Cambridge Univ Press. 2016. http://www.inference.org.uk/itprnn/book.pdf

On stochastic predator-prey models: U.C. Täuber 2011 J. Phys.: Conf. Ser. 319 012019 https://iopscience.iop.org/article/10.1088/1742-6596/319/1/012019/pdf

R. Erban, J. Chapman & P. Maini. "A practical guide to stochastic simulations of reaction-diffusion processes" https://arxiv.org/abs/0704.1908

Vestergaard CL, Génois M (2015) Temporal Gillespie Algorithm: Fast Simulation of Contagion Processes on Time-Varying Networks. PLoS Comput Biol 11(10): e1004579. https://doi.org/10.1371/journal.pcbi.1004579 Code @ https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5473341/

TA Witten and LM Sanders, Diffusion-Limited Aggregation, a Kinetic Critical Phenomenon, Phys Rev Lett 47, 1400 (1981) https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.47.1400

K Binder. Applications of Monte Carlo methods to statistical physics. Rep. Prog. Phys. 60 (1997) 487–559 https://pdfs.semanticscholar.org/4921/99353dec6e405e557c7de1b517148fb6b957.pdf