Computational Physics (PHYS6350)

Lecture 1: Introduction, Syllabus, Technical Details

January 14, 2025

Instructor: Volodymyr Vovchenko (vvovchenko@uh.edu)

Course description

Description: Simulation of classical and quantum mechanical problems on digital computers using numerical and modern programming techniques.

Topics:

- General introduction to scientific programming and visualization.
- Function interpolation.
- Linear algebra and matrices.
- Numerical solutions to (systems of) non-linear equations.
- Numerical integration and differentiation.
- Numerical solutions to ordinary and partial differential equations.
- Molecular dynamics and Monte Carlo simulations.
- Problems from classical, statistical, and quantum mechanics.
- Data analysis, processing, and parameter estimation. Bayesian analysis.
- Introduction to parallel computing and machine learning. *(tentative)*

Textbook: No mandatory textbook but recommend *Computational Physics* by Mark Newman (Some parts of this text are available on the author's website: http://www-personal.umich.edu/~mejn/cp/index.html)

Requirements

- A laptop to run where you can write, compile, and run code.
- Plotting of the obtained results.

Preferred languages:

- Python within Jupyter Notebook (most of the examples will be given in this format)
- Pure Python (.py code)
- C/C++
- Other languages possible with prior approval (e.g. for assignments)

The operating system is up to you, I will use Mac.

Useful links:

- Python/Jupyter Notebook: one may use **Anaconda** distribution https://www.anaconda.com/
- C/C++/Python: **Visual Studio Code** https://code.visualstudio.com/
- Plotting: **matplotlib** (part of Python), **gnuplot** (http://www.gnuplot.info/)

Class schedule

Lecture: TuTh 10 AM – 11:30 AM

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Lab: Tu 9:00 AM – 10 AM

Instructor: Volodymyr Vovchenko (vvovchenko@uh.edu)

Office Hours: Wednesday 12-1 PM or by appointment (office SR1 629C)

Lecture notes and the solution to sample problems
will be posted after each lecture

Course materials:

- Teams
- https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Class schedule II

Tentative Schedule (Last update 1/13/2025)

1/14	Introduction, Syllabus, Technical Details
1/16	Visualization of Data, Machine Precision
1/21	Function Interpolation
1/23, 1/28	Linear Algebra and Matrices
1/30, 2/4	Nonlinear Equations
2/6, 2/11, 2/13	Numerical Calculus
2/18, 2/20	Numerical Differential Equations
2/25, 2/27	Problems in Classical Mechanics
3/4	Molecular Dynamics
3/6	Midterm Exam
3/11, 3/13	Spring Break – no classes
3/18, 3/20	Partial Differential Equations
3/25, 3/27	Random Numbers and Monte Carlo Methods
4/1, 4/3	Problems in Statistical Physics
4/8, 4/10	Problems in Quantum Mechanics
4/15	Data Analysis and Curve Fitting, Bayesian Methods
4/20	Selected Topics
4/22	Selected Topics
4/24	Review, Final Projects
5/6	Final Exam

Grading

- Homework (40%)
  - Every 1-2 weeks, due on Friday of the following week
  - Should include code and where applicable plot/tabulated output
  - The instructor may ask to explain how the submitted code works
- Final project (20%)
  - A numerical solution to a problem on a pre-approved topic
  - Or exploration of some of the advanced methods that we did not cover
  - Should include both the code and a report
  - Due on last day of class
- Mid-term (15%) and Final (25%)
  - Multiple choice, short and long answer questions
  - May include a quick programming exercise