Computational Physics (PHYS6350)

Lecture 1: Introduction, Syllabus, Technical Details

January 17, 2023

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.
- Numerical solutions to (systems of) non-linear equations.
- Numerical integration and differentiation.
- Numerical solutions to ordinary and partial differential equations.
- Linear algebra and matrices.
- Molecular dynamics and Monte Carlo simulations.
- Problems from classical, statistical, and quantum mechanics.
- Data analysis, processing, and curve fittings.
- Introduction to parallel computing. *(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 one)
- 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 Ubuntu.

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 4 PM – 5:30 PM

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Lab: Tu 5:30 PM – 7 PM

Instructor: Volodymyr Vovchenko (vvovchenko@uh.edu)

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

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

Class schedule II

Tentative Schedule (Last update 1/16/2023)

1/17	Introduction, Syllabus, Technical Details
1/19	Visualization of Data, Machine Precision
1/24	Function Interpolation
1/26, 1/31	Nonlinear Equations
2/2, 2/7, 2/9	Numerical Calculus
2/14, 2/16	Numerical Differential Equations
2/21, 2/23	Problems in Classical Mechanics
2/28	Molecular Dynamics
3/2, 3/7	Partial Differential Equations
3/9	Midterm Exam
3/14, 3/16	Spring Break – no classes
3/21, 3/23	Linear Algebra and Matrices
3/28, 3/30	Random Numbers and Monte Carlo Methods
4/4, 4/6	Data Structures, Data Analysis and Curve Fitting
4/11, 4/13	Problems in Statistical Mechanics
4/18	Problems in Quantum Mechanics
4/20, 4/25	Selected Topics
4/27	Review
5/9	Final Exam

2/7 and 2/9 virtual
(pre-recorded lecture)

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
  - 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