PY2105 Projects

The possible projects are all based on selected sections of the book of
N. J. Giordano/H. Nakanishi “*Computational Physics*”.

General requirements (minimal):

- First weekly report: description of the physical setting and the numerical problem to be solved. Outline:
    - A solution to the problem and the strategy which will be used to solve it
    - The equations that are needed to describe the physics of the problem
    - Results/graphs that will be generated.
      Deadline: Tuesday, 05th Nov., 18:00

- Second weekly report: working programme for minimum goals (at least)
  Deadline: Tuesday, 12th Nov., 18:00

- Third weekly report: working programme for minimum goals and results for minimum goals (at least)
  Deadline: Tuesday, 19th Nov., 18:00

- Final report and final C/C++-file(s)
  Hard Deadline: Friday, 29th November 2018, 18:00
  no late submissions will be accepted

- Personal meeting with the supervisor and presentation of the current status of the project on **Tuesday, 12th Nov., 14:00-16:00/ Friday, 15th Nov., 13:00-14:00**

All report should to be submitted in PDF format (Word also acceptable) via Canvas. The C/C++ programmes have to be also submitted via Canvas.

The project and the report have to be done individually.
Copying or any form of plagiarism will result in zero marks for the whole project.

Project 1: Billiard Problem

Ref.: Section 3.7 from *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; numerical simulation of a billiard on a square table; reproduce Figs. 3.20 and 3.21

Stretch Goals: billiard on circular and stadium-shaped tables, reproduce Figs. 3.22, 3.23, 3.24, 3.25, exercise 3.30 (Lyapunov exponent)

Project 2: Two- and three-body Solar System

Ref.: Sections 4.1, 4.2 and 4.4 from *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; numerical simulation of the solar system with Earth and fixed Sun using Euler-Cromer method; reproducing Figs. 4.2, 4.4, 4.5

Stretch Goals: examination of Earth, Jupiter and fixed sun; numerical simulation of the motion of Earth and Jupiter using Euler-Cromer method; reproduce Fig.4.12 and 4.13

Project 3: Chaotic Tumbling of Hyperion

Ref.: Sections 4.1, 4.2 and 4.6 from *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; derivation of eq. (4.24), examine the model of Hyperion shown in Fig. 4.16 (Saturn and two connected particles) based on eq. (4.24); reproduce figures similar to Fig. 4.17, 4.18

Stretch Goals: reproduce Fig. 4.19; Exercise 4.19 (Lyapunov exponent)

Project 4: Laplace equation

Ref.: Section 5.1 of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; numerical simulation of the Laplace equation in two dimensions using the (Jacobi) relaxation method; using setting of Fig. 5.2 (idealised parallel plates): reproduce Figures 5.3; using setting of 5.4 (hollow metallic prism): reproduce Fig. 5.5

Stretch Goals: Setting of Fig. 5.6 (finite capacitor): reproduce Fig. 5.7 and Exercise 5.4

Project 5: Waves on a string

Ref.: Section 6.1 of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; numerical simulation of the one dimensional wave equation (6.1) using the algorithm described in the book assuming fixed ends; reproduce Fig. 6.2; setting of a composite string: reproduce Fig. 6.3

Stretch Goals: Exercises 6.1 (string with free ends) and 6.5 (fixed and oscillating end)

Project 6: 2-D random walks, diffusion and entropy

Ref.: Section 7.4 and 7.5 (and exercises 7.12 to 7.14) of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

A 2-D random walk on a square lattice involves a walker that can take steps of fixed length in 2 dimensions, each with equal probability. This project focuses on modelling of diffusion in 2-D using random walks and calculation of the entropy vs time.

Minimum Goals: Develop a programme that reproduces the results shown in Fig. 7.13 to 7.16 of *Computational Physics*, N.J. Giordano & H. Nakanishi, 2nd ed., i.e., the evolution of the positions of 400 diffusing particles on a 200 x 200 square lattice versus time, where the particles are initially confined in a square "drop" close to the centre of the lattice. Calculate the root mean square displacement for each particle versus time and show how this distribution evolves.
By dividing the lattice into grid cells (e.g., 8 x 8), calculate the entropy as a function of time for this system.

Stretch Goals: Show that the time taken for the entropy to reach equilibrium varies as the square of the lattice size.
For the 2-D random walk simulation, show that the size of the "drop" varies as the square root of time as long as the drop is smaller than the size of the lattice. Show that the behaviour changes when the particles have spread out to uniformly fill the lattice.

Project 7: Percolation

Ref.: Section 7.8 of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Percolation theory is widely used, e.g., to describe the fluid flow through porous networks, charge transport in mixtures of conducting and insulating materials or the spread of forest fires. This project focuses on studying percolation in a 2-D square lattice.

Minimum Goals: Write a programme to sequentially occupy random sites on a 2-D square lattice with each site occupied with a probability p . Identify and record cluster formation (ie new occupied site has at least one neighbour site occupied) and also cluster "bridging" where the occupation of a given site links two (or more) clusters. Percolation occurs when a single cluster spans the lattice, i.e. touches all four edges. Reproduce Figure 7.26 and show how to estimate the smallest probability at which a spanning cluster will form (the critical probability, pc)

Stretch Goals: Following Figure 7.27, calculate the number of occupied sites (F) which are in the spanning cluster as a fraction of the total number of occupied sites on the lattice and show how this varies as p approaches p_c.

Project 8: Normal modes of vibration of a membrane

Ref.: Section 11.4 of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference; numerical simulation of the one-dimensional setting shown in Fig. 11.12, reproduce Fig. 11.13; numerical simulation of the two-dimensional setting shown in Fig. 11.14, reproduce Figs. 11.15 and 11.16

Stretch Goals: modify programme to solve Exercise 11.13 (circular membrane in polar coordinates)

Project 9: Numerical Simulation of Quantum Mechanics

Ref.: Sections 10.1, 10.2 of *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd ed.

Minimum Goals: read and understand the reference, solving the stationary, one-dimensional Schrödinger equation using the shooting method, reproduce a figure similar to Figs. 10.4, 10.5, 10.6

Stretch Goals: implement the matching method and produce a figure similar to Fig. 10.8, apply it to the potential Fig. 10.9