1 Location and Timetable

Wed-Fri, 10-12, Pierce 100F

2 Course Description and Motivation

In this Course, we shall familiarise with the main computational tools which permit to simulate and analyse the dynamic behaviour of a wide range of physical problems involving fluids, solids, soft matter and quantum systems, as well as the dynamics of (some) biological and social systems. Special attention will be paid to the modelling/programming techniques involved with the generation of massive amounts of data which result from large-scale simulations of the above systems, as well as to the techniques to analyse and extract physical knowledge from such datasets.

3 Learning goals

The main goal of the course is to make the student acquainted with major computational techniques for solving a broad range of complex problems involving fluids, solids, waves, quantum systems, as well as biological and social systems with internal degrees of freedom (psycho-physics). Techniques to analyse the corresponding large sets of data will also be presented.

At the completion of the course, the student is expected to be able to:

1. Employ and develop concepts and methods for the large scale simulations of the dynamic behaviour of complex systems, as well as the corresponding data analysis techniques.

2. Read the current literature and appreciate the various approaches to large-scale simulation of scientific and engineering applications.

3. Choose and code the most appropriate computational techniques for modelling and data-analysing complex problems in physics, engineering biology and also social sciences.

4. Contribute to research projects involving the simulation and data analysis of complex natural and social systems.
4 Contents

• Grid methods for classical and quantum fields

  1. Finite Difference Method (Project 1a: Numerical simulation of advection-diffusion-reaction transport phenomena)
  2. Finite Volume Method
  3. Quantum Wave Equations (Project 1b: Numerical simulation of quantum scattering and tunnelling)

• Analysing and learning from data

  1. Signals: time-series and probability distribution functions
  2. (Multi)fractal analysis of turbulent signals (Project 2: Statistical analysis of turbulent time-series)
  3. Rudiments of Machine Learning

• Simulating complex states of matter

  1. Lattice Boltzmann I: Fluids
  2. Lattice Boltzmann II: Soft matter (Project 3: Lattice Boltzmann simulation of multiphase flow)
  3. Agent-based Models for Active Matter

• Computational psycho-physics

  1. Finite Differences as Social Networks
  2. Predicting X-events
  3. Neural networks: the Hopfield model (Project 4: Simulating the Hopfield neural network)

5 References

T. Pang, Computational Physics, Cambridge Univ. Press,
6 Pre-requisites

None, although some foreknowledge of numerical analysis and coding practice (Fortran, C, C++, Matlab, Mathematica, Python, Julia...) will help.

7 Grading policy

- Weekly assignments: 30%
- Running projects (every three weeks): 30%
- Final project (second week of December): 40%

The final project may be related to an ongoing PhD thesis, on the strict condition that it represents original work.

8 Lecture plan

Most subjects will be illustrated through a Theory lecture (2h), followed by a Practice lecture (2h) based on the use of warm-up computer programs. Starting from these practical examples, the student is expected to write up her/his own programs for further practice.

8.1 Lecture schedule

L1: Sept 2: Introduction to AC274

Part I: Grid Methods for Classical and Quantum Fields

L2-3: Sept 7-9: Finite Difference Method

L4-5: Sept 14-16: Finite Volume Method

L6-7: Sept 21-23: Quantum Wave Equations

Part II: Data Analysis and Learning

L10-11: Oct 5-7: Time series, correlations and probability distributions
L12: Oct 12: (Multi)-fractal analysis of turbulent time-series
L13-14: Oct 14-19: Machine Learning

Part III: Complex States of Matter

L15-16: Oct 21-26: Lattice Boltzmann for Fluids
L19-20: Nov 4-9: Agent-based Models for Active Matter

Part IV: Computational Psycho-Physics

L22: Nov 16: Predicting X-events
L23-24: Nov 18-25: The Hopfield Neural Network
L25: Nov 30: Wrap-up Lecture