Computational Physics (AC274)

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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, (https://www.amazon.com/Introduction-Computational-Physics-Tao-Pang/dp/0521532760)

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

L8-9: Sept 28-30: Numerical Solution of Compressible Flows (P. Mocz)

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

L17-18: Oct 28-Nov 2: Lattice Boltzmann for Soft Matter (G. Falcucci)

L19-20: Nov 4-9: Agent-based Models for Active Matter

Part IV: Computational Psycho-Physics

L21: Nov 11: The Social Rules of Finite Difference Methods

L22: Nov 16: Predicting X-events

L23-24: Nov 18-25: The Hopfield Neural Network

L25: Nov 30: Wrap-up Lecture