Computational methods for the physical sciences (AM227)

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1 Location and Timetable

W/F, 10.30-11.45, Crufts 309

2 Course Description and Motivation

In this Course, we shall familiarise with the main computational methods which permit to simulate and analyse the behaviour of a wide range of problems involving *fluids, solids, soft matter, classical and quantum waves as well as the dynamics of (some) biological and, as time allows, also social systems*. Special attention will be paid to the modelling/programming techniques involved in the simulation of complex systems, as well as to methods to analyse simulation data and extract knowledge therefrom. In addition, we shall provide the opportunity of hands-on on a multi scale codes for *extreme simulations at the interface between physics and molecular biology.*

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 leading-edge problems at the frontier between physics and biology (biopolymer translocation, protein crowding). Techniques to analyse the corresponding large sets of data will also be presented, along with some introductory notions of (physics-aware) machine learning.

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 General contents

1. **Grid methods for classical and quantum fields**

   (a) *Fundamentals of grid-discretization: Finite Differences (FD)*

   (b) *FD for linear classical PDE's (advection-diffusion-reaction)*

   (c) *FD for nonlinear PDE's (fluids and waves)*

   (d) *FD for linear quantum PDE's (wave functions)*

   (e) *Introduction to Finite Volume and Finite Element methods*

2. **Mesoscale methods**

   (a) *Lattice Boltzmann for fluids and soft matter*

   (b) *Multiscale Lattice-Boltzmann-Particle-Methods*

   (c) *Extreme simulations at the physics-biology interface*

   (d) *Stochastic Particle Methods*

3. **Data analysis and Machine Learning**

   (a) *Time-series and probability distribution functions*

   (b) *Statistical analysis of chaotic and turbulent signals*

   (c) *Physics-Aware machine Learning*

5 References

- P. Moin, Fundamentals of Engineering Analysis, Cambridge U.P., 2001 (https://www.amazon.com/Fundamentals-Engineering-Numerical-Analysis-Parviz/dp/0521711231)

- T. Pang, Computational Physics, Cambridge Univ. Press, 2006, (https://www.amazon.com/Introduction-Computational-Physics-Tao-Pang/dp/0521532760)

- S. Succi, The lattice Boltzmann Equation, Oxford Univ. Press, 2001 and 2018 (https://www.amazon.com/Boltzmann-Numerical-Mathematics.../dp/0198503989)
- Y. Abu-Mostafa et al, Learning from Data, 2012 (https://www.goodreads.com/book/show/15 learning-from-data)

6 Pre-requisites

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

The course is a natural complement and follow on to AM225.

7 Grading policy

- Weekly assignments: 65%
- Final Project (second week of December): 35%

  The weekly assignments are due out on friday of the week after the lectures are delivered. They should be provided in the form of a paper-lookalike short report (pdf preferred) of about 10 pages, with i) Statement of the problem, ii) Motivation of the chosen numerical technique, iii) Convergence and performance analysis, iv) Data analysis, v) Brief summary.

  The preparation of the weekly assignments is expected to take no less than 10h work.

  The final project consists in the solution of a research-oriented problem of choice. Projects related to an ongoing PhD thesis are encouraged, on the *strict* condition that they report original work, potentially liable to publication in a scientific journal (with follow-on work).

8 Lecture plan

Each theory lecture will be accompanied by short warm-up codlets. Starting from these practical examples, the student is expected to write up her/his own programs to complete the weekly assignments.

8.1 Lecture schedule

Note: The schedule is tentative; (a few) new lectures can be added in place of planned ones should the need arise.

Sep 5-7: Introduction to AM227 and Computational Physics

Sept 10-Oct 5: Grid methods for classical and quantum Fields

- Generalities of the Finite Difference (FD) method
- FD for linear transport problems
- FD for nonlinear conservation laws
- Practical application to fluids, waves and irreversible growth phenomena
- FD for non-relativistic and relativistic quantum mechanics

Oct 8-19: Advanced grid methods

- Introduction to the Finite Volume and Element Method
- Applications to transport and fluid problems (hands on on COMSOL code)

Oct 22-Nov 9: Mesoscale methods

- Introduction to the Lattice Boltzmann (LB) method
- LB for fluids and soft matter
- Extreme multiscale simulations of biological systems (hands-on on MUPHY code)
- Stochastic Particle Dynamics and the Fokker-Planck equation

Nov 12-30: Data analysis and machine learning

- Statistical analysis of time series and turbulent signals
- Introduction to Physics Aware Machine Learning
- Machine learning for turbulence modelling