Computational Physics (AC274)

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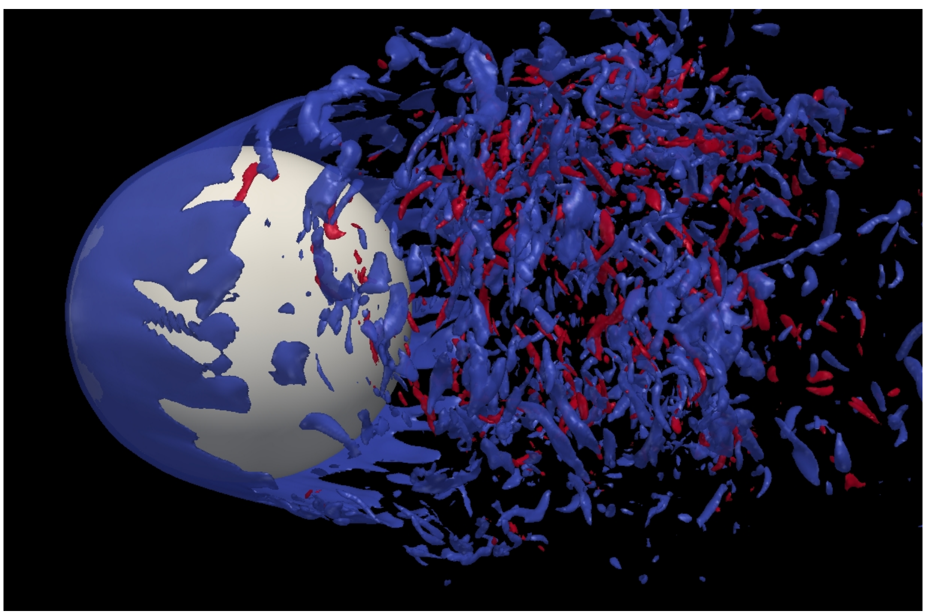

Lattice Boltzmann Simulation of a turbulent flow past a sphere

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 methods which permit to simulate and analyse the behaviour of a wide range of problems involving *fluids, solids, soft matter and quantum systems, 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.

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 (some) biological and social systems. 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 General contents

- **Grid methods for classical and quantum fields**
    1. *Basics of grid-discretization*
    2. *Finite Difference Method for linear PDE's (transport phenomena)*
    3. *Finite Difference Method for nonlinear PDE's (fluids and waves)*
- **Advanced Grid methods**
    1. *Numerical Electromagnetics (NEM)*
    2. *Finite Volume Method (FVM)*
    3. *Finite Element Method (FEM)*
- **Simulating complex states of classical and quantum matter**
    1. *Lattice Boltzmann for Fluids and Soft Matter*
    2. *Molecular and Langevin Dynamics*
    3. *Quantum many-body methods and quantum computing*
- **Data analysis and machine learning**
    1. *Rudiments of Machine Learning*
    2. *Time-series and probability distribution functions*
    3. *Analysis of turbulent signals*

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 (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.

7 Grading policy

- Weekly assignments: 60%
- Final Project (second week of December): 40%

  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 about 8h-12h 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

All subjects will be illustrated through a theory lecture (2h) followed by practical exercises 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 (weekly assignments).

8.1 Lecture schedule

9/1, **L01:** Introducing AC274: What is Computational Physics?

Part I: **Grid Methods for Classical and Quantum Fields**

9/06, **L02**: Generalities of the Finite Difference (FD) method

9/08, **L03**: FD for linear transport problems

9/13, **L04**: FD for nonlinear conservation laws

9/15, **L05**: Practical examples (fluids, waves, growth phenomena)

9/20, **L06**: FD for non-relativistic quantum mechanics

9/22, **L07**: FD for relativistic quantum mechanics

Part II: **Advanced Grid Methods**

9/27, **L08**: Numerical Electromagnetics: basic notions (*)

9/29, **L09**: Numerical Electromagnetics: applications (*)

10/04, **L10**: Introduction to the Finite Volume Method

10/06, **L11**: Applications to transport and fluid problems

10/11, **L12**: Introduction to the Finite Element Method

10/13, **L13**: Applications to fluids and quantum gravity

Part III: **Simulating complex states of matter**

10/18, **L14**: Introduction to the Lattice Boltzmann Method (LBM)

10/20, **L15**: LBM for fluids

10/25, **L16**: LBM for soft matter

10/27, **L17**: Basics of Molecular and Stochastic Particle Dynamics

11/01, **L18**: Applications to biological and social systems (*)

11/03, **L19**: A brief intro to the quantum many-body problem (*)

Part IV: **Data Analysis and Learning**

11/08, **L20**: Introduction to Machine Learning (*)

11/10, **L21**: Application of ML to material science simulations (*)

11/15, **L22**: Statistical analysis of time series

11/17, **L23**: From time series to probability distribution functions

11/22, **L24**: Statistical analysis of chaotic and turbulent signals

11/24, **L25**: Predicting extreme events

11/29, **L26**: Wrap-up and project preview Lecture

(*) Guest lectures