Physique Numérique — Computational Physics (M1)

Lecturer: Tommaso Roscilde (tommaso.roscilde@ens-lyon.fr)
TDs: Benjamin Guiselin (benjamin.guiselin@ens-lyon.fr)

Web-page: https://sites.google.com/site/roscilde/home/teaching/computational-physics-m1

Guidelines for choosing the project / writing the report

The main goal of the final project for the exam could be to use some of the numerical techniques that you have learnt during the lectures/TD, or to learn new ones related to the methods that we have seen in class, in order to tackle a (simple) physical problem; and/or it could be to test (possibly in the context of a physical problem) the performance of numerical methods which are widely used in different fields of physics and beyond.

In any case, the project should involve the *practical coding of a method on the computer*, and the *obtention of original numerical results,* which should be presented in graphs and discussed critically in the report.

The choice of the project topic is up to you, and you should feel free to follow your scientific interests and curiosity. But you should also be pragmatic in the choice of the subject, as the whole operation is already rather ambitious! Dont forget that you are asked to implement a method, and obtain original numerical results, during a limited amount of time. Adding a lot of scientific ambition to this task may easily make the whole operation very difficult! Hence I would recommend that you set yourself *simple* scientific goals; and that you make your numerical simulations on *small* system sizes, so that you are not limited by computational time. Only after you have obtained satisfactory results in simple instances of your problem of interest, you can think of going “bigger” (in terms of the scientific questions that you want to address, or of the system sizes you want to simulate, etc.).

You can work on your project *alone* or in a *2-people team* (*exceptionally* also in a *3-people team*). The final note will be the same for each member of the team. The content of the report being the same, projects that have been conducted by single persons will obviously be evaluated differently (= more generously) than projects conducted by teams. At the same time we encourage you to form teams in order to vastly improve your chances to learn from the whole experience, and to have better fun.

The final report should be **max. 10 pages long** (including title page and bibliography), and it should be structured in: 1) an introductory chapter describing the problem of interest; 2) an introductory chapter describing the numerical technique, and why it is appropriate to use it for the problem at hand; and 3) a chapter describing the original results that you have obtained.

The presentation style of the project should be inspired by the following idea: you are not writing for us the teachers, but you are rather describing *to your colleagues* what you have done. In this perspective, whenever it is appropriate, you can/should use as many references as possible to the material of the lectures, given that this is the common ground between you and your colleagues.

A LaTeX template for the project can be found on the webpage of the lectures.

You can write your report in English - *ou vous pouvez l'écrire en français, à votre gout!*

Some ideas for the final project

Quantum mechanics

1) Lanczos diagonalisation of a quantum spin model (e.g. quantum phase transitions in quantum spin chains);
2) Lanczos diagonalisation of a few-electron atom;
3) Variational Monte Carlo / exact diagonalization study: ground state of a quantum particle in an anharmonic potential;
4) Numerical solution of the time-dependent Schrödinger equation for a single particle: tunneling, self-trapping, localization, etc.;
5) Gross-Pitaevskii equation: search for the equilibrium configuration of Bose-Einstein condensate in an external potential (imaginary-time evolution and split-operator method);
6) Gross-Pitaevskii equation: dynamics of a Bose-Einstein condensate (vortices, solitons, etc.);

etc.

Statistical / non-linear physics

1) Monte Carlo study of phase transitions: 2d Ising model, 2d XY model;
2) Simulated annealing of a spin glass, or of other combinatorial optimization problems;
3) Application of the Verlet algorithm to molecular dynamics: e.g. some interacting classical particles in an external potential;
4) Korteweg-de Vries equation (solitons, etc.);
5) Sine-Gordon equation (solitons, etc.);
6) Study of the Fermi-Pasta-Ulam-Tsingou problem (chain of anharmonic oscillators);

etc.

Astrophysics

1) Internal structure of stars with spherical symmetry and chemical homogeneity: equation of state, opacity, energy production, convection (write the equations in the stationary regime and numerically integrate them starting from the center of the star and from its surface to achieve continuity afterwards);
2) Image of a disc around a blackhole (trace the light rays in a curved space-time described by the Schwarzschild metric); possibility to extend the study to the disc "spectrum" (if at each point we place a blackbody radiation source; or if at each point there is an infinitely thin ray);
3) Thermal instability of a Sakura-Sunyaev accretion disc (start from a model of a stable and stationary disc, and then increase the accretion rate up to an instability; implicity and/or explicit methods will be necessary);
4) Solar wind: start from a spherically symmetric fluid which is stationary, not magnetized and isothermal, as a function of the wind velocity at the basis of the Solar Corona and of the gaz temperature;
5) Radiative transfer (rewriting as a flux conservation, then discretisation: e.g. Lax-Wendroff and Godunov schemes, leap-frog method, depending on the instability);
6) Collapse (e.g. of a star);

etc.