Summary of course and the final oral exam

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Learning outcomes

Our ideal about knowledge on computational science

Does that match the experiences you have made this semester?

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Topics we have covered this year

- Introduction to c++ programming and object orientation
- How to write scientific reports
- Linear algebra and eigenvalue problems. (Lecture notes chapters 6.1-6.5 and 7.1-7.5 and projects 1 and 2).
- Ordinary differential equations (Lecture notes chapter 8 and projects 3 and 4)
- Monte Carlo methods in physics (Lecture notes chapters 11, 12 and 13, project 4)

Linear algebra and eigenvalue problems, chapters 6.1-6.5 and 7.1-7.5

- How to handle vectors and matrices
- Gaussian elimination and LU decomposition (project 1)
- How to solve linear equations (project 1)
- How to obtain the inverse and the determinant of a real symmetric matrix
- Cubic spline
- Tridiagonal matrix decomposition (project 1)
- Householder's tridiagonalization technique and finding eigenvalues based on this
- Jacobi's method for finding eigenvalues (project 2)

Monte Carlo methods in physics (Chapters 11, 12 and 13)

- Random walks and Markov chains
- Generation of random numbers
- Monte Carlo integration
- Probability distributions and their properties
- Errors in Monte Carlo calculations (statistical errors)
- Metropolis algorithm (project 4)
- Applications to statistical physics systems (project 4)
- Brief excursion into quantum mechanical systems (project 4)

Ordinary differential equations (Chapter 8)

- Euler's method and improved Euler's method, truncation errors (projects 3 and 4)
- Runge Kutta methods, 2nd and 4th order, truncation errors (projects 3 and 4)
- Leap-frog and Verlet algoritm (projects 3 and 4)
- How to implement and solve a second-order differential equation, both linear and non-linear.
- How to make your equations dimensionless.

Partial differential equations, chapter 10, not covered this year

- Set up diffusion, Poisson and wave equations up to 2 spatial dimensions and time
- Set up the mathematical model and algorithms for these equations, with boundary and initial conditions. The stability conditions for the diffusion equation.
- Explicit, implicit and Crank-Nicolson schemes, and how to solve them. Remember that they result in triangular matrices (project 4).
- Diffusion equation in two dimensions.

Final presentation

Select the project you liked the most among projects 2-4. Alternatively, if there are other topics of relevance you would like to present, feel free to suggest (send me an email however). Your presentation (bring your own laptop) should include

- Introduction with motivation
- Give an overview of the theory and numerical algorithms employed
- Discuss the implementation of your algorithm and how you verified it and validated it. Discuss for example various tests you made.
- Present and discuss your results
- Summary, conclusions and perspectives
- Anything else you think is important. Useful to have backup slides

In total your talk should have a duration of 20-25 minutes, but longer is also ok. The style for the final presentation follows very much the way the lay out your reports.

What? Me worry?

Computational science courses at MSU

- PHY905 section 004 High-Performance computing
- New department offers degrees in Computational Science and many new courses
- See special courses offered now
- Undergraduate courses
- Graduate courses

Best wishes to you all and thanks so much for your efforts this semester