

# Computers in Science Education A New Way to Teach Science?

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# Acknowledgements

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## Administration

Annik Myhre, Dean of Education

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# Principles

## MATNAT21@UiO

Our school of Science and Math has singled four basic principles for the future organization of our research and education

- Quality
- Research based teaching
- Academic freedom
- Discipline based research

# Principles

## Three central aims behind our CSE reform

Computational thinking as a way to

- Enhance instruction based teaching
- Introduce Research based teaching from day one
- Trigger further insights in math and other disciplines

Alan Perlis (first Turing award recipient), 1962: Argued that programming was an exploration of a given process, a topic that concerned everyone and that the automated execution of a given process by a machine was going to change everything. He saw programming as a step toward understanding a 'theory of computation', which would lead to students recasting their understanding of a variety of topics in terms of computations.

# Research based teaching

## How do we define it?

One possible definition: It is coupled to a direct participation in actual research and builds upon established knowledge and insights about scientific methods.

- It is the standard situation at all universities and takes normally place at the senior undergraduate/graduate level
- It is seldom done in undergraduate courses.
- Taught by a researcher
- The student starts seeing the contour of the scientific approach leading him/her to make new interpretations, develop new insights and understandings that lead to further research.

# Research based education

## What should the education contain?

The standard situation we meet at an almost daily basis:

- Theory+experiment+simulation is almost the norm in research and industry
- To be able to model complex systems with no simple answers on closed form. Solve real problems.
- Emphasis on insight and understanding of fundamental principles and laws in the Sciences.
- Be able to visualize, present, discuss, interpret and come with a critical analysis of the results, and develop a sound ethical attitude to own and other's work.

Our education should reflect this.

# Computers and science teaching

## Education

- During the last 25 years there has been considerable focus on technology at all levels in the educational ladder.
- Calculators, text processing, email, digital learning environments etc.
- Much focus on means and technologies, but what about the content, or more importantly, insight into physical systems?
- The basic topics (math, chemistry, physics, . . . ) are taught more or less in the same fashion as before — unchanged over several decades!

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# Some observations

## Computation in the sciences

- Calculations have always been a central ingredient in science and mathematics.
- The computer has brought a new dimension to the different fields and we can nowadays do immensely many floating-point operations per second. Petascale computers are here now (Roadrunner, U.S.A.), with  $10^{15}$  floating-point operations per second.
- Many problems which previously were insolvable are now solved in a routine-like fashion within seconds or minutes.
- Modern science has become a three-legged animal consisting of experiment, numerical modelling and theory.

# More observations

## Computation in the Sciences

- Computations is a fundamental tool to gain new insights
- Computer simulations can act as a lab — can save both time and resources
- Computations is a central component in modern industry and research in the sciences, spanning almost every field: *Materials science and nanotechnology, weather forecasting, earthquake simulations and forecasting, medical technology, industrial design, design of new computers, the entertainment industry, almost all aspects of our modern society!!*

# Further observations

## Computations should enter science education

- Our teaching should include an education in basic numerical methods, normally taught in different departments, and often disconnected. In the US several smaller university colleges have implemented something similar to our project, see Computing in Science and Engineering, Vol. **8**, sept/oct issue 2006.
- The students should also learn to develop new methods and learn new tools when needed.
- Need an adequate computational platform.(Python as computing language).

# More observations

## Observations about implementations

- One creates different physics courses and graduate programs which bake in computations, typically various Computational Physics courses from sophomore to graduate level. The problem is that these courses are not compulsory. The result is often an uneven background of the students.
- Dedicated teachers incorporate numerical exercises (at different levels) in their physics courses. When new teachers take over, the whole initiative may disappear.
- Quite many physics departments teach their own math and computer science courses! But have still not been able to coordinate properly computational topics.

# Can we catch many birds with one stone?

## HPC at early stages in our educational ladder

- How can we include and integrate a computational perspective in our basic education?
- Can this enhance the students' understanding of mathematics and science?
- Own hobby horse: And can we enhance the visibility of a high-performance computing perspective? (students come with dual-core laptops and quad-core PCs are standard now!)

# Preliminary summary

## Computations should enter basic science education

- Computation is a fundamental tool to gain new insights and should be included in our elementary teaching.
- Requires development of algorithmic thinking.
- Basic numerical methods should be part of the compulsory curriculum.
- The students should also learn to develop new numerical methods and adapt to new software tools.
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# What is needed?

## Programming

A compulsory programming course with a strong mathematical flavour. Should give a solid foundation in programming.

## Mathematics and numerics

Mathematics is at least as important as before, but should be supplemented with development and analysis of numerical methods.

## Sciences

Training in modelling and problem solving with numerical methods and visualisation, as well as traditional methods.



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# Implementation

## Crucial ingredients

- Support from governing bodies
- Cooperation across departmental boundaries
- Willingness by individuals to give priority to teaching reform

# Implementation in Oslo: Organization

## University of Oslo's (UiO) information and communication technology (ICT) strategy

Two of five strategic goals involve ICT.

- *ICT should be integrated as a pedagogical tool in our education*
- *UiO wishes to develop and increase its employee's competence and motivation in the usage of ICT in educational matters.*

From the Faculty of Math and Sciences' strategic plan 2005-2009

*Integrate central modern computational tools, instrumentation and techniques, in order to modernize our Math and Science education. Computations and numerical modelling has a central place here.*

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# Implementation in Oslo: The CSE project

## Goals

- Include and integrate a computational perspective in the bachelor curriculum in the mathematically oriented sciences.
- Give the students realistic examples from our research, this brings our research into the undergraduate teaching at a much earlier stage than before.
- Upgrade the staff's competence on computational topics.
- Focus on fundamental (long-lasting) knowledge that prepares the students for a long professional career, also in the area of computer use.
- Aim at strengthening instruction based teaching.

# Implementation in Oslo: The CSE project

## What we do

- Coordinated use of computational exercises and numerical tools in many undergraduate courses.
- Help update the scientific staff's competence on computational aspects and give support (scientific, pedagogical and financial) to those who wish to revise their courses in a computational direction.
- Develop courses and exercise modules with a computational perspective, both for students and teachers.
- Basic idea: mixture of mathematics, computation, informatics and topics from the physical sciences.

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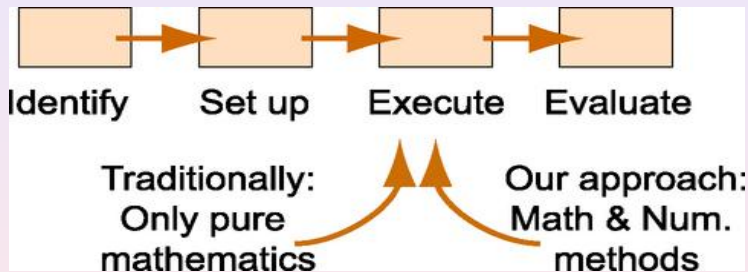
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# What do we want to achieve?



# Organizational framework

## Educational Reform

- The reform in 2003 (Bachelor+Master+Phd) paved the way for coordinated introduction of computational topics in several bachelor programs.
- There are six major bachelor programs in the sciences with several common mathematics, physics and informatics courses in the first 3–4 semesters.
- Modern software has a low learning threshold and it is easy to visualize and program complicated systems.

## Centers of excellence

The Faculty (co-)hosts four (++) centers of excellence where computations are central. These play an important role in catalyzing cross-disciplinary research and educational projects.

# Example of bachelor program

## Physics, Astronomy and Meteorology, sorry for Norwegian text

6. semester	Se ønsket studieretning	<a href="#">EXPHIL03 - Examen philosophicum</a> /Valgfritt	Valgfritt
5. semester	Se ønsket studieretning	Se ønsket studieretning	Valgfritt/ <a href="#">EXPHIL03 - Examen philosophicum</a>
4. semester	Se ønsket studieretning	Se ønsket studieretning	Se ønsket studieretning
3. semester	<a href="#">FYS1120 - Elektromagnetisme</a>	<a href="#">AST1100 - Innføring i astrofysikk</a> / <a href="#">GEF1000 - Klimasystemet</a>	<a href="#">MAT1120 - Lineær algebra</a>
2. semester	<a href="#">FYS-MEK1110 - Mekanikk</a>	<a href="#">MEK1100 - Feltteori og vektoranalyse</a>	<a href="#">MAT1110 - Kalkulus og lineær algebra</a>
1. semester	<a href="#">INF1100 - Grunnkurs i programmering for naturvitenskapelige anvendelser</a>	<a href="#">MAT-INF1100 - Modellering og beregninger</a>	<a href="#">MAT1100 - Kalkulus</a>
	10 studiepoeng	10 studiepoeng	10 studiepoeng

- First semester common for six out of 12 Bachelor programs (Math, Physics, Materials Science, Nanotechnology, Math and economy, electronics)
- The mathematics courses MAT1100, MAT1110, MAT1120 and MEK1100 are also common to many Bachelor programs.

# Example: Computations from day one

## Differentiation

Three courses the first semester: MAT1100, MAT-INF1100 og INF1100.

- Definition of the derivative in MAT1100 (Calculus and analysis)

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

- Algorithms to compute the derivative in MAT-INF1100 (Mathematical modelling with computing)

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

- Numerical differentiation and use in applications in the programming course INF1100 (Numerical methods and scientific computing)

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# Other Examples

## Integration by Trapezoidal Rule

- Definition of integration in MAT1100 (Calculus and analysis).
- The algorithm for computing the integral vha the Trapezoidal rule for an interval  $x \in [a, b]$

$$\int_a^b (f(x))dx \approx \frac{1}{2} [f(a) + 2f(a+h) + \dots + 2f(b-h) + f(b)]$$

is taught in MAT-INF1100 (Mathematical modelling)

- The algorithm is then implemented in INF1100 (programming course):

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# Coordination

## More Examples

- The courses MAT1100, MAT-INF1100 og INF1100 have many common examples and topics, amongst these ordinary differential equations. They solve the pendulum at the end of INF1100.
- Differential equations are in turn used widely in our mechanics course, which comes in the second semester, with examples spanning from the classical pendulum to rocket launching.
- Differential equations (partial and ordinary) are in turn used in many many other courses, from electromagnetism to quantum physics.
- The central mathematics courses MEK1100, MAT1110 og MAT1120 develop further numerical exercises and problems, from linear algebra to multi-dimensional integration.

# Coordination

- Teachers in other courses need therefore not use much time on numerical tools— it is naturally included in other courses.

# Learning outcomes three first semesters

## Knowledge of basic algorithms

- Differential equations: Euler, modified Euler and Runge-Kutta methods
- Numerical integration: Trapezoidal and Simpson's rule, multidimensional integrals
- Random numbers, random walks, probability distributions and Monte Carlo integration
- Linear Algebra and eigenvalue problems: Gaussian elimination, LU-decomposition, SVD, QR, Givens rotations and eigenvalues, Gauss-Seidel.
- Root finding and interpolation etc.
- Processing of sound and images.

The students have to code several of these algorithms during the first three semesters.

# Later courses

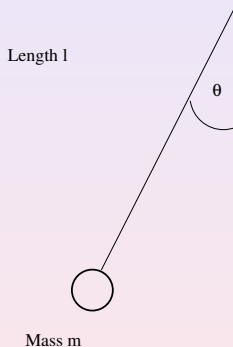
Later courses should build on this foundation as much as possible.

In particular, the course should not be too basic! There should be progression in the use of mathematics, numerical methods and programming, as well as science.

Computational platform: Python, fully object-oriented and allows for seamless integration of c++ and Fortran codes, as well as Matlab-like programming environment. Makes it easy to parallelize codes as well.



## FYS-MEK1100 (Mechanics), Second Semester



## Realistic Pendulum

Classical pendulum with damping and external force

$$ml \frac{d^2\theta}{dt^2} + \nu \frac{d\theta}{dt} + mgsin(\theta) = Asin(\omega t).$$

Easy to solve numerically without classical simplification, and then visualize the solution. Done in first semester!

Same equation for an RLC circuit

$$L \frac{d^2Q}{dt^2} + \frac{Q}{C} + R \frac{dQ}{dt} = V(t).$$

# What can we do with the pendulum?

## Many interesting problems

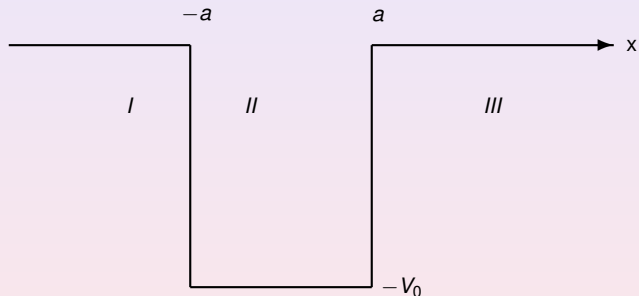
- Can study chaos, theoretically, numerically and experimentally, can choose 'best' parameters for experimental setup.
- Can test different algorithms for solving ordinary differential equations, from Euler's to fourth-order Runge Kutta methods. Tight connection with algorithm and physics.
- Can make classes of differential equation solvers.
- Can make a general program that can be applied to other scientific cases in later courses, such as electromagnetism (RLC circuits). Students realize that much of the same mathematics enters many physics cases.

# More Examples from Physics Courses, 2-5 semester

## Second-fourth semester

- 1 Air resistance in two and three dimensions with quadratic velocity dependence.
- 2 Rocket launching with realistic parameters
- 3 How to kick a football and model its trajectory.
- 4 Planet motion and position of planets
- 5 Magnetic fields with various geometries based on Biot-Savart's law
- 6 Harmonic oscillations and various forms of electromagnetic waves.
- 7 Combined effect of different potentials such as the electrostatic potential and the gravitational potential.
- 8 Simple studies of atoms and molecules, and much more

# Quantum Physics: Particle in a Box, fourth semester



# Box Potential

For bound states the time-dependent Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + V(x)\psi(x) = -|E|\psi(x),$$

or slightly rewritten

$$\frac{\partial^2}{\partial x^2} \psi(x) - \frac{2m}{\hbar^2} (V(x) + |E|) \psi(x) = 0.$$

# Box Potential

After a series of manipulations and usage of various requirements on the solution, the students arrive at a set of transcendental equations

$$\beta = k \tan(ka),$$

for even solutions and

$$-\beta = k \cot(ka),$$

for odd solutions. The variables  $k$  and  $\beta$  contain the energy  $E$ .

These equations cannot be solved analytically for a general case and most students stop here and move on to the next exercise What is gained? Any new insight about the physics?

# New wisdom/insight?

- A computational environment like our Python framework allows one to solve differential equations with boundary conditions. Alternatively the students can use Matlab (students learn Matlab in addition to Python) As in many applications, the physics case is in the boundary conditions. The students have to understand these and solve the problem with different boundary conditions. Requires a better understanding of the problem and more interactions and discussions among students and teachers.
- This example can easily be transferred to other single-particle problems, such as the harmonic oscillator, the hydrogen atom etc. Increases the capability to make abstractions.
- The students can play with the parameters and uncover relations between various constants (here potential strength and extension) which most students normally never do.
- It brings our research closer to the students as well. Much more fun to teach. But much work for teachers and students.
- Can easily extend to atoms and molecules.

# Can we bake in Parallelization at an early stage?

## Late: Fifth semester, FYS3150 Computational Physics

Quad-core is standard now for most supermarket PCs!! Should bake in parallelization.

The integral we need to solve is the quantum mechanical expectation value of the correlation energy between two electrons, namely

$$\left\langle \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right\rangle = \int_{-\infty}^{\infty} d\mathbf{r}_1 d\mathbf{r}_2 e^{-2\alpha(r_1+r_2)} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

Students use either Python, C++ or Fortran95 as programming languages on our supercomputing cluster (educational nodes, with MPI-2).

**It took the students on average 1-2 hours at the lab to become operative with their first MPI program.** [http:](http://www.uio.no/studier/emner/matnat/fys/FYS3150/h07/)

[//www.uio.no/studier/emner/matnat/fys/FYS3150/h07/](http://www.uio.no/studier/emner/matnat/fys/FYS3150/h07/), see under projects, project 2 and 4.



# Can we bake in Parallelization at an early stage?

## Late: Fifth semester, FYS3150 Computational Physics

The tasks they are to solve

- Use Gauss-Legendre quadrature and compute the integral by integrating for each variable  $x_1, y_1, z_1, x_2, y_2, z_2$  from  $-\infty$  to  $\infty$ .
- Compute the same integral but now with brute force Monte Carlo and compare your results with those from the previous point. Discuss the differences. With brute force we mean that you should use the uniform distribution.
- Improve your brute force Monte Carlo calculation by using importance sampling. Hint: use the exponential distribution. Does the variance decrease? Comment your results.
- Parallelize your code from the previous point and compare the CPU time needed with that from point [c)]. Do you achieve a good speedup?**

# Can we bake in Parallelization at an early stage?

## Late: Fifth semester, FYS3150 Computational Physics

- Integration and Monte carlo methods are embarrassingly trivial (ET), only few students had problems when parallelizing.
- The students found it easy to implement MPI as long as support was given.
- To use MPI or similar libraries, it is important that the infrastructure has a as low as possible threshold. On average they used 1-2 hours to have MPI running.
- Solving quantum mechanical problems by Variational Monte Carlo or study phase transitions (ising and Potts model).

# Challenges ...

## ... and objections

- Standard objection: computations take away the attention from other central topics in 'my course'.

CSE incorporates computations from day one, and courses higher up do not need to spend time on computational topics (technicalities), but can focus on the interesting science applications.

- The students become better qualified than their teachers. Good teaching assistants aid to improve this aspect.
- Pedagogical courses which can aid university teachers are under development.

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- Continuity is important when teachers change. New textbooks are being written.
- Major challenge: How to reflect computational exercises in grading and final evaluations?
- What about students from other universities?

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# Challenges

- The project depends crucially on a few individuals.
- Need to get more teachers involved, not only good TAs.
- How to implement a CSE perspective in other programs like Chemistry, Geology, Molecular Biology, and Biology. Work in progress, but depends on scientific profile.

# Summary

## CSE

- Try to accommodate an international trend.
- Make our research visible in early undergraduate courses, enhance research based teaching
- Possibility to focus more on understanding and increased insight.
- Impetus for broad cooperation in teaching.
- Strengthening of instruction based teaching (expensive and time-consuming).
- Give our candidates a broader and more up-to-date education with a problem-based orientation, often requested by potential employers.
- And perhaps the most important issue: does this enhance the student's insight in the Sciences?

# Selected Material



Python and our programming course, first semester

<http://www.uio.no/studier/emner/matnat/ifi/INF1100/h08/>.



Mathematical modelling course, first semester [http:](http://www.uio.no/studier/emner/matnat/math/MAT-INF1100/h08/)

[//www.uio.no/studier/emner/matnat/math/MAT-INF1100/h08/](http://www.uio.no/studier/emner/matnat/math/MAT-INF1100/h08/)



Computational Physics I, fifth semester,

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