UPPSALA
UNIVERSITET

Institutionen för informationsteknologi
Teknisk databehandling
Malin Ljungberg

Besöksadress:
MIC hus 2, Polacksbacken
Lägerhyddsvgen 2

Postadress:
Box 337
751 05 Uppsala

Telefon:
018–471 62 09

Telefax:
018–52 30 49

Hemsida:
http://user.it.uu.se/~malinl

Epost:
Malin.Ljungberg@it.uu.se

Department of Information Technology
Scientific Computing
Malin Ljungberg

Visiting address:
MIC bldg 2, Polacksbacken
Lägerhyddsvgen 2

Postal address:
Box 337
SE-751 05 Uppsala
SWEDEN

Telephone:
+46 18–471 62 09

Telefax:
+46 18–52 30 49

Web page:
http://user.it.uu.se/~malinl

Email:
Malin.Ljungberg@it.uu.se

Masters program in Computational Science and Engineering, CSE

This document

This outline for a masters program within the area of Computational Science and Engineering (CSE) is part of an effort by the Bologna task force at the IT department to formulate Bologna compliant masters programs, in fields connected to computer science.

The proposal is the result of discussions between Sverker Holmgren (director of UPPMAX), Malin Ljungberg (coordinator), Per Lötstedt (professor in Numerical Analysis and chairman of the Scientific Computing subject advisory group) and Stefan Pålsson (director of studies, Scientific Computing) from the IT department, and also Hans Karlsson (director of studies, Quantum Chemistry). Stefan Seipel (division of Human Computer Interaction) and Hans Norlander (director of studies, Systems and Control) were asked to participate, but were unable to.

This outline is also part of the ongoing development of a joint internet based masters program together with ICME (Institute of Computational Mathematics in Engineering) at Stanford University School of Engineering [**?**].

Lennart Edsberg (director of studies, Masters of Science, Scientific Computing, KTH) has also been involved in the discussions concerning collaboration with KTH, mentioned below.

Background

CSE is now widely accepted, along with theory and experiment, as a crucial third mode of scientific investigation and engineering design. In many industrial sectors, companies are relying on simulation for development and technical decision support. Also, in many new areas such as medicine, the life sciences, management and marketing and finance techniques and algorithms from CSE are of growing importance.

CSE is by nature interdisciplinary. It grows out of applications and it depends on computer systems, but at its heart are powerful algorithms. Much of CSE has so far involved simulations for analysis, but the future also includes using computational methods for optimization and engineering design. The demand for expertise in computational methods and

simulations is growing world wide, as more cost efficient computer simulations replace experiments. In response to this there is a trend at international educational institutions for introducing programs within this field. The internationally adopted name CSE is used world-wide. This is also the name that we use here [**?**]. The suggested name in Swedish is "Tekniskt-vetenskapliga datorberäkningar".

Background material which has been considered includes

- reports from subject advisory groups (ämnesråd) at the IT department, particularly from the scientific computing group [**?**, **?**],
- Bachelor and Master of Engineering physics (Förslag på utformning av bachelor- och masterutbildning i teknisk fysik i Uppsala) [**?**],
- SIAM overview of Graduate Education for Computational Science and Engineering [**?**],

Purpose

The goals of the CSE program are formulated in terms of the professions and tasks that students will be suited for after graduation. A selection of these are currently being formulated in cooperation with the UPPMAX [**?**] industry reference group. Some skills that have already been identified as particularly requested in connection with Computational Science in Engineering are mathematical modeling, problem solving using computers, project work, cooperation with experts in other fields, working towards a specification, validation, and presentation of results. These skills shall, in additional to numerical methods, be given particular emphasis in the CSE Masters program at Uppsala University.

The main aim of the program is to provide the skills necessary for performing computer simulations within a wide range of fields. These include (examples of companies performing these types of computations within parenthesis)

- combustion (Scania, Volvo Aero)
- high voltage electric field simulations (ABB)
- fluid flow simulations (engines, turbines, aerodynamics, etc.) (Volvo, SAAB, ABB, FOI)
- electromagnetic wave propagation (radio coverage) (Ericsson, TeliaSonera, AerotechTelub)
- materials science, metallurgy (Sandvik)
- molecular modeling (Biovitrum, GE Healthcare, AstraZeneca)
- bioinformatics (Carlson Research)

- geology (SKB)
- rendering and modeling for the entertainment industry (Starbreeze, Ongame)
- pharmaceutical modeling (NeoPharma)
- prototype design, e.g. equipment for medical analysis (Biotage)

The larger research institutes also constitute a potential market for computational scientists. We have for example FOI (Totalförsvarets forskningsinstitut), SMHI (Sveriges Meteorologiska och Hydrologiska Institut), SIMR (Swedish Institute for Metals Research), STFI (Skogsindustrins Tekniska ForskningsInstitut), and SP (Statens Provnings- och Forskningsinstitut).

Finally there are a number of high profile consulting agencies that welcome computational scientists, such as for example Ånpanneföreningen, Enea and Prevas.

Within the program there is also space for specialization within the field of methods, algorithms and programs for computational experiments. Such a specialization will be a suitable background for work within the companies that develop software for large scale computations (COMSOL, FOI).

Students from the CSE Program will also be well suited for continuing within research. This could be within a specific application area, such as computational physics, chemistry or biology, and also within the field of Scientific Computing.

Goals, summarized

The CSE program will provide the necessary skills in principles, methodologies, and algorithms for computer simulations within various areas, e.g. physics, chemistry, biology, and technology. A graduate from the program will have acquired proficiency within the following areas

- algorithms and numerical methods,
- mathematical modeling,
- use, development and maintenance of complex and efficient software systems,
- the use of various types of computers and computer architectures suitable for large computations,
- applying numerical computational techniques for problem solving in at least one application field in science and technology,
- validation and presentation of results, e.g. using advanced visualization techniques.

Prerequisites

Students entering the CSE Masters program are required to have a background in one or more application fields, as well as a good level of mathematical background, including

- basic algebra,
- calculus of one variable,
- calculus of several variables,
- linear algebra,
- ordinary differential equations, and
- statistical theory and methods.

Prerequisites from the area of computation are

- introductory computer programming
- scientific computing I
- scientific computing II

where the second course in scientific computing differs from that which is now offered in the F program by putting more emphasis on applications.

The three year Bachelor program suggested in [**?**] forms a strong background for a student specializing in the application area of physics, but a similar level of expertise from another area, such as biology, chemistry, also forms a suitable background for the program.

Students lacking the sufficient background in mathematics or computation will need to broaden their Bachelors by adding these courses before commencing the CSE Masters program, or alternatively within the program. In support of this, a basic package of required courses will be offered for such students. Examples of areas included in this basic package are

- scientific computing II
- ordinary differential equations
- linear algebra
- calculus of several variables

Content of the program

Within the program there will be a number of core courses, most of which are currently available within today's Computational Science track of the Engineering physics program. The main part of the courses will be within the field of computer science and scientific computing. The other two major subject areas are mathematics, including applied mathematics, and computational courses within a specific application field, e.g. physics, biology or chemistry. Mathematical modeling will be considered in relationship to a particular application field. The division of courses between the different areas will be, in broad figures, 40 p Computer and Computational Science, 5-10 p courses specific to the application area and 10 p mathematics, including applied mathematics.

That a course is in the core curriculum does not mean that it is mandatory. It is important to leave some freedom of choice, so as to allow for specialization, e.g. towards computer science or mathematics. The requirements for assuring that students take an sufficient amount of relevant courses will be introduced in coordination with other master programs in order to ensure a consistent set of rules between the different programs.

Areas within Computer and Computational Science

- High Performance Computing (Högprestandaberäkningar)
- Programming of parallel computers (Programmering av parallelldatorer)
- Visualization (Vetenskaplig visualisering) Focusing on practical experience in visualization.
- Computer programming II (Programmeringsteknik II)
- Optimization (Optimering) This also includes the use of optimization for model construction and design.
- Applied finite element methods (Tillämpad FEM) More applied than the FEM course currently offered.
- Scientific Computing, advanced level (Tekniskt vetenskapliga datorberäkningar) This also includes sections on project steering and presentation techniques.

Areas within Mathematics

- Complex analysis and transforms (Komplexanalys och Transformmetoder)
- Applied mathematics and mathematical modeling (Tillämpad matematik och matematisk modellering)

Application area specific

- Computational chemistry (beräkningskemi)
- Computational physics (beräkningsfysik)
- Computational biology (beräkningsbiologi)

Computational courses that are application area specific will be developed as extensions of existing courses given at the relevant departments. In general there may be a need to extend the theoretical background for the description of the numerical methods used in these courses.

Integration with todays engineering programs

The CSE Masters program will fit well within an engineering program, such as the Engineering physics program (F) or the Material Science Engineering physics program (Q). A background in mathematics and biology, as provided by today's Molecular Biotechnology Engineering program (X), will also be well suited. We forsee a need to supply incoming students with an opportunity to supplement their Bachelors degree with the second course in scientific computing, which is a prerequisite for the program.

If the structure of todays engineering programs remains intact it will be possible for a student graduating from the Engineering Physics program to add 6 months of courses and receive a CSE masters as well, provided that the student fulfills the course requirements.

Coordination with existing and new programs

Since the program will be offered as a joint program together with ICME at Stanford University School of Engineering [**?**] we forsee opportunities of offering masters theses projects (Examensarbete) in collaboration with Stanford. This will form an opportunity for students from both sides of the Atlantic to gain international experience as part of their education.

Uppsala University also has a long tradition of collaboration with computational groups at KTH, e.g., including collaborative courses at the graduate level. A collaboration on CSE masters eduction is currently also being set. The goal is to mutually offer CSE courses to students at both UU and KTH, and to collaborate on, e.g., development of course material and modules in courses.

There are natural connections between the CSE Masters program and masters programs in Computer Science, Mathematics, Bioinformatics and Physics at UU, if such are created. Students from the CSE program should be able to take certain courses from these programs, and vice versa. We also expect these programs to contain computationally oriented courses.

A particularly strong connection will be with the masters program in Mathematics and Scientific Computing suggested by the department of

Mathematics. The relationship between the two programs can in simple terms be described as theory vs. practice. The basis of the CSE program is the application of numerical methods for problem solving, whereas the more mathematical program has more focus on the analysis and development of the numerical methods themselves. This will provide an opportunity for collaboration with respect to courses, but also with respect to the definition of the external interface, i.e. towards potential students and their potential employers.

Opportunities for post graduate studies

A student from the CSE program is expected to fulfill the requirements to continue in a post graduate program in one on the fields *Scientific Computing*, *Physics*, *Chemistry*, or *Biology*, depending both on the background the student had when entering the CSE program, and on the course selection within the program. Our aim is to also provide a means of ensuring competence for the field of *Systems and Control*, but at this point the details of how this can be done have not been worked out.

Time plan

We expect the CSE Masters program will consist to a large extent of existing courses, or courses which are constructed from existing courses. All of the required competence is available. Because of this the specification and development of the new courses for the program will not require a significant amount of time. The first instance of the first year of the program can be given in the fall of 2006.