Group discussions KCSE Annual Meeting 2008

Topic: CSE Courses at KTH

A. Present Status – Courses:

Numerics

Parallel Computations for Large-Scale Problems I (DN2264, 6, C)

The overall goal of the course is to provide a basic understanding of how to develop algorithms and how to implement them in distributed memory computers using the message-passing paradigm.

Advanced Numerical Analysis (DN2290, 7.5, D)

This is an advanced course in numerical methods focusing on efficient algorithms for large scale algebraic problems often arising in the numerical treatment of partial differential equations, including Fast Multipole, Krylov and Multigrid methods.

Numerical Solutions of Differential Equations I (DN2225, 6, C)

The course gives the students knowledge of problem classes, basic mathematical and numerical concepts and properties, modern numerical methods, and software for solution of engineering and scientific problems formulated as ordinary or partial differential equations (PDEs).

Numerical Solutions of Differential Equations II (DN2255, 7.5, D)

This course follows DN2225. It emphasizes finite difference methods and finite volume schemes for solving PDEs of importance in applications. The goal is to give an understanding of the mathematical concepts, properties and tools for analyzing differential equations and their discretizations and a working knowledge and experience of implementing finite difference schemes with various boundary conditions.

The Finite Element Method (DN2260, 6, C)

This FEM course aims to provide the student both with theoretical and practical skills, including the ability to formulate and implement adaptive FEM algorithms for an important family of PDEs.

Applications

Computational Physics (MH2102, 7.5, D)

This advanced course in numerical analysis is focusing on the computer simulation of condensed matter systems using particles. The main part of the course concerns the molecular dynamics simulation technique (MD).

Computational Physics (SI2530, 7.5, D)

This course treats: The Monte Carlo and molecular dynamics methods, simulations in different statistical mechanical ensembles, computation of free energies, stochastic dynamics. Applications are to spin systems, fluids, polymers and biological macromolecules.

Computational Chemistry (BB2300, 7.5, D)

The goal with this course is to acquire knowledge in Computational Chemistry and some basic skills in carrying out calculations on problems of chemical interest. Except for learning some basic theoretical models, the emphasis is to actually carry out the calculations, and to learn about possible applications and limitations. The course contains a number of theoretical problems and descriptions how to solve these problems.

Computational Fluid Dynamics (SG2212, 7.5, D)

An in-depth course on numerical methods for computer simulation of fluid flows. Together with 5C1213 Applied Computational Fluid Dynamics, a comprehensive course on theory and practice of computational fluid dynamics.

Computational Techniques in Materials Science (4H5919, 2007)

This course is meant as an introduction and overview to the computational techniques in common use in materials science. Emphasis is placed on how and when to apply the different techniques and implementation.

Computational Aerodynamics (SD2610, 9, D)

Aerodynamics is a very central topic in Aeronautics, but is also important in design of cars, trains, boats and bridges. Aerodynamic properties of an aircraft and its components can in many cases be computed by solving the governing differential equations for the flow with numerical methods. This course covers methods for and applications of Computational Fluid Dynamics (CFD) in design of aircraft and other vehicles.

Numerical Methods in Nuclear Engineering (SH2774, 6, D)

The course focus is on computational methods for problems arising in nuclear reactor system analysis. Topics include numerical methods for solving large, sparse systems of linear equations that result from the discretization of partial differential equations, numerical solution of nonlinear algebraic equations, eigenvalue problems, ordinary differential equations and partial differential equations. Applications include heat conduction, fluid mechanics, neutron diffusion and neutron kinetics.

Computational Methods from Micro to Macro Scales (DN3249, 7.5, D)

The course presents computational methods from Schrödinger's equation for nuclei-electron systems over molecular dynamics to continuum partial differential equations, using a unified mathematical method to derive and explain the coupling between the models on the different scales.

Computational Electromagnetics and Photonics (2009)

The new course focuses on modern electromagnetic engineering of microwave and lightwave circuits, antennas, and photonics. The computational tools are now becoming more mature, and require less detailed knowledge of specific numerical methods. It is possible to introduce more realistic applications and have the students develop CEM engineering skills in modeling and understanding and to treat more advanced theoretical approaches.

Advanced Simulation Methods in Statistical Physics (2009)

This is a proposal to develop a new course for PhD students in advanced simulation methods in statistical physics with possible applications in condensed matter physics, material science, biophysics, chemistry, etc. The course would cover more advanced methods and applications that would usefully complement our basic course SI2530 Computational Physics.

Summer/Winter School on Multiscale Modelling (2009)

A winterschool in multiscale modelling will be held in November 2009 at Albanova, together with Nordita and NGSSC. Tutorials on topics in chemistry, biology, materials science and numerical analysis will be given, followed by group projects led by senior scientists. More information will be provided later.

Computer

Introduction to High Performance Computing / PDC Summer School (DN2258, 7.5, C)

This course covers algorithms and techniques for high performance computing. The goal of this course is to give the student a basic introduction to the skills needed to utilize high performance computing resources for own projects.

PRACE Petascale Summer School (2008)

The course will focus on porting an application to a massively parallel computer. Students are encouraged to bring their own applications to the Summer School. The last two days will focus on advanced parallel programming and are concurrent with the final two days of the two week "Introduction to High-Performance Computing" Summer School. Topics covered include hybrid programming (MPI and OpenMP) and performance measurement tools and techniques.

Visualization (DD2257, 6, C)

The course focuses on visualization of scientific measurements and computations, including basic concepts, methods, visualisation systems.

GPU Programming (short course June/November 2008 plus workshop 2009)

This summer course for PhD students and researchers interested in high-performance and parallel computing was given in June 2008. Specifically, the course did introduce and give a hands-on experience with the massively parallel computing hardware found in a modern graphics card (the GPU).

Introduction to Makefiles/Compilers etc. (tutorial, 2009)

“Practical HPC”: Programming, Implementation, Optimisation, Interpretation (2009)

Complementary Courses

Teaching and Learning (LH201V, 7.5)

Course Design is a practical exercise where you develop a course in which you teach. The goal is that you will be able to make conscious and informed design choices and motivate them from a student learning perspective. Reflective Practice aims to deepen the learning perspective through further investigation and application to other areas. You will start on your Teaching Portfolio.

Basic communication and teaching (LH200V, 3)

This course is aimed for PhD students who also work with different kinds of teaching. The course consists of group meetings and field studies. The main objective with the course is to provide an opportunity to develop a foundation which enables the development of the participants’ lectures and their students’ learning.

Innovation and entrepreneurship

Travel Grants for external schools

B. Group Discussion:

Start with either point 1 or 3, and continue with 2 and 3 or 1, respectively.

1. **Courses in KCSE**
   Discussion about the curriculum of the KCSE Graduate School, in particular related to the available courses, desired/missing courses in the various areas
   a. **Numerics**: Basic numerical analysis which is useful/necessary for all further HPC studies.
      Topics: level of the NA courses (too detailed, too basic, too complete, more overview courses), example-based courses/projects. Overlap with application courses, coordination?
   b. **Applications**: Research topics of the various departments, to provide an introduction.
      Topics: Entrance knowledge level, "pre"-tutorials, focus on interdisciplinarity, level of courses (too advanced, too easy, too much repetition). Additional application areas?
   c. **Computer**: HPC in practice; computer architectures, scientific programming, tools for visualisation, debugging, optimisation, parallelisation.
      Topics: Addition to PDC summer school, advanced topics, overview of new techniques/architectures. Tutorials for beginning students, programming languages (Matlab, Fortran)
   d. **Complementary Courses**: Education for future working live
      Topics: Tailored/existing courses (presentation techniques, economics, teaching, supervision). Media training?

2. **School organisation**
   a. Social events/Information: Desired activities? What format?
   b. Seminar series/Information/Mailing/Web: Present status, future organisation?
   c. Formalia: Requirements for KCSE degree. Support for students (travel grant for summer schools).

3. **KCSE – PDC – SNIC**
   a. Architectures – PDC Support
      Information/Meetings about new machines, information on website, how-to guides: more necessary?
   b. Applications – PDC Support
      Would there be a need for further support? Application support, optimisation, debugging, "segmentation fault"-cures etc.
      Correct application on appropriate system?
   c. SNIC Systems
      Information in research groups about available architectures within SNIC; sharing of experience with different centres/machines. Group meetings to exchange ideas/tricks?
      User environment/login at various centres different, application procedures.
   d. PDC Generalities
      General views on PDC, what is good, what could be improved? What could KCSE contribute to it (users group, etc.)
   e. Storage of data
      How do you solve it? Spread over various places (SNIC Centres, PDC HSM, local resources at the department, private harddisks)

C. Panel Discussion

Discussion about

- the available courses; in particular how one can coordinate the courses and make sure the prerequisites of each course can be met by the students.
- Seminar series, how to attract an audience and speakers
- Course suggestions, how to find people to give courses, how to advertise a given course
- Interdisciplinary courses (with various teachers): Good thing, or rather split into two courses that are taken sequentially.
- Course formats: Shorter overview courses ←→ longer, more thorough courses. Attract more students via shorter courses?
- Future of HPC education? Is soon everybody doing HPC in some way.
- What is HPC compared to normal “matlab” usage?
- Provide course suggestions to Director of Studies

KCSE annual meeting, discussion in the evening, 2008-12-11

Group 1

- Are overlapping courses really needed in KCSE?
- 30ECTS feels much if you are in a specialized area.
- Linear algebra is a focal point, everybody does that, make numerical linear algebra a requirement
- Recommendations: a) Course in Visualization tools; b) 2 full day courses (Workshop style).
- Travel grants – good idea! Travels also can give insight. Little information about them is available at the moment. Right now, they can only be used to traveling to summer schools.
- Idea: go to another university and take a course there – not sure whether it does not cross a boundary.

Group 2

Applications:

- computational physics – we see 2 courses?
- CFD course – too easy for a graduate student
- GPU course was too early, the technology is not mature yet.
- HPC course: good intro to MPI.
- A new course on Makefile/compilers – good idea (just keep it short).
- Complementary course suggestion: Basic communication – good if you are going to do teaching.

School Organization:

- more social events.
- Seminars - hold them both in Albanova and Main Campus.
- Communication should be improved – check whether all the participants are on the mailing list.
- Requirement of 30 ECTS points feels too many.

PDC:

- some users want more computers with fast interconnect.
- Better library support (MPI, lapack, parpack was not installed).
- SNIC: should unify the user interface (same queuing system etc).
- AFS: too slow, too small, too *bad*. (20GB is too little). Better user support for how to mount AFS on your desktop would be desired.

Group 3

Recommendation for PDC:

- Specialise in some types of calculations if possible (“profile”).
- Investigate application experts. They reduce “waste” of computational resources. However, a career path for them does not seem clear, they would lose competitiveness without doing own research. It is difficult to find good, commited candidates for the job, too.
- Support “user groups” (research areas), help them to find a way to collaborate. Application expert could act as a moderator in a forum.
- Café type meeting, or lunch meetings with a sandwich.

Course suggestions:

- “Getting started with Gromacs/Dalton/Gaussian” - as a follow-up for a more theoretically oriented course.
- Basic media training to make a presentation of own work to people outside of the field possible (example forum: KCSE seminars).

Group 4

- PDC support responsive but the web page is a mess. No need for meetings but better website needed.
- Consider more active mailing lists for better communication.
- Storage of data: many store data on local disks (outside of PDC); national storage in Sweden would be desired.
- KCSE organization: clarity desired – what does one gain from the participation.

Group 5

- FORUM or “wiki” to help on basic problems (makefiles, coding,...).
- More general seminars by guest lecturers. Ask *everybody* for suggestions! NADA people are not thrilled with the current Albanova location.

Courses - new topics to cover:

- spectral methods.
- optimization, large-scale inverse problems:
  - Courses must not ignore existing libraries (LAPACK is so basic).
  - Introduction to software development.

Group 6

- bimonthly KCSE social meeting (dinner/pub).
- Bigger room for the KCSE seminar.
- Stricter guidelines for making seminar to make them less specialized.
- KCSE students should get something tangible (t-shirt?)

- PDC website generally good
- Suggest a meeting twice a year to get info about new systems and other snic systems. It will be an opportunity to ask questions.
- Workshop on profiling/optimization – you bring your code.
- info/web – how to use standard codes (“user groups”).
- More uniform user environment among snic centers.
- Very common to use local storage with no back-up.

Final day discussion

- Application experts.
- Seminar series: more accessible talks, feel free to suggest speakers. We need a larger screen than the one in theochem.
- Courses: “proper” course vs “tutorial”. Both have their place.
- Interdisciplinary “intro”-courses, mixed-projects. Example: CFD. Can it be made interesting for a broader audience without dumbing it down.