**KTH Computational Science
and Engineering Centre**

Annual report KCSE 2004

The KTH Computational Science and Engineering Centre (KCSE) was constituted in 2004 by the president of KTH among a number of departments at KTH; today of the departments of Mechanics, Numerical Analysis and Computer Science, Aeronautical and Vehicle Engineering, Materials Science and Engineering and Biotechnology. KCSE started its activities in August 2004 with an initial 500kkr/year funding from the president of KTH. Already during the few months of activity, the contact between the participating institutions has been improved significantly.

Summary of activities during 2004

Most of the activities have focused on getting the centre started and initialize the communication and collaboration between the different departments involved.

The main activities and the people involved are described in the appendices.

- *Kick-off* (Appendix A, p.5)
  At the kick-off in Lovik, Lidingö there were about 40 participants, of which about half were PhD students. An invited speaker, Professor Risto Nieminen, HUT gave an inspiring talk about computational science. Key activities of KCSE departments were also presented. Several common themes between departments were identified

- *Seminar series* (Appendix B, p.7)
  During the fall of 2004 three seminars were held in the multidisciplinary seminar series, initiated by KCSE. The series has become a success with 40-60 participants.

- *Formation of a graduate school* (Appendix C, p.8)
  The goal of the graduate school is to widen the competence and perspectives of the participating PhD students within the area of computational science and engineering and to provide an opportunity to network with potential collaboration partners in academia and industry. About 20 graduate students from the five participating departments have been enrolled and the work to identify a common curriculum has been initiated.

- *Applications to funding agencies* (Appendix D, p.10)
  KCSE is part of a consortium which has proposed a Simulation Centre to the Swedish Foundation for Strategic Research (SSF).

- *Active participants* (Appendix E, p.11)

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KCSE Vision

Simulations have, together with theoretical analysis and traditional experimental research, become an independent and extremely useful tool to gain new knowledge. This new multi-disciplinary field is often called Computational Science and Engineering or CSE. Recently, CSE has been established as a discipline in its own right with research centers, departments and education programs around the world.

The KCSE vision can be summarized as

> *"KTH as a leading university in research and education within CSE."*

This requires that
- KTH recruits internationally world leading scientists in the area of CSE
- KTH is on top of the list for students making their choice for where to study computational science and engineering
- KTH creates and sustains environments in which world leading research groups in CSE can both evolve and collaborate with each other

Board and Directors of KCSE

The board and directors of KCSE are the following

Björn Engquist, NADA, *Chairman*
Börje Johansson, Materials Science and Engineering, *Vice Chairman*
Anders Eriksson, Department of Mechanics
Hans Ågren, Department of Biotechnology
Gunilla Efraimsson, Aeronautical and Vehicle Engineering
Per Öster, PDC
Bengt Finnström, International Relations

Dan Henningson, Mechanics, *Director*
Jesper Oppelstrup, NADA, *Deputy Director*
Anna Delin, Materials Scince and Engineering, *Director of Studies*

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About KCSE

To promote efficient CSE activities at KTH, KCSE works actively to improve and encourage collaboration between different disciplines and departments. This is realized through the following activities.

Graduate School in CSE
The collaboration and exchange of knowledge between PhD students
are enhanced via an active graduate program in CSE. This program contains common graduate courses within the different disciplines, coordinated research projects with common advisors as well as seminar series with both invited speakers and presentations by the PhD students.

Development of undergraduate education and Master's programs with CSE profile
There are a number of undergraduate courses as well as Master's programs in the area of CSE given at the departments comprising KCSE. The coordination and renewal of these courses is an essential part of the KCSE activities.

Post-doc, visiting research program and international collaboration
A post-doc and visiting researchers program will be associated with KCSE as well as collaboration with researchers in other CSE centers internationally.

Collaboration with industry
Collaboration with industry is an important basis for e.g. choice of research areas, exploitation of academic results within industry and demonstrating industrial research and development for students at both undergraduate and graduate level. Today the natural starting point for industrial collaboration is through the competence centers existing within the KCSE group.

Main research areas in KCSE

The research at KCSE is mainly conducted in 4 areas. Several common themes between departments were identified, such as multiscale problems and computations involving the Schrödinger, Navier-Stokes and Maxwell equations. The main research areas, which are further described at www.kcse.kth.se, are

- *Simulations of biological systems (life science)*
- *Simulations of properties of materials (materials science)*
- *Simulations of fluid systems*
- *Simulation in engineering design and optimization*

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Appendix A: Kick-off Lovik, Nov 25-26, 2004

At the kick-off in Lovik, Lidingö there were about 40 participants, of which about half were PhD students. An invited speaker, Professor Risto Nieminen, HUT gave an inspiring talk about computational science. Key activities of KCSE departments were also presented. Several common themes between departments were identified, such as multiscale problems and computations involving the Schrödinger, Navier-Stokes and Maxwell equations.

Group activities: discussions about future activities of KCSE

An important goal with the kick-off was to inspire free discussion among the participants. The group discussions focused on the following topics. Many of the ideas that were suggested are now being transformed into activities with KCSE.

Curriculum for the Graduate School
Common graduate/master courses
Core courses with broader appeal identified

Future activities of KCSE
Seminar series and annual (multidisciplinary) meeting
Lobbying for CSE at KTH
Computer resources: Kallsup III proposal
SUS-initiative at SSF: proposal with UU
Coordination with future Vinn X centres

Role of KCSE in CSE education
Integrating computations in undergraduate mathematics teaching
Coordination of masters programs dealing with aspects of CSE
Computational majors for F- and T- students within School of Science?

Research activities within KCSE
Possibilities for coordination and synergy of research projects
Networking and multidisciplinary projects

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Kick-off program

Thursday 25/11

12:00   Lunch

13:00   Welcome and KCSE Presentation
Börje Johansson,Vice chairman
Dan Henningson, Director

13:30   Computational science and its role in modern research
Risto Nieminen, HUT

14:30   Coffee

15:00   Computational Biology
Hans Ågren, Biotechnology

15:30   Computational Fluid Dynamics
Luca Brandt, Mechanics

16:00   Computational Electromagnetics
Jesper Oppelstrup, NADA

16:30- Group activities: Getting to know each other
18:00

19:00   Dinner

Friday 26/11

8:30   Group activities: Future activities of KCSE
Coffee during discussions

11:00   Aerodynamic and aeroacoustic computations
Art Rizzi, Gunilla Eframinsson, Aeronautical and Vehicle Engineering

11:30   Computational Materials Science
*David Andersson, Materials Sicence and Engineering*

12:30   Lunch

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Appendix B: Seminar series

We have initiated a multidisciplinary seminar series, which has become a success with 40-60 participants each time. The first three seminars are listed below, taken from the homepage announcement. The seminar program for the spring semester 2005 has already been finalized.

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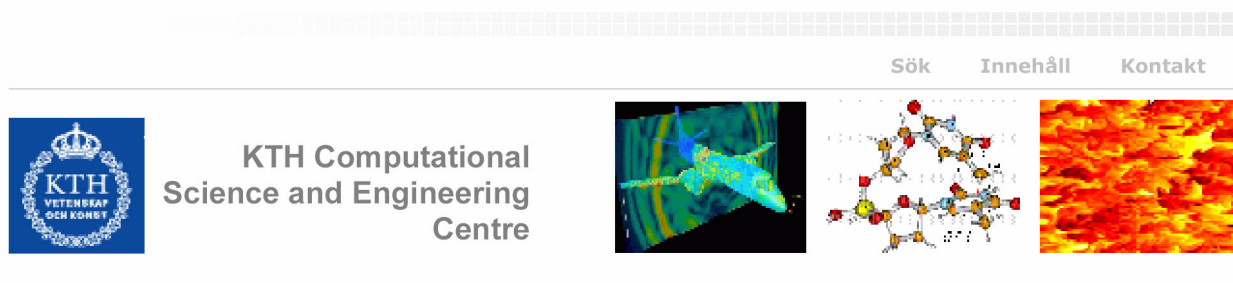
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Seminars

Title	Speaker	Date/Time/Place
Atomistic modelling of materials *The inaugural KCSE seminar.*	Börje Johansson Materials Science	2004-11-10 (wed) 15.30 (coffee at 15:00) Room E3, Osquarsbacke 18, level 5
Computational science and its role in modern research	Risto Nieminen, HUT	KCSE Kick-off, Lovik, Lidingö 25-26 Nov.
The hetrogeneous multiscale method	Björn Engquist, NADA	2004-12-08 (wed) 15.30 (coffee at 15:00) PDC seminar room, Teknikringen 14, level 3

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Appendix C: Graduate school

The goal of the graduate school is to widen the competence and perspectives of the participating PhD students within the area of computational science and engineering and to provide an opportunity to network with potential collaboration partners in academia and industry. Often, different sub-fields of computational science consider similar problems in very different ways, and use different terminology to describe their problems. The scientific focus can also vary greatly, from pure method development issues to applications. By organizing coordinated activities among a group of students from different departments we expect that they will benefit both from learning about each others point of view and from cooperation's initiated between their different research projects.

Initial activities:

Courses

The research school will have its own course curriculum, consisting of selected courses from the participating departments as well as courses in innovation strategies, patent rights, scientific writing, and project planning. Students participating in the school are expected to take courses from this curriculum, initially courses worth in total at least 5 points. This (these) additional course (courses) must be from another department than the student's own. The core courses identified so far are listed below. The plan is to develop these courses so that they can be given on a very high level to a multidisciplinary student group, for instance by starting each couse with a few introductory lectures to non-specialist students. We hope that this strategy will produce true excellence among the students.

Seminar series

There are several reasons why we have initated a seminar series. A series of multi-disciplinary seminars with a certain focus makes a lot of sense, both for senior researchers and PhD students. Apart from that, the series aims at giving students training in presenting their research for a wider audience. The frequency is currently 9 seminars per semester, i.e. approximately two per month. Every other seminar will be given by a leading scientist from academia or industry, and every other seminar by a PhD student active in the research school. PhD students participating in the research school are expected to attend these seminars, and will obtain 3 points for active participation in the series, i.e. for having given one seminar, and having participated in 15 other seminars in the series.

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PhD students who have completed both the seminar series and the course work obtain a certificate/diploma as a proof of their participation. The points accumulated within the research school are of course counted as part of the normal PhD or licentiate course work.

Core courses

2D1258 Introduction to High Performance Computing, 5 credits
2D1263 Program Construction for Scientific Computing, 4 credits
2D1290 Advanced Numerical Analysis, 4 credits
2D1225 Numerical Solutions of Differential Equations, 4 credits
2D1255 Numerical Solutions of Differential Equations, 5 credits
2D1260 The Finite Element Method, 4 credits
2D1272 Computational Physics, 5 credits
3A1640 Computational Chemistry, 5 credits
5C1212 Computational Fluid Dynamics, 5 credits
4H5919 Computational Techniques in Materials Science
4E1212 Aerodynamics, 6 credits

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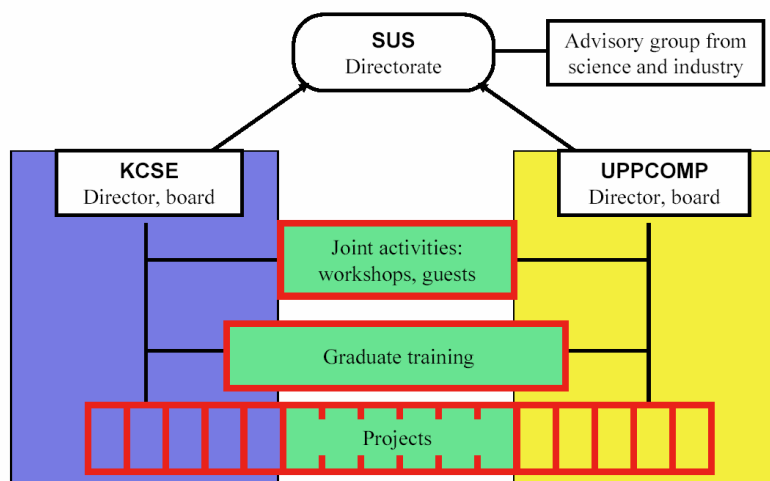and Engineering Centre**

Appendix D: SUS consortium

KCSE is part of a consortium which has proposed a Simulation Centre to the Swedish Foundation for Strategic Research.

Strong and dynamic CSE environments exist not only at the Royal Institute of Technology (KTH) but also at Uppsala University (UU). Just as KCSE was established with the vision to further establish KTH as a leading university for research and education in CSE, the excellence of CSE research groups at UU is the basis for the Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX). The new Uppsala Program for Computational Methods in Science and Engineering (UPPCOMP), building on Uppsala's strong tradition in numerical analysis, has been formed to complement UPPMAX, in focusing on the development of methodologies for CSE.

These local initiatives now pave the way for establishing a strong Simulation Consortium in the Stockholm-Uppsala region, through a Stockholm-Uppsala Simulation (SUS) consortium, enabling CSE research at the internationally highest level. This will strongly enhance the multi-disciplinary cross-fertilization, which is most central for the CSE development, and allow for a regional distribution of cutting edge research activities. Cooperating groups in CSE from KTH and UU already exist, and the consortium will add value by improving the research environment for the cooperation and including other groups and researchers. This consortium fits well into the recently formed Stockholm-Uppsala University Network.

The figure below show the organization of the consortium, with the red boarder representing proposed joint activities.

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Appendix E: Active participants

The table below give a summary of the number of active participants, and the following list are the ones now listed on the homepage.

	MEK	*NADA*	*AVE*	*MSE*	*BIO*	*Σ*
Professors	4	5	1	2	2	**14**
Lecturers and Assistant lecturers	1	3	1		1	**6**
Researchers and Research Assistants	3	3		9	1	**16**
Graduate students	6	5	3	3	4	**21**
Σ	**14**	**16**	**5**	**14**	**8**	**57**

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