



**KTH Computational Science  
and Engineering Centre**

## Annual report KCSE 2005

The year 2005 was the first full year of KCSE operation and several activities have reached maturity. The seminar series has the dual role of bringing together researchers within the area of CSE at KTH, and also to serve as a corner stone of the activities in the graduate school. In addition the graduate program involves common courses which have been identified as interesting for a wider audience, giving the students a broader perspective on computational science. Multidisciplinary research is another cornerstone, although it has so far proved difficult to obtain funding directly to KCSE for such projects. The year ended with a workshop where industrial issues within computational science were in focus. The opportunity for graduate students to meet with industrial researchers responsible for computational research proved to be a success and will be developed further in the future. During the year it was also identified that KCSE must be involved as a lobby group for increased High Performance Computing (HPC) capacity in Sweden. This is one of the focal points of the activities during 2006, in addition to the developments of a common CSE centre with Beijing University in China.

Stockholm, May 2006

Dan Henningson, Director KCSE  
Gunilla Efraimsson, Co-director KCSE  
Olof Runborg, Co-director KCSE  
Anna Delin, Director of Studies KCSE



**KTH Computational Science  
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**KCSE 2005**



**Vision**

The KTH center KCSE was established to realize the vision of

***KTH as a leading university in Computational Science and Engineering (CSE)***

by means of

- *Graduate program*  
Educate students to obtain a dual expertise in scientific computing and applications
- *Multidisciplinary research*  
Stimulate cooperative research projects between the departments in KCSE
- *High performance computing (HPC)*  
Strengthening the computational infrastructure in collaboration with PDC
- *Workshops and seminars*  
Widening and strengthening the network of computational scientists
- *Industrial focal point*  
Facilitate the dialogue between industry and KTH within CSE



## KTH Computational Science and Engineering Centre

### Motivation

The remarkable evolution of large scale computations has in recent years created a new and revolutionary way of performing research. 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.

KCSE was constituted 2004 among a number of departments at KTH, today it consists of the departments of [Mechanics](#), [Numerical Analysis and Computer Science](#), [Aeronautical and Vehicle Engineering](#), [Materials Science and Engineering](#), [Biotechnology](#) and [Electromagnetic Engineering](#).

### Board and directors of KCSE

Björn Engquist, NADA, *Chairman*  
 Börje Johansson, Materials Science and Engineering, *Vice Chairman*  
 Anders Eriksson, Department of Mechanics  
 Hans Ågren, Department of Biotechnology  
 Art Rizzi, Aeronautical and Vehicle Engineering  
 Per Öster, PDC  
 Gustav Amberg, School of Engineering Sciences

Dan Henningson, Mechanics, *Director*  
 Gunilla Efraimsson, Aeronautical and Vehicle Eng., *Deputy Director*  
 Olof Runborg, Nada, *Deputy Director*  
 Anna Delin, Materials Science and Engineering, *Director of Studies*

### Contact

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**KTH Computational Science  
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## Activities 2005

### **Graduate school in CSE**

The graduate program aims to educate students to obtain dual expertise in scientific computing and applications. The graduate 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.

#### *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

The graduate school had 26 active students at the end of 2005. Eight students (Elias Rudberg, Astrid Herbst, Elin Olsson, Klara Asp, Thomas Melin, Freddy Guimaraes, Emanuel Rubensson, Daniel Ahlman) have given a seminar on their research within the KCSE seminar series. On average, each KCSE seminar was attended by about 10 KCSE students.

#### *Graduate school contact:*

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## KTH Computational Science and Engineering Centre

### Multidisciplinary research

The research at KCSE is mainly conducted in 4 areas. Several common themes between departments have been 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](http://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*

### High performance computing

KCSE aims to strengthen the computational infrastructure at KTH in collaboration with PDC. In 2005 KCSE has worked on bringing in new computer resources to KTH, directly through an application to the Wallenberg Foundation for new hardware, and indirectly by starting to profile itself as a lobbying group towards SNIC. To support the latter aim, KCSE has begun a detailed investigation into the computational needs of the individual research groups of KCSE. The goal is to highlight the importance of better computer infrastructure by showing some concrete examples of new scientific undertakings it would allow and the possible new discoveries and breakthroughs these could lead to. KCSE staff has also participated in a seminar on e-Science and grid computing organized by the Swedish Research Council.

### Workshop and seminars

#### *Seminars spring 2005*

1. *Linear Scaling Quantum Modelling*, Elias Rudberg, BIO.
2. *The phase field method: A general idea for free boundary problems in fluid mechanics and materials science*, Gustav Amberg, MEK.
3. *Advances in the Application of Higher-Order Finite-Difference Schemes to Multidisciplinary Simulation on General Geometries*, Miguel Visbal, Air Force Research Laboratory, Ohio.
4. *Simulation and control of turbulent separated flow in a diffuser*, Astrid Herbst, MEK.
5. *A conservative level set method for two-phase flow*, Elin Olsson, NADA.



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6. *First-principles calculations of materials properties*, Andrei Ruban, MSE.
7. *Phase-field simulation of sintering and related phenomena – a vacancy diffusion approach*, Klara Asp, MSE.
8. *Body&Soul: Utbildningsprogram i CSE*, Claes Johnson, Chalmers.
9. *Emerging Role of Simulation in Conceptual Aerospace Design*, Thomas Melin, AVE.

### *Seminars fall 2005*

1. *Ethics in CSE*, Michael Thuné, UU.
2. *Numerical Climate Simulation - An example of computational physics or hokus-pokus?* Michael Tjernström, SU.
3. *Calculations of Quantum Wave Packets, with Applications*, Freddy Guimaraes, BIO.
4. *Sparse Matrices with Applications in Quantum Chemistry*, Emanuel Rubensson, BIO.
5. *Simulation of mixing in a plane, turbulent and compressible wall jet*, Daniel Ahlman, MEK.
6. *Modeling and numerical simulation of shockwave lithotripsy (getting rid of kidney stones)*, Tim Colonius, Caltech.

### **Industrial focal point**

KCSE aims to facilitate the dialogue between industry and KTH within the area of CSE. 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. Within the framework of the KCSE annual meeting, see below, representatives from Swedish industry were invited to give a presentation of their CSE related activities. Also, a networking session with the KCSE PhD students were arranged, see below. The overall reaction from industry was very positive and several representatives expressed a wish for a closer dialogue between the industry and KCSE.



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**Annual meeting, Dec 8-9, 2005**

The Annual meeting was held at the [Lovik conference](#) center, Lidingö, with schedule

***Thursday 8/12***

- 12.00 Lunch
- 13.00 Björn Engquist, KCSE
- 13.30 Dan Henningson, KCSE
- 14.00 Mats Jirstrand, FCC Chalmers
- 14.30 Timothy Lovell, Astra Zeneca
- 15.00 Coffee
- 15.30 Peter Löfgren, ABB
- 16.00 Pavel Korzhavyi, KTH MSE
- 16.30 Göran Bengtsson, SAAB
- 17.00 Group discussions: graduate students and industry representatives
- 19.00 Dinner

***Friday 9/12***

- 7.30 Breakfast
- 8.30 Presentation of the group discussions
- 9.30 Adam Wikström, Scania
- 10.00 Coffee
- 10.30 Carmen Medina, BioVitrum
- 11.00 Lars Thylén, KTH IMIT
- 11.30 Discussion: “What role can KCSE play for industrial contacts”
- 12.30 Lunch
- 13.30 KCSE Board Meeting

The networking sessions at the workshop between KCSE students and the industrial contacts showed that there is a vital interest in the competence of the KCSE students within Swedish industry. KCSE therefore aims to repeat and expand the concept. of networking between KCSE students and representatives from industry.



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## Active participants

The table below give a summary of the number of active participants as of 060401.

	<i>MEK</i>	<i>NA/PDC</i>	<i>AVE</i>	<i>MSE</i>	<i>BIO</i>	<i>EE</i>	$\Sigma$
<b><i>Professors</i></b>	4	5	1	2	2	1	15
<b><i>Lecturers and Assistant lecturers</i></b>	1	4	1		1	1	8
<b><i>Researchers and Research Assistants</i></b>	3	2		9	1	1	16
<b><i>Graduate students</i></b>	7	6	4	4	4		25
$\Sigma$	15	17	6	15	8	3	64

### Professors

Anders Eriksson, MEK  
Anders Lansner, NA  
Anders Szepessy, NA  
Arne Johansson, MEK  
Arthur Rizzi, AVE  
Björn Engquist, NA  
Börje Johansson, MSE  
Dan Henningson, MEK  
Faris Gel'mukhanov, BIO  
Gunilla Kreiss, NA  
Gustav Amberg, MEK  
Hans Ågren, BIO  
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Sailing He, EE

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### Lecturers and Assistant Lecturers

Björn Sjögreen, NA  
Erik Lindborg, MEK  
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Lennart Edsberg, NA  
Martin Norgren, EE  
Mikhail Dzugutov, NA  
Olof Runborg, NA  
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## KTH Computational Science and Engineering Centre

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**Economic results 2004 and 2005, budget 2006**

<b>Budget for KCSE (kkkr)</b>	<b>2004</b>	<b>2005</b>	<b>2006</b>	<b>Total</b>
Director (20%,10% 06)	78	241	120	439
Co-director (5%)	0	32.5	49	81.5
Co-director (5%)	0	32.5	49	81.5
Director of studies (15%)	0	102	102	204
Yearly workshop	85	100	100	285
Consultants	0	50	50	100
HSG (17%)	27.71	94.86	79.9	202.47
<b>TOTAL</b>	<b>190.71</b>	<b>652.86</b>	<b>549.9</b>	<b>1393.47</b>
Remaining				106.53