



**KTH Computational Science  
and Engineering Centre**

## Annual report KCSE 2006

In 2006, its third year of operation, the focus of KCSE has been on lobbying for increased high performance computer (HPC) resources and on establishing international collaboration with China and India in the field of computational science and engineering (CSE). A number of initiatives have been taken to promote larger investment in HPC at KTH and on the national level as well as to advertise the importance of CSE. HPC was also the theme at the KCSE annual meeting where representatives from SNIC and EU participated. The foundation has been laid for a Joint Centre in CSE together with Peking University and the Indian Association for the Cultivation of Science. Meanwhile, the core activities of KCSE have continued. The seminar series brings together CSE researchers at KTH for talks on the use of computational methods in different subject areas. The KCSE graduate program acts as an informal graduate school, where computational courses with wider appeal is promoted to KCSE students across member departments to give the students a broader perspective on computational science. During 2006 KCSE has also grown with three new member departments.

**KCSE**

*Workshops/Seminar*

*Graduate Program*

*Multidisciplinary Research*

*Industrial Focal Point*

*International Contacts*

*HPC*

Stockholm, May 2007

Olof Runborg, Director KCSE



**KTH Computational Science  
and Engineering Centre**

**KCSE 2006**



**Vision**

The KTH centre 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



## KTH Computational Science and Engineering Centre

- *Industrial focal point*  
Facilitate the dialogue between industry and KTH within CSE
- *International contacts*  
Establish contacts with CSE researchers abroad

### 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 the KTH departments of Mechanics (MEK), Numerical Analysis (NA), Aeronautical and Vehicle Engineering (AVE), Materials Science and Engineering (MSE) and Theoretical Chemistry (TC). In 2006 another three departments have joined KCSE: Electromagnetic Engineering (EE), Theoretical Physics (TP) and Nuclear Power Safety (NPS).

### KCSE Board and Executives

The board 2006 was composed of:

Björn Engquist, NA, *Chairman*  
 Börje Johansson, MSE, *Vice Chairman*  
 Anders Eriksson, MEK  
 Hans Ågren, TC  
 Art Rizzi, AVE  
 Per Öster, PDC  
 Gustav Amberg, School of Engineering Sciences

The executive committee was:

Dan Henningson, MEK, *Director*  
 Gunilla Efraimsson, AVE, *Deputy Director*



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Olof Runborg, NA, *Deputy Director*  
 Anna Delin, MSE, *Director of Studies*  
 Hans Ågren, TC  
 Per Öster, PDC

A new board and executive committee were installed 2007-01-01:

Dan Henningson, MEK, *Chairman*  
 Börje Johansson, MSE, *Vice Chairman*  
 Hans Ågren, TC  
 Gunilla Efraimsson, AVE  
 Per Öster, PDC  
 Gustav Amberg, School of Engineering Sciences  
 Johan Hoffman, NA

Olof Runborg, NA, *Director*  
 Anna Delin, MSE, *Deputy Director*  
 Philipp Schlatter, MEK, *Director of Studies*  
 Pawel Salek, TC  
 Per Öster, PDC  
 Mats Wallin, TP

### *Contact*

Olof Runborg, Director KCSE  
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 Sweden

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## Activities

### **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 as well as a seminar series with both invited speakers and presentations by the PhD students (see below). The set of core courses are:



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2D1258	Introduction to High Performance Computing, 5 credits
2D1264	Parallel Computations for Large-Scale Problems, Part 1, 4 credits
2D1290	Advanced Numerical Analysis, 4 credits
2D1225	Numerical Solutions of Differential Equations, 4 credits
2D1255	Numerical Solutions of Differential Equations, 5 credits
DD2260	The Finite Element Method, 4 credits
MH2102	Computational Physics, 5 credits
3A1640	Computational Chemistry, 5 credits
SG2212	Computational Fluid Dynamics, 5 credits
4H5919	Computational Techniques in Materials Science, 6 credits
SD2610	Computational Aerodynamics, 6 credits
	Numerical Methods in Nuclear Engineering, 4 credits

The graduate school had 34 active students at the end of 2006. Eight students (Erik von Schwerin, Måns Elenius, Jun Jiang, Simone Crippa, Kalle Pettersson, Vitalij Bajkov, Jakob Wohlert and Anders Odell) have given a seminar on their research within the KCSE seminar series (see below).

### *Graduate school contact:*

Philipp Schlatter, Director of Studies KCSE  
 KTH Mechanics  
 SE-100 44 Stockholm  
 Sweden  
 email: pschlatt@mech.kth.se  
 phone: +46-8-7907176

### **Multidisciplinary research**

The research at KCSE is conducted in five broad areas stretching over eight departments. Several common themes can be 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*
- *Numerical analysis and general algorithm development*



## KTH Computational Science and Engineering Centre

### High performance computing

KCSE aims to strengthen the computational infrastructure at KTH in collaboration with PDC. In 2006 KCSE has worked on bringing in new computer resources to KTH directly through applications but also indirectly by lobbying towards SNIC and the Swedish Research Council (VR). The activities included

- An application to the Research Infrastructure (KFI) panel of VR for a major investment in CSE infrastructure (hardware, software and education) at KTH. In this application KCSE also forcefully argued that the CSE field in Sweden is starved of resources and that funding agencies has failed to respond to the increased importance of CSE.
- A presentation of the application's message at a SNIC workshop targeted at user groups with "extreme needs for and demands on HPC resources", 2006-04-14. The purpose of the workshop was for SNIC to identify such users and their needs and to develop strategies to handle HPC support for them.
- Submitting a response to VR/KFI's long-term plan for research infrastructure investments. KCSE again urged a major increase in funding for CSE. In addition to all members of the KCSE board and executive committee, the response was signed by the president of KTH, the principal secretary of VR's subcommittee for Natural Sciences and Technology and the director of PDC.
- Encouraging KCSE members to submit applications to the Nordic Computational Grand Challenge, a survey commissioned by the Nordic research councils to "identify outstanding problems in science whose solution will greatly benefit from the use of large-scale e-Infrastructure". The survey will be used to motivate new funding for CSE on a Nordic level. Six proposals were submitted with KCSE members as PI and one additional with a KCSE co-PI. This amounts to almost half of the 14 applications from Sweden. The KCSE applications were:
  - ATMOTURB — *From Kolmogorov theories to fluid mechanics of climate change*, Erik Lindborg, MEK.
  - BRAINSIM — *Full scale, biologically detailed neocortex simulation*, Anders Lansner, NA.
  - CMPQ — *Computation of novel materials with predictive quality*, Olle Eriksson, Department of Physics, Uppsala University (co-PI: Börje Johansson, MSE)
  - GRAMS — *GRAnd and not so grand challenges in computational Materials Science*, Anatoly Belonoshko, MSE
  - LOWSOUND — *Generation and propagation of sound in low Mach number internal flows*, Gunilla Efraimsson, AVE
  - NANOQUANT — *Understanding nanomaterials from the quantum perspective*, Hans Ågren, TC



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- TURBSIM — *Direct numerical simulation of turbulence, transition and separation for flows around bodies*, Dan Henningson, MEK.
- Inviting representatives from SNIC and EU to the KCSE annual meeting for presentations and discussions about the Swedish HPC situation with KCSE researchers.

### Seminars

KCSE organizes a seminar series where the speakers are mixed senior researchers and PhD students. The seminars 2006 are listed below.

#### *Seminars spring 2006*

1. *Computational Electromagnetics at TET, KTH and KTH-Zhejiang University Joint Centre of Photonics*, Sailing He, EE
2. *Adaptive Monte Carlo Algorithms for Stopped Diffusion*, Erik von Schwerin, NA
3. *Computational Neuroscience: Goals, Methodology and Challenges*, Anders Lansner, NA
4. *Computational Multi-fluid Dynamics: Recent Advances, Challenges, and Opportunities*, Nam Dinh, NPS
5. *Atomistic Simulation of Simple Liquids*, Måns Elenius, NA
6. *Adaptive Computational Methods for Turbulent Incompressible Flow*, Johan Hoffman, NA
7. *Electron Transport in Nanostructures*, Jun Jiang, TC
8. *Numerical Methods for Quantum Molecular Dynamics*, Sverker Holmgren, TDB, UU
9. *The Role of Computational Engineering in Aeronautics and Focus on CFD*, Simone Crippa, Kalle Pettersson, AVE

#### *Seminars fall 2006*

1. *Cluster Monte Carlo simulation of phase transitions in disordered systems*, Mats Wallin, TP
2. *Ab initio calculation of thermochemistry of IVB transition metal-oxygen solid solutions*, Vitalij Bajkov, MSE



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3. *Scientific Computing at KTH, FOI, UU and CTR*, Jan Nordström, AVE
4. *Computer modeling of lipid bilayers*, Jakob Wohlert, TP
5. *Simulations of flexible structure in space*, Gunnar Tibert, MEK
6. *The overturning circulation of the global ocean*, Jonas Nycander, Department of Meteorology, SU
7. *Calculation of transport properties - application to organic molecules attached to metallic leads*, Anders Odell, MSE

### Workshop

The annual meeting of KCSE took place on 7-8 December at Lovik, Stockholm. The topic of the meeting was Computations in Biotechnology and Large Scale Computing. Invited speakers for the Biotechnology area were Anders Lansner, KTH and Erik Sonnhammar, Stockholm Bioinformatics Centre. Invited presentations regarding the High Performance Computing situation at KTH, in Sweden, the Nordic Countries and in Europe were given by Lennart Johnsson, PDC, Sverker Holmgren, SNIC, Leif Laaksonen and Enric Mitjana, EC.

The program consisted also of group discussions on the HPC situation at KTH. The conclusion from these discussions is that the HPC users at KTH are in general happy with the work performed at the staff of PDC, but more computational power is needed. Also, a concluding panel discussion on the HPC situation in Europe was held.

The annual meeting assembled around 45 participants.

The detailed meeting schedule is given below.

*Thursday 7/12*

- |       |  |
|-------|--|
| 12.00 | Lunch  |
| 13.00 | Börje Johansson, Professor, Condensed Matter Theory, |
| 13.15 | Dan Henningson, Director KCSE                        |
| 13.30 | Lennart Johnson, Director PDC                        |
| 14.15 | Coffee   |



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- 15.00 Group discussion: HPC at KTH
- 16.00 Presentation of the results of the group discussions
- 17.00 Break
- 17.15 Anders Lansner, Professor, Computational Biology
- 18.00 Erik Sonnhammer, Director, Stockholm Bioinformatics Center
- 19.00 Dinner

### *Friday 8/12*

- 7.30 Breakfast
- 8.30 Mr Enric Mitjana, European Commission
- 9.15 Sverker Holmgren, Director SNIC
- 10.00 Coffee
- 10.45 Leif Laaksonen, Chariman eIRG
- 11.30 Concluding discussion
- 12.00 Lunch

### **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.

### **International contacts**

During 2006 KCSE has established co-operation with China and India. After initial contacts in the spring, a KCSE delegation of seven people took part in a workshop at Peking University (PKU) in October to determine mutual interests and discuss a possible collaboration. From KTH the vice-president for international affairs, Ramon Wyss, participated and presented KTH's China programme. The Indian Association for the Cultivation of Science (IACS), Kolkata, India was also represented.



## KTH Computational Science and Engineering Centre

The outcome of the workshop was a draft of a letter of intent to create a Joint Center for Computational Science and Engineering between KTH (through KCSE), PKU and IACS. The center would comprise cooperation in research and graduate education with joint international research projects, workshops and training schools. It was envisaged that the centre could make important contributions within CSE, gathering the best expertise in the three countries in the related fields. From KTH's perspective it would be a strategic partnership that widens the international networks of KTH researchers by bringing in leading scientists from China and India. It could also be a source for recruiting students.

The letter of intent has been signed by the presidents of KTH and IACS, and it is currently (May 2007) in the process of being signed also by PKU.

## Active participants

The table below give a summary of the number of active participants as of 070510.

	<i>MEK</i>	<i>NA/PDC</i>	<i>AVE</i>	<i>MSE</i>	<i>TC</i>	<i>EE</i>	<i>TP</i>	<i>NPS</i>	$\Sigma$
<b><i>Professors</i></b>	4	5	1	2	3	1	3	1	20
<b><i>Lecturers and Assistant lecturers</i></b>	1	4	1		1	1	1		9
<b><i>Researchers and Research Assistants</i></b>	4	1		8	1	1	2	1	18
<b><i>Graduate students</i></b>	8	9	3	3	2	2	4	1	32
$\Sigma$	17	19	5	13	7	5	10	3	79

<b>Professors</b>	<b>Lecturers and Assistant Lecturers</b>	<b>Researchers and Research Assistants</b>
<a href="#">Anders Eriksson</a> , MEK	<a href="#">Anna-Karin Tornberg</a> , NA	<a href="#">Anatoly Belonoshko</a> , MSE
<a href="#">Anders Lansner</a> , NA	<a href="#">Erik Lindborg</a> , MEK	<a href="#">Andrei Ruban</a> , MSE
<a href="#">Anders Rosengren</a> , TP	<a href="#">Gunilla Efraimsson</a> , AVE	<a href="#">Anna Delin</a> , MSE
<a href="#">Anders Szepessy</a> , NA	<a href="#">Johan Hoffman</a> , NA	<a href="#">Famhi Himo</a> , TC
<a href="#">Arne Johansson</a> , MEK	<a href="#">Lennart Edsberg</a> , NA	<a href="#">Geert Brethouwer</a> , MEK
<a href="#">Arthur Rizzi</a> , AVE	<a href="#">Martin Norgren</a> , EE	<a href="#">Gunnar Tibert</a> , MEK
<a href="#">Björn Engquist</a> , NA	<a href="#">Olof Runborg</a> , NA	<a href="#">Henrik Larsson</a> , MSE
<a href="#">Börje Johansson</a> , MSE	<a href="#">Patrik Henelius</a> , TP	<a href="#">Jack Lidmar</a> , TP
<a href="#">Dan Henningson</a> , MEK	<a href="#">Pawel Salek</a> , TC	<a href="#">Lars Höglund</a> , MSE
<a href="#">Faris Gel'mukhanov</a> , TC		<a href="#">Levente Vitos</a> , MSE
<a href="#">Gustav Amberg</a> , MEK		<a href="#">Luca Brandt</a> , MEK



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<a href="#">Hans Ågren</a> , TC		<a href="#">Malin Selleby</a> , MSE
<a href="#">Jesper Ooppelstrup</a> , NA		<a href="#">Patrik Persson</a> , EE
<a href="#">John Ågren</a> , MSE		<a href="#">Pavel Korzhavyi</a> , MSE
<a href="#">Mats Wallin</a> , TP		<a href="#">Per Öster</a> , PDC
<a href="#">Mikhail Dzugutov</a> , NA		<a href="#">Per-Håkan Lundow</a> , TP
<a href="#">Olle Edholm</a> , TP		<a href="#">Philipp Schlatter</a> , MEK
<a href="#">Sailing He</a> , EE		<a href="#">Tomasz Kozłowski</a> , NPS
<a href="#">Truc-Nam Dinh</a> , NPS		
<a href="#">Yi Luo</a> , TC		

### Graduate Students

Name	Dept	Adm year	Research subject	Advisor
Anders Biltmo	TP	2005	Monte Carlo simulation of disordered magnetic materials	Anders Rosengren, Patrik Henelius
Anders Odell	MSE	2005	Spin molecular electronics	Anna Delin
Andreas Andersson	TP	2007	Modeling and simulation of low-dimensional quantum liquids	Mats Wallin, Jack Lidmar
Axel Kierkegaard	AVE	2006	Studies of sound generation in internal low-Mach number flows via numerical solutions of the Navier-Stokes equations	Mats Åbom, Gunilla Efraimsson
Daniel Ahlman	MEK	2002	Simulation and modeling of turbulent flow and combustion	Geert Brethouwer, Arne Johansson
Elias Rudberg	TC	2004	Methods for linear scaling evaluation of the Fock matrix	Pawel Salek
Emanuel Rubensson	TC	2005	Error control in density purification methods and self-consistent field method as used in Hartree-Fock and Kohn-Sham methods	Pawel Salek
Erik Brandt	TP	2007	Molecular dynamics simulations of biological membrane proteins	Olle Edholm, Mats Wallin
Erik von Schwerin	NA	2001	Adaptivity for stochastic and partial differential equations with applications to phase transitions	Anders Szepessy
Espen Åkervik	MEK	2004	Control of open flows using global modes	Luca Brandt, Dan Henningson
Francesco	NPS	2006	Development of a multi-scale simulation	Truc-Nam Dinh.



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Cadinu			methodology for nuclear reactor thermal hydraulic and safety analysis	Tomasz Kozlowski
Henrik Holst	NA	2006	Multiscale methods for the wave equation	Björn Engquist
Jelena Popovic	NA	2006	Numerical methods for high frequency waves	Olof Runborg
Jun Song	EE	2006	Photonic integrated circuits for optical communications	Sailing He
Kalle Pettersson	AVE	2004	RANS methods to obtain aerodynamic data	Arthur Rizzi
Klara Asp Grönhagen	MSE	2004	Phase-field simulations of structural evolution in alloys	John Ågren
Lars-Uve Schrader	MEK	2006	Receptivity of three-dimensional boundary layers	Luca Brandt, Dan Henningson
Linus Marstorp	MEK	2004	Subgrid-scale modelling for large-eddy simulation including scalar mixing in rotating turbulent shear flows	Geert Brethouwer, Arne Johansson
Måns Elenius	NA	2004	Molecular dynamics, glass formation and supercooled liquids	Mikhail Dzugutov
Marco Kupiainen	NA	2001	LES for compressible turbulent and reactive flow	Björn Sjögreen
Martin Lindén	TP	2003	Modeling and computations for biological motors	Mats Wallin
Mattias Jansson	MEK	2004	Rotation-free shell elements for thin-film structures and simulations of centrifugally deployed space webs	Gunnar Tibert, Anders Ericsson
Mohammad Motamed	NA	2003	Numerical methods and theory for creeping and surface waves	Olof Runborg
Murtazo Nazarov	NA	2006	Adaptive computation of turbulent flow	Johan Hoffman
Sara Zahedi	NA	2006	A conservative level set method for two-phase flow	Gunilla Kreiss
Shervin Bagheri	MEK	2006	Flow control and stability	Dan Henningson
Simone Crippa	AVE	2005	RANS and DES methods in aerodynamic applications	Arthur Rizzi
Tomas Ooppelstrup	NA		Molecular dynamics	Mikhail Dzugutov



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Vitalij Bajkov	MSE	2002	Electronic structure of diluted magnetic semiconductors	Börje Johansson
Walter Villanueva	MEK	2003	Diffuse-interface simulations of capillary phenomena	Gustav Amberg
Xin Hu	EE	2006	Metamaterial transmission lines	Sailing He
Yuan Lin	MEK	2004	Modeling and simulation of dielectrophoresis of micro and nano particles	Gustav Amberg

## Economic results 2004-2006, budget 2007

All sums are in kSEK.

<b>Item</b>	<b>2004</b>	<b>2005</b>	<b>2006</b>	<b>2007</b>	<b>Total</b>
Director	78	242	240	130	690
Co-director		32.5	85	85	202
Co-director		32.5	38		70
Director of studies		102	41	85	228
Yearly workshop	85	98	92	100	375
Consultants		50			50
International contacts			58	30	88
Other costs		10	2	10	22
HSG (17%)	28	86	79	85	278
<b>Total</b>	<b>191</b>	<b>653</b>	<b>635</b>	<b>525</b>	<b>2004</b>

KCSE is funded by 500 kSEK per year from KTH. In addition it has accumulated 10 kSEK on interest. The remaining funds at the end of 2007 would therefore be ca +6 kSEK.