KTH Computational Science and Engineering Centre

Annual Report KCSE 2007

For KCSE the most important moment of 2007 came in November when Vetenskapsrådet (VR) announced they would award KCSE a five-year grant of 2.5 MSEK/year to set up an expanded graduate school in Computational Science and Engineering (CSE). This is an exciting opportunity for KCSE to strengthen and shape the education in this important field. It will doubtless be in the focus of much of KCSE's work in the next few years.

Otherwise the main activities in 2007 concerned international collaboration and lobbying activities at KTH. The creation of a trilateral Joint Center for CSE together with Peking University (PKU) and the Indian Association for the Cultivation of Science (IACS) picked up speed as the presidents of the three institutes signed a letter of intent to set up the center, and students from PKU and IACS participated in a summer school on high performance computing (HPC) at PDC. KCSE took an active role in discussions about the HPC environment at KTH, contributing to the commission that was set up by the KTH President to determine the future organization of PDC. In the process, KCSE also secured a three year prolonged financial support from KTH at 300 kSEK/year.

Stockholm, May 2008

Olof Runborg, Director KCSE

KTH Computational Science and Engineering Centre

KCSE 2007

The remarkable evolution of large-scale computing has created in recent years a new and revolutionary way of performing research. Together with theoretical analysis and traditional experimental research, computer simulations have 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.

At KTH the centre KCSE was established to realize the vision of

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

It was created in 2004 and now comprises eight KTH departments: Mechanics (MEK), Numerical Analysis (NA), Aeronautical and Vehicle Engineering (AVE), Materials Science and Engineering (MSE), Theoretical Chemistry (TC), Electromagnetic Engineering (EE), Theoretical Physics (TP) and Nuclear Power Safety (NPS).

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The activities within KCSE can be grouped into the following points:

- *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*
  Strengthening the computational infrastructure in collaboration with PDC

- *Workshops and seminars*
  Widening and strengthening the network of computational scientists

- *International collaborations*
  Be a focal point at KTH for international contacts within CSE research and education.

KCSE Board and Executives

The board and executive group 2007 was composed of the following people.

Board

Dan Henningson, MEK, *Chairman*
Börje Johansson, MSE, *Vice Chairman*
Hans Ågren, TC
Gunilla Efraimsson, AVE
Per Öster, PDC (replaced by Peter Graham in Nov 07)
Gustav Amberg, School of Engineering Sciences
Johan Hoffman, NA

Executive group

Olof Runborg, NA, *Director*
Anna Delin, MSE, *Deputy Director*
Philipp Schlatter, MEK, *Director of Studies*
Pawel Salek, TC
Per Öster, PDC (replaced by Peter Graham in Nov 07)
Mats Wallin, TP

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Contact

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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. It has run on an informal basis since the start of KCSE in 2004. In 2007 KCSE made applications to Vinnova and VR for funds to expand and modernize the school's curriculum. A grant of 2,5 MSEK/year (2008-2012) for these activities was awarded KCSE from VR in November 2007. This will allow KCSE to significantly improve and develop CSE education in the years ahead.

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:

DN2258 Introduction to High Performance Computing, 5 credits
DN2264 Parallel Computations for Large-Scale Problems, Part 1, 4 credits
DN2290 Advanced Numerical Analysis, 5 credits
DN2225 Numerical Solutions of Differential Equations I, 4 credits
DN2255 Numerical Solutions of Differential Equations II, 5 credits
DN2260 The Finite Element Method, 4 credits
MH2102 Computational Physics, 5 credits
BB2300 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

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The graduate school had 37 active students at the end of 2007. Five students (Tomas Oppelstrup, Walter Villanueva, Espen Åkervik, Mohammad Motamed, Mattias Gärdsback) 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
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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, are

- *Simulations of biological systems (life science)*
- *Simulations of properties of materials (materials science)*
- *Simulations of fluid systems*
- *Simulations of electromagnetic fields*
- *Numerical analysis and general algorithm development*

With the aim of stimulating cross-disciplinary research, in 2007 KCSE has begun setting up research subgroups with scientists from different departments working on similar topics. A first example would be an *Atomistic Simulation Group* with a focus on molecular dynamics simulations, where members come from the departments of Materials Science, Theoretical Physics and Numerical Analysis.

High performance computing

KCSE aims to strengthen the computational infrastructure at KTH in collaboration with PDC. In 2007 KCSE has worked on bringing in new computer resources to KTH directly through applications but also indirectly by lobbying towards SNIC and VR. The work included the following results:

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- KCSE coordinated an application to SNIC/KAW for a large computer system dedicated to *Complex Dynamical Systems*. The partners involved in the proposal were the KCSE groups from Theoretical Chemistry, Materials Science, Mechanics and the Stockholm Brain Institute (related to NA), as well as PDC.
- KCSE Deputy Director Anna Delin (MSE) was appointed to serve on the SNIC board and Philipp Schlatter, Director of Studies in KCSE, became a member of the SNUG (SNIC User Group) committee. Previously, neither of these bodies had representatives from KTH.
- KCSE was given financial responsibility for the operation costs of the BlueGene *Hebb* computer at PDC, with a budget of about 1 MSEK/year.
- VR solicited a response from KCSE to the Nordic eScience Strategy draft document, proposed by the Nordic Council of Ministers. KCSE argued that the most important components of the strategy were the programmes on CSE education and on research for grand challenge problems, emphasizing the role of computer hardware and development of numerical algorithms/software. KCSE also cautioned against directing too much resources towards grid technology for grand challenge problems.
- KCSE took an active role in the commission on the future organization of PDC in the fall of 2007. Out of 8 commission members, 4 are active in KCSE.
- Anna Delin presented KCSE and the proposed KCSE graduate school at the SNIC Interaction meeting November.

Seminars

KCSE organizes a seminar series where the speakers are mixed senior researchers and PhD students, both from inside and outside KTH. The seminars 2007 are listed below.

Seminars spring 2007

1. *Large-eddy simulation: Application to bypass transition*, Philipp Schlatter, MEK

2. *First-passage kinetic Monte-Carlo: Diffusion simulation without the tiny steps*, Tomas Oppelstrup, NA

3. *Interatomic interaction potentials for molecules and solids*, Pavel Korzhavyi, MSE

4. *7th EU Research Framework Programme - in brief and some relevant details*, Christian Hansen, VINNOVA Brussels

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5. *Ab-Initio Molecular Dynamics Simulations of Nucleic Acids*, Håkan Hugosson, TC

6. *Negative refractive index materials*, Kevin Webb, Purdue University

7. *Phase-field modeling and simulation of capillary-driven flows*, Walter Villanueva, MEK

8. *The VINNOVA Excellence Center "Hierarchic design of Industrial Materials"*, Hans Ågren, MSE

Seminars fall 2007

1. *Recent advances in many-body theory*, Debashis Mukherjee, IACS, India

2. *Large scale eigenvalue computations for flow stability*, Espen Åkervik, MEK

3. *Thermodynamical properties of biological molecules through loosely coupled or distributed simulations: protein folding and insertion in biomembranes*, Erik Lindahl, Stockholm Bioinformatics Center

4. *Computation of Creeping Waves on Smooth Objects*, Mohammad Motamed, NA

5. *Computational Thermodynamics*, Malin Selleby, MSE

6. *ELMER - an Open Source Finite Element software for Multi Physics Problems*, Peter Råback, CSC Finland

7. *Using patches of Finite Elements - instead of just elements*, Mattias Gärdsback, MEK

Workshop

The annual meeting of KCSE took place on 6-7 December 2007 at Lovik, Stockholm. The topic of the meeting was “Computational Science and Engineering in Europe”, and “Graduate Schools in Computational Science and Engineering”. Invited speakers were Kenneth Ruud (Chemistry, University of Tromsø), Alexander Reinefeld (Konrad Zuse Zentrum, Berlin), Hans Karlsson (NGSSC, Uppsala), David Wales (Chemistry, University of Cambridge), Petros Koumoutsakos (Computational Science, ETH Zurich), and Sinisa Krajnovic (SNIC/SNUG, Fluid Dynamics, Chalmers).

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The program consisted also of group discussions on how to perform interdisciplinary research and various ideas about the forthcoming KCSE graduate school.

The annual meeting assembled around 45 participants.

The detailed meeting schedule is given below.

Thursday 6/12

12.00 Lunch

13.00 Olof Runborg, Director KCSE
Dan Henningson, Chairman of the Board, KCSE

13.30 Kenneth Ruud, Department of Chemistry, University of Tromsø

14.15 Coffee

14.45 Alexander Reinefeld, Konrad-Zuse-Zentrum für Informationstechnik, Berlin

15.30 Hans Karlsson, Director NGSSC, Department of Physical Chemistry, Uppsala University

16.15 Break

16.30 Group Discussions: Research Schools

17.30 Discussion of the results of the discussions

19.00 Dinner

Friday 7/12

7.30 Breakfast

8.30 David Wales, Department of Chemistry, University of Cambridge
9.15 Petros Koumoutsakos, Institute for Computational Science, ETH Zurich

10.00 Coffee

10.30 Sinisa Krajnovic, Department of Fluid Dynamics, Chalmers

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11.15 Concluding discussion

12.00 Lunch

International collaboration

During 2007 KCSE strengthened its co-operation with Peking University (PKU), China and the Indian Association for the Cultivation of Science (IACS), India. A letter of intent was signed by the presidents of KTH, PKU and IACS to set up a Joint Center for Computational Science and Engineering, where KCSE would be the KTH partner. The center will comprise cooperation in research and graduate education with joint international research projects, workshops and training schools. It is envisaged that the centre can make important contributions within CSE, gathering the best expertise in the three countries in the related fields. From KTH's perspective it is a strategic partnership that widens the international networks of KTH researchers by bringing in leading scientists from China and India.

As a first concrete activity of this collaboration six students from PKU and IACS were invited to KTH in August to take part in PDC's summer school on high performance computing. The IACS director Prof. Debashis Mukherjee also came and gave a guest lecture in the course. This effort was supported financially by VR, KAW, Wenner-Gren as well as the CSC and SCI Schools at KTH.

In the fall of 2007 a Memorandum of Understanding to set up the Joint Center was drafted. The goal is to get external financing for the center, and in December KCSE together with IACS and PKU wrote a joint proposal to STINT for funding. In case external funds cannot be found, the SCI School at KTH gave a guarantee of limited funding to initiate the activities in the center (150 kSEK/year, 2008-2010).

Active participants

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

	MEK	NA/PDC	AVE	MSE	TC	EE	TP	NPS	Σ
Professors	4	5	1	2	3	1	3	1	**20**
Lecturers and Assistant lecturers	1	4	1		1	1	1		**9**

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Researchers and Research Assistants	5	1		8	1	1	2	1	**19**
Graduate students	12	9	3	4	2	2	4	1	**37**
Σ	**22**	**19**	**5**	**14**	**7**	**5**	**10**	**3**	**85**

Professors	**Lecturers and Assistant Lecturers**	**Researchers and Research Assistants**
Anders Eriksson, MEK	Anna-Karin Tornberg, NA	Anatoly Belonoshko, MSE
Anders Lansner, NA	Erik Lindborg, MEK	Andrei Ruban, MSE
Anders Rosengren, TP	Gunilla Efraimsson, AVE	Anna Delin, MSE
Anders Szepessy, NA	Johan Hoffman, NA	Famhi Himo, TC
Arne Johansson, MEK	Lennart Edsberg, NA	Geert Brethouwer, MEK
Arthur Rizzi, AVE	Martin Norgren, EE	Gunnar Tibert, MEK
Björn Engquist, NA	Olof Runborg, NA	Henrik Larsson, MSE
Börje Johansson, MSE	Patrik Henelius, TP	Jack Lidmar, TP
Dan Henningson, MEK	Pawel Salek, TC	Lars Höglund, MSE
Faris Gel´mukhanov, TC		Levente Vitos, MSE
Gustav Amberg, MEK		Luca Brandt, MEK
Hans Ågren, TC		Malin Selleby, MSE
Jesper Oppelstrup, NA		Patrik Persson, EE
John Ågren, MSE		Pavel Korzhavyi, MSE
Mats Wallin, TP		Peter Graham, PDC
Mikhail Dzugutov, NA		Per-Håkan Lundow, TP
Olle Edholm, TP		Philipp Schlatter, MEK
Sailing He, EE		Tomasz Kozlowski, NPS
Truc-Nam Dinh, NPS		Minh Do-Quanq, MEK
Yi Luo, TC		Johan Jansson, NA

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	Modelling and simulation of low-dimensional quantum liquids	Mats Wallin, Jack Lidmar

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Andreas Vallgren	MEK	2007	Studies in chaotic atmospheric dynamics: The quasi-geostrophic approximation	Erik Lindborg and Geert Brethouwer
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
Cecilia Århammar	MSE	2007	Atomistic modelling of solid oxides	Börje Johhansson
Daniel Ahlman	MEK	2002	Simulation and modelling of turbulent flow and combustion	Geert Brethouwer, Arne Johansson
David Tempelmann	MEK	2007	Receptivity of 3D boundary layers using parabolised stability equations	Ardeshir Hanifi, Dan Henningson
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 Cadinu	NPS	2006	Development of a multi-scale simulation methodology for nuclear reactor thermal hydraulic and safety analysis	Truc-Nam Dinh, 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

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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	Modelling and computations for biological motors	Mats Wallin
Mattias Gärdsback	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
Outi Tammisola	MEK	2007	Hydrodynamic stability of a plane liquid jet in a surrounding gas	Fredrik Lundell, Daniel Söderberg, Henrik Alfredsson
Qiang Li	MEK	2007	Turbulent wall-bounded flows with passive-scalar transport	Philipp Schlatter, Dan Henningson
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 Oppelstrup	NA		Molecular dynamics	Mikhail Dzugutov
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	Modelling and simulation of dielectrophoresis of micro and nano particles	Gustav Amberg

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Economic results 2004-2007, budget 2008

Below is the income statement for KCSE 2004-2007 and a budget for KCSE proper (without the graduate school) 2008. All sums are in kSEK.

Revenues	**2004**	**2005**	**2006**	**2007**	**2008**
KTH President	500	500	500	500	300
KTH Schools				111	150
External funds				62	
Interest		3	7	55	45
Total revenues	**500**	**503**	**507**	**728**	**495**
Expenses					
Director	78	242	240	160	160
Co-director		32	85	100	80
Co-director		32	38		
Director of studies		102	41	100	
Consultants		50			
Other staff				40	
Annual meeting	85	98	92	101	50
International contacts			58	111	150
Course fees				10	
Other costs		10	2	6	5
HSG (17%)	28	86	79	75	75
Total expenses	**191**	**653**	**635**	**704**	**520**
Net income	**309**	**-150**	**-128**	**24**	**-25**
Unused funds prev years		**309**	**159**	**31**	**55**
Total unused funds	**309**	**159**	**31**	**55**	**30**