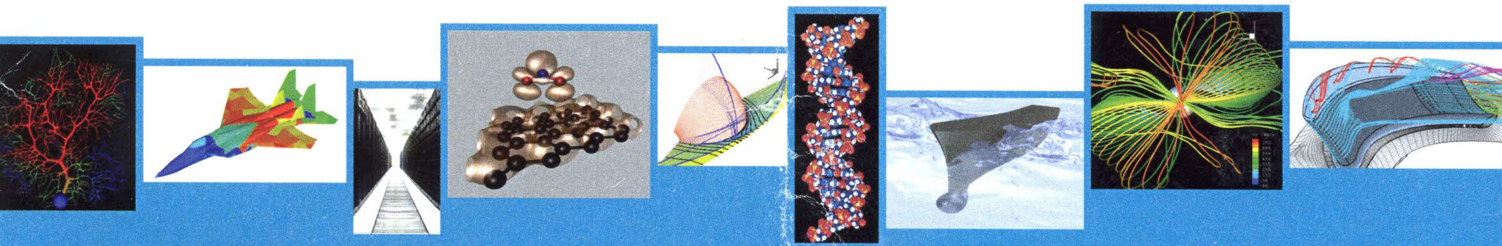
Vlaams Supercomputer Centrum

23 March 2009

Launch Vlaams Supercomputer Centrum



PROGRAM

Program:

14.15	**Scientific program**
14.15	Dr. ir. Kurt Lust (Vlaams Supercomputer Centrum) - Presentation of the VSC
14.30	Prof. dr. Patrick Bultinck (Universiteit Gent) - *In silico* Chemistry: Quantum Chemistry and Supercomputers
14.45	Prof. dr. Wim Vanroose (Universiteit Antwerpen) - Large scale calculations of molecules in laser fields
15.00	Prof. dr. Stefaan Tavernier (Vrije Universiteit Brussel) - Grid applications in particle and astroparticle physics: The CMS and IceCube projects
15.15	Prof. dr. Dirk Van den Poel (Universiteit Gent) - Research using HPC capabilities in the field of economics / business and management science
15.30	Dr. Kris Heylen (K.U.Leuven) -Supercomputing and Linguistics
15.45	Dr. ir. Lies Geris (K.U.Leuven) - Modeling in biomechanics and biomedical engineering
16.00	Prof. dr. ir. Chris Lacor (Vrije Universiteit Brussel) and Prof. dr. Stefaan Poedts (K.U.Leuven) - Supercomputing in CFD and MHD
16.15	**Coffee break**

17.00 Academic session

17.00	Prof. dr. ir. Karen Maex, Chairman of the steering group of the Vlaams Supercomputer Centrum
17.10	Prof. dr. dr. Thomas Lippert, Director of the Institute for Advanced Simulation and head of the Jülich Supercomputer Centre, Forschungszentrum Jülich. European view on supercomputing and PRACE
17.50	Prof. dr. ir. Charles Hirsch, President of the HPC Workgroup of the Royal Flemish Academy of Belgium for Sciences and the Arts (KVAB)
18.00	Prof. dr. ir. Bart De Moor, President of the Board of Directors of the Hercules Foundation
18.10	Minister Patricia Ceysens, Flemish minister for economy, enterprise, science, innovation and foreign trade

18.30 Reception

Prof. dr. Patrick Bultinck. *In silico* Chemistry: Quantum Chemistry and Supercomputers

Universiteit Gent/Ghent University, Faculty of Sciences, Department of Inorganic and Physical Chemistry

Abstract: Quantum Chemistry deals with the chemical application of quantum mechanics to understand the nature of chemical substances, the reasons for their (in)stability but also with finding ways to predict properties of novel molecules prior to their synthesis. The working horse of quantum chemists is therefore no longer the laboratory but the supercomputer. The reason for this is that quantum chemical calculations are notoriously computationally demanding. These computational demands are illustrated by the scaling of computational demands with respect to the size of molecules and the level of theory applied. An example from Vibrational Circular Dichroism calculations shows how supercomputers play a role in stimulating innovation in chemistry.

Prof. dr. Patrick Bultinck (°Blankenberge, 1971) is professor in Quantum Chemistry, Computational and Inorganic Chemistry at Ghent University, Faculty of Sciences, Department of Inorganic and Physical Chemistry. He is author of roughly 100 scientific publications and performs research in quantum chemistry with emphasis on the study of concepts such as the chemical bond, the atom in the molecule and aromaticity. Another main topic is the use of computational (quantum) chemistry in drug discovery. In 2002 and 2003, P. Bultinck received grants from the European Center for SuperComputing in Catalunya for his computationally demanding work in this field.

Prof. dr. Wim Vanroose. Large scale calculations of molecules in laser fields

Universiteit Antwerpen, Department of Mathematics and Computer Science

Abstract: Over the last decade, calculations with large scale computer have caused a revolution in the understanding of the ultrafast dynamics that play at the microscopic level. We give an overview of the international efforts to advance the computational tools for this area of science. We also discuss how the results of the calculations are guiding chemical experiments.

Prof. dr. Wim Vanroose is BOF-Research professor at the Department of Mathematics and Computer Science, Universiteit Antwerpen. He is involved in international efforts to build computational tools for large scale simulations for ultrafast microscopic dynamics. Between 2001 and 2004 he was a computational scientist at NERSC computing center at the Berkeley Lab, Berkeley USA.

Prof. dr. Stefaan Tavernier. Grid applications in particle and astroparticle physics: The CMS and IceCube projects

Vrije Universiteit Brussel, Faculty of Science and Bio-engineering Sciences, Department of Physics, Research Group of Elementary Particle Physics

Abstract: The large hadron collider LHC at the international research centre CERN near Geneva is due to go into operation at the end of 2009. It will be the most powerful particle accelerator ever, and will give us a first glimpse of the new phenomena that are expected to occur at these energies. However, the analysis of the data produced by the experiments around this accelerator also represents an unprecedented challenge. The VUB, UGent and UA participate in the CMS project. This is one of the four major experiments to be performed at this accelerator. One year of CMS operation will result in about 106 GBytes of data. To cope with this flow of data, the CMS collaboration has set up a GRID computing infrastructure with distributed computer infrastructure scattered over the participating laboratories on 4 continents.

The IceCube Neutrino Detector is a neutrino observatory currently under construction at the South Pole. IceCube is being constructed in deep Antarctic ice by deploying thousands of optical sensors at depths between 1,450 and 2,450 meters. The main goal of the experiment is to detect very high energy neutrinos from the cosmos. The neutrinos are not detected themselves. Instead, the rare instance of a collision between a neutrino and an atom within the ice is used to deduce the kinematical parameters of the incoming neutrino. The sources of those neutrinos could be black holes, gamma ray bursts, or supernova remnants. The data that IceCube will collect will also contribute to our understanding of cosmic rays, supersymmetry, weakly interacting massive particles (WIMPS), and other aspects of nuclear and particle physics. The analysis of the data produced by IceCube requires similar computing facilities as the analysis of the LHC data.

Prof. dr. Stefaan Tavernier is professor of physics at the Vrije Universiteit Brussel. He obtained a PhD at the Faculté des sciences of Orsay (France) in 1968, and a "Habilitation" at the VUB in 1984. He spent most of his scientific career working on research projects at the international research centre CERN in Geneva. He has been project leader for the CERN/NA25 project, and he presently is the spokesperson of the CERN/Crystal Clear (RD18) collaboration. His main expertise is in experimental methods for particle physics. He has over 160 publications in peer reviewed international journals, made several contributions to books and has several patents. He is also the author of a textbook on experimental methods in nuclear and particle physics.

Prof. dr. Dirk Van den Poel. Research using HPC capabilities in the field of economics / business and management science

Universiteit Gent/Ghent University, Faculty of Economics and Business Administration, Department of Marketing, www.crm.UGent.be and www.mma.UGent.be

Abstract: HPC capabilities in the field of economics / business and management science are most welcome when optimizing specific quantities (e.g. maximizing sales, profits, service level, or minimizing costs) subject to certain constraints. Optimal solutions for common problems are usually computationally infeasible even with the biggest HPC installations, therefore researchers develop heuristics or use techniques such as genetic algorithms to come close to optimal solutions.

One of the nice properties they possess is that they are typically easily parallelizable. In this talk, I will give several examples of typical research questions, which need an HPC infrastructure to obtain good solutions in a reasonable time window. These include the optimization of marketing actions towards different marketing segments in the domain of analytical CRM (customer relationship management) and solving multiple-TSP (traveling salesman problem) under load balancing, alternatively known as the vehicle routing problem under load balancing.

Prof. dr. Dirk Van den Poel (°Merksem, 1969) is professor of marketing modeling / analytical customer relationship management (aCRM) at Ghent University. He obtained his MSc in management / business engineering as well as his PhD from K.U.Leuven. He heads the modeling cluster of the Department of Marketing at Ghent University.

He is program director of the Master of Marketing Analysis, a one-year program in English about predictive analytics in marketing. His main interest fields are aCRM, data mining (genetic algorithms, neural networks, random forests, random multinomial logit: RMNL), text mining, optimal marketing resource allocation and operations research.

Dr. Kris Heylen. Supercomputing and Linguistics

Katholieke Universiteit Leuven, Faculty of Arts, Research Unit Quantitative Lexicology and Variational Linguistics (QLVL)

Abstract: Communicating through language is arguably one of the most complex processes that the most powerful computer we know, the human brain, is capable of. As a science, linguistics aims to uncover the intricate system of patterns and structures that make up human language and that allow us to convey meaning through words and sentences. Although linguists have been investigating and describing these structures for ages, it is only recently that large amounts of electronic data and the computational power to analyse them have become available and have turned linguistics into a truly data-driven science. The primary data for linguistic research is ordinary, everyday language use like conversations or texts. These are collected in very large electronic text collections, containing millions of words and these collections are then mined for meaningful structures and patterns. With increasing amounts of data and ever more advanced statistical algorithms, these analyses are no longer feasible on individual servers but require the computational power of interconnected supercomputers.

In the presentation, I will briefly describe two case studies of computationally heavy linguistic research. A first case study has to do with the pre-processing of linguistic data. In order to find patterns at different levels of abstraction, each word in the text collection has to be enriched with information about its word class (noun, adjective, verb,..) and syntactic function within the sentence (subject, direct object, indirect object...). A piece of software called a parser can add this information automatically. For our research, we wanted to parse a text collection of 1.3 billion words, i.e. all issues from a 7-year period of 6 Flemish daily newspapers, representing a staggering 13 years of computing on an ordinary computer. Thanks to the K.U.Leuven's supercomputer, this could be done in just a few months. This data has now been made available to the wider research community.

Dr. Kris Heylen obtained a Master in Germanic Linguistics (2000) and a Master in Artificial Intelligence (2001) from the K.U.Leuven. In 2005, he was awarded a PhD in Linguistics at the K.U.leuven for his research into the statistical modelling of German word order variation. Since 2006, he is a postdoctoral fellow at the Leuven research unit Quantitative Lexicology and Variational Linguistics (QLVL), where he has further pursued his research into statistical language modelling with a focus on lexical patterns and word meaning in Dutch.

Dr. ir. Lies Geris. Modeling in biomechanics and biomedical engineering

Katholieke Universiteit Leuven, Faculty of Engineering, Department of Mechanical Engineering,
Division of Biomechanics and Engineering Design

Abstract: The first part of the presentation will discuss the development and applications of a mathematical model of fracture healing. The model encompasses several key-aspects of the bone regeneration process, such as the formation of blood vessels and the influence of mechanical loading on the progress of healing. The model is applied to simulate adverse healing conditions leading to a delayed or nonunion. Several potential therapeutic approaches are tested in silico in order to find the optimal treatment strategy. Going towards patient specific models will require even more computer power than is the case for the generic examples presented here.

The second part of the presentation will give an overview of other modeling work in the field of biomechanics and biomedical engineering, taking place in Leuven and Flanders. The use of supercomputer facilities is required to meet the demand for more detailed models and patient specific modeling.

Dr. ir. Liesbet Geris is a post-doctoral research fellow of the Research Foundation Flanders (FWO) working at the Division of Biomechanics and Engineering Design of the Katholieke Universiteit Leuven, Belgium. From the K.U.Leuven, she received her MSc degree in Mechanical Engineering in 2002 and her PhD degree in Engineering in 2007, both summa cum laude. In 2007 she worked for 4 months as an academic visitor at the Centre of Mathematical Biology of Oxford University. Her research interests encompass the mathematical modeling of bone regeneration during fracture healing, implant osseo-integration and tissue engineering applications. The phenomena described in the mathematical models reach from the tissue level, over the cell level, down to the molecular level. She works in close collaboration with experimental and clinical researchers from the university hospitals Leuven, focusing on the development of mathematical models of impaired healing situations and the in silico design of novel treatment strategies. She is the author of 36 refereed journal and proceedings articles, 5 chapters and reviews and 18 peer-reviewed abstracts. She has received a number of awards, including the Student Award (2006) of the European Society of Biomechanics (ESB) and the Young Investigator Award (2008) of the International Federation for Medical and Biological Engineering (IFMBE).

Prof. dr. ir. Chris Lacor[1] and Prof. dr. Stefaan Poedts[2]. Supercomputing in CFD and MHD.

1 Vrije Universiteit Brussel, Faculty of Applied Sciences, Department of Mechanical Engineering
2 Katholieke Universiteit Leuven, Faculty of Sciences, Department of Mathematics, Centre for Plasma Astrophysics

Abstract: CFD is an application field in which the available computing power is typically always lagging behind. With the increase of computer capacity CFD is looking towards more complex applications – because of increased geometrical complication or multidisciplinary aspects e.g. aeroacoustics, turbulent combustion, biological flows, etc – or more refined models such as Large Eddy Simulation (LES) or Direct Numerical Simulation (DNS). In this presentation some demanding application fields of CFD will be highlighted, to illustrate this.

Computational MHD has a broad range of applications. We will survey some of the most CPU demanding applications in Flanders in the context of examples of the joint initiatives combining expertise from multiple disciplines the VSC will hopefully lead to, such as the customised applications built in the COOLFluiD and AMRVAC-CELESTE3D projects.

Prof. dr. ir. Chris Lacor obtained a degree in Electro-mechanical Engineering at VUB in 1979 and his PhD in 1986 at the same university. Currently he is Head of the Research Group Fluid Mechanics and Thermodynamics of the Faculty of Engineering at VUB. His main research field is Computational Fluid Dynamics (CFD). He stayed at the NASA Ames CFD Branch as an Ames associate in 1987 and at EPFL IMF in 1989 where he got in contact with the CRAY supercomputers. In the early 90's he was co-organizer of supercomputing lectures for the VUB/ULB CRAY X-MP computer. His current research focuses on Large Eddy Simulation, high-order accurate schemes and efficient solvers in the context of a variety of applications such as Computational Aeroacoustics, Turbulent Combustion, Non-Deterministic methods and Biological Flows. He is author of more than 100 articles in journals and on international conferences. He is also a fellow of the Flemish Academic Centre for Science and the Arts (VLAC).

Prof. dr. Stefaan Poedts obtained his degree in Applied Mathematics in 1984 at the K.U.Leuven. As 'research assistant' of the Belgian National Fund for Scientific Research he obtained a PhD in Sciences (Applied Mathematics) in 1988 at the same university. He spent two years at the Max-Planck-Institut für Plasmaphysik in Garching bei München and five years at the FOM-Instituut voor Plasmafysica 'Rijnhuizen'. In October 1996 he returned to the K.U.Leuven as Research Associate of the FWO-Vlaanderen at the Centre for Plasma Astrophysics (CPA) in the Department of Mathematics. Since October 1, 2000 he is Academic Staff at the K.U.Leuven, presently a Full Professor. His research interests include solar astrophysics, space weather and controlled thermonuclear fusion. He co-authored two books and 170 journal articles on these subjects. He is president of the European Solar Physics Division (EPS & EAS) and chairman of the Leuven Mathematical Modeling and Computational Science Centre. He is also member of ESA's Space Weather Working Team and Solar System Working Group.

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