VSC Echo

Januari 2015
January 2015

Voorwoord

Grote rekencapaciteit is één van de pijlers waarop de vierde industriële revolutie wordt gebouwd. Om haar welvaart te behouden moet Vlaanderen hier volop op inspelen. Daarom hebben de overheid en de universiteiten de voorbije jaren fors geïnvesteerd in de uitbouw van het Vlaams Supercomputercentrum (VSC). In dit virtueel centrum staan de universiteiten en de Herculesstichting samen in voor de exploitatie van het geïntegreerd netwerk van krachtige computers. De ingebruikname begin 2013 van de eerste Vlaamse supercomputer vervolledigde de HPC infrastructuur. Het VSC voorziet ook in de opleiding en de ondersteuning van gebruikers uit de publieke kennisinstellingen en de bedrijven.

Om bedrijven bewust te maken van de mogelijkheden van grote rekencapaciteit en van de diensten die het VSC biedt om efficiënter nieuwe producten of diensten te ontwikkelen of om bestaande te verbeteren, organiseert het VSC op 27 januari 2015 een evenement rond industriële HPC (high performance computing) toepassingen.

Enkele Vlaamse bedrijven zullen aan de hand van voorbeelden het belang van HPC illustreren en buitenlandse HPC centra zullen succesverhalen brengen over de samenwerking met bedrijven. Het VSC zal de Vlaamse aanpak presenteren. Dit evenement is ook een uitstekende gelegenheid om contacten te leggen met Vlaamse onderzoekers actief in HPC toepassingen.

In dit nummer wordt het programma van dit evenement toegelicht en worden de sprekers kort aan u voorgesteld. Zo hebt u reeds een voorproefje van wat die dag u te bieden heeft. Ik hoop u er dan ook persoonlijk te mogen begroeten.

Bart De Moor
Voorzitter Herculesstichting

Foreword

Large computing capacity is one of the cornerstones on which the fourth industrial revolution is being built. To maintain its prosperity, Flanders must fully participate in this development. Therefore, the government and the universities have heavily invested in the development of the Flemish Supercomputer Center (VSC) in recent years. In this virtual centre, the universities and the Hercules Foundation share the responsibility for the operation of the integrated network of powerful computers. The commissioning in early 2013 of the first Flemish supercomputer completed the HPC infrastructure. The VSC also provides training and support for users from the public research institutions and from enterprises.

To make companies aware of the possibilities of large computing capacity and of the services that VSC offers to more efficiently develop new products or services or to improve existing ones, VSC organizes an event focused on industrial HPC (High Performance Computing) applications on 27 January 2015.

Through examples, several Flemish companies will illustrate the importance of HPC. HPC centres from abroad will present success stories about cooperation with industry. VSC will present the Flemish approach. This event is also an excellent opportunity to establish contacts with Flemish researchers active in HPC applications.

In this issue, the programme of this event is presented and the speakers are briefly introduced. This gives you a taste of what the day has to offer. I look forward to welcoming you personally.

Bart De Moor
Chairperson Herculesstichting

Inhoud

Contents

Editor's Column

In naam van het VSC team wens ik alle lezers een gelukkig 2015.

Wij plannen een excellent VSC jaar! We starten met een evenement gericht naar de industrie maar kondigen ook al de volgende gebruikersdag aan. Er is ook volop keuze aan interessante opleidingen. Wij hopen dat jullie ook inspiratie vinden in de getuigenissen van Tier 1 gebruikers om de stap naar supercomputing te maken. Laat mij er nog aan toevoegen dat er gewerkt wordt aan de aankoop van een nieuwe Tier 1 en 2015 kan niet meer stuk.

In name of the VSC team I wish all the VSC Echo readers a happy 2015.

We plan an excellent VSC year! We start with an event focussed on the industry and we already announce the next users day. Our course calendar presents a large choice of interesting courses. We hope that the testimonials of Tier 1 users inspire you to take the step to the use of supercomputing. Let me add that work is being done for the acquisition of a new Tier 1 and 2015 cannot go wrong.

Rosette Vandenbroucke

Vlaams Supercomputer Centrum

Tier 1 nieuws—Tier 1 News

Aanpassingen bij de aanvraag van rekentijd

- Verhoging van de standaard "scratch" schijfopslag tot 1 TB. Extra opslag wordt aangerekend;
- Facturatie voor de kosten van de helft van de toegekende rekentijd bij toekenning van het project;
- Aanpassing van het aanvraagformulier gedeeltelijk op basis van suggesties van de Gebruikerscommissie.

Het volledige reglement, het aanvraagformulier en bijkomende informatie onder meer over de samenstelling van de evaluatiecommissie vindt u op https://vscentrum.be/nl/tier1-rekenen.

Afsluitdata voor Tier 1 rekenaanvragen

Rekenaanvragen kunnen permanent worden ingediend, maar de afsluitdata voor evaluaties in 2015 zijn: 2 februari, 1 juni en 5 oktober.

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HERCULES STICHTING

Adjustments for the application of computing time

- Increase of the standard "scratch" disk space to 1TB. Additional storage is charged;
- Billing for the cost of half of the allocated computing project at acceptance;
- Adaptation of the application form partly on the basis of suggestions from the User Committee.

The complete rules, the application form and additional information including the composition of the evaluation committee can be found on https://vscentrum.be/en/tier1-allocation/overview.

Cut-off dates for Tier 1 computing time applications

Applications may be made on a permanent basis but the closing dates for evaluations in 2015 are: February 2, June 1 and October 5.

Gebruik van de Tier 1 Use of the Tier 1

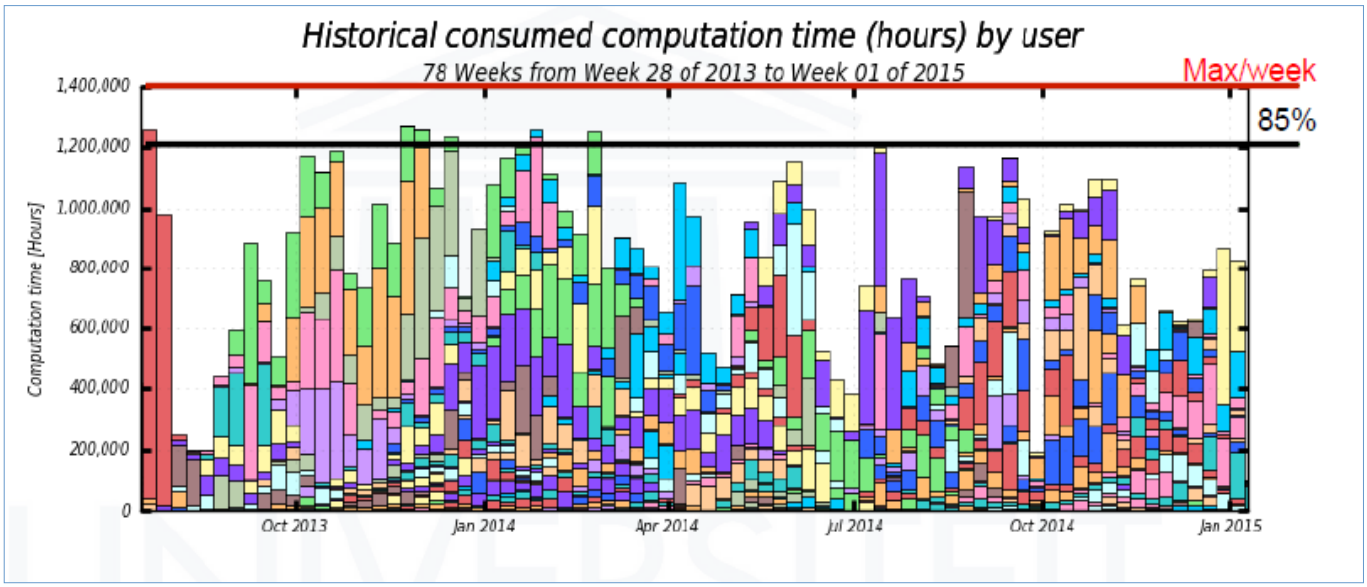


Fig. 1 Historisch overzicht van gebruikte rekentijd op Tier-1 sinds 15 juli 2013.

Approved node days per scientific field

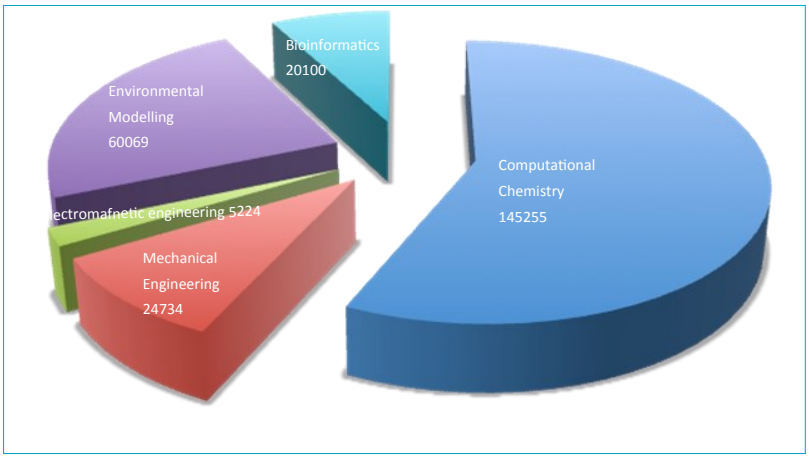


Fig. 2

Toegekende rekentijd per wetenschappelijk domein

Approved computing time per scientific domain

Used node days per scientific field

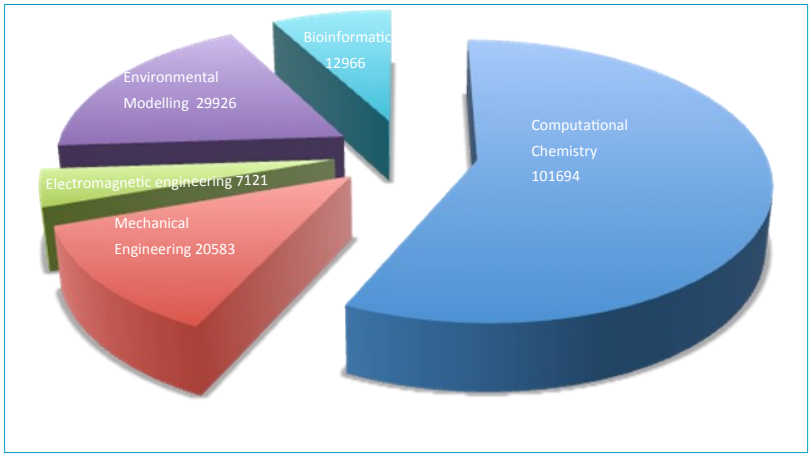


Fig. 3

Gebruikte rekentijd per wetenschappelijk domein

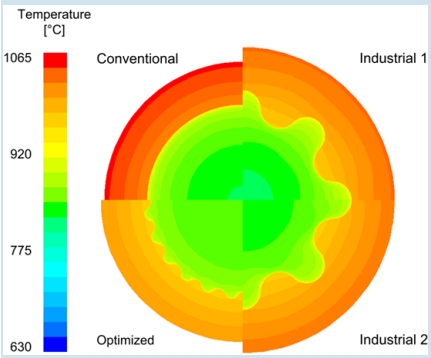
Used computing time per scientific domain

Resultaten van het gebruik van de VSC Tier 1 bij het aangaan van wetenschappelijke uitdagingen

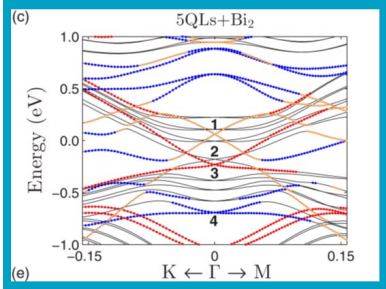
Carl Schietekat is een PhD-fellow bij het Laboratorium voor Chemische Technologie (LCT) aan de Universiteit Gent (promotors: prof. dr. ir. Guy B. Marin, prof. dr. ir. Kevin M. Van Geem). Het onderzoek van het LCT is gericht op het ontwerpen van nieuwe en het optimaliseren van bestaande industriële processen op het gebied van brandstoffen, energiedragers en functionele materialen. Carl's onderzoek richt zich op Computational Fluid Dynamics simulaties van stoomkraak reactoren. Stoomkraken is het belangrijkste commerciële proces om koolwaterstoffen om te zetten naar platform chemicaliën zoals lichte olefinen. Deze platform chemicaliën zijn de bouwstenen voor de meeste polymeren en de startmoleculen voor de productie van vele additieven, oplosmiddelen en andere hoogwaardige chemicaliën.

Een belangrijke factor in de energie-efficiëntie van het stoomkraakproces is de vorming van een koolstofhoudende cokes laag op de binnenwand van de buisvormige reactoren. Carl onderzoekt de toepassing van driedimensionale reactor configuraties om de snelheid van cokesvorming te verlagen. Door de warmteoverdracht te verbeteren, worden lagere temperaturen bekomen in de gas-cokes interface van het proces, en worden zo geringere coking rates verkregen vergeleken met conventionele buisreactoren. Anderzijds leidt de hogere drukval van deze reactoren tot een verlies aan selectiviteit voor het hoofdprodukt van het proces, ethyleen. Omdat experimentele kwantificering van dit selectiviteitsverlies moeilijk is, worden de prestaties van verschillende reactorgeometrieën geëvalueerd met behulp van Computational Fluid Dynamics (CFD) simulaties, zowel voor de gasfase chemie als voor de cokes vorming.

Om rekening te kunnen houden met gedetailleerde chemie in complexe stromingssimulaties zijn extreem lange CPU tijden vereist, maar dankzij parallellisatie op de Tier 1 van het Vlaams Supercomputer Centrum, is het mogelijk om de simulaties tijdig te voltooien. Een studie over gevinde reactorpijpen resulteerde zo in een optimaal ontwerp, genaamd 'SmallFins'. Zoals weergegeven in de figuur, is de metaaltemperatuur in een SmallFins reactor lager dan in een conventionele buis en twee andere industrieel toegepaste ontwerpen, waardoor de laagste coking rating verkregen wordt.

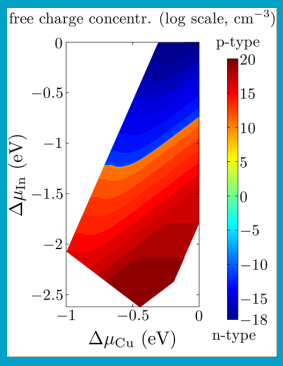


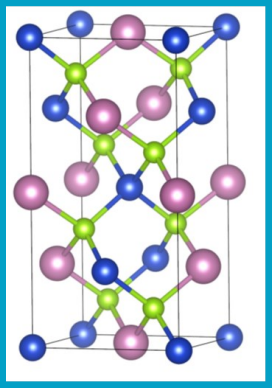
De onderzoeksgroepen Electron Microscopy for Materials Science (EMAT) en de Condensed Matter Theory (CMT) van de Universiteit Antwerpen werken nauw samen voor een aantal projecten met als doel het berekenen van materiaaleigenschappen die rechtstreeks gebaseerd zijn op de elektronische structuur van vaste stoffen.
Veel van deze vaste stoffen zijn veelbelovende innovatieve materialen voor toepassingen zoals fotovoltaïsche energie, fotokatalyse, spintronica, quantum computers, plasma gebaseerde depositietechnieken. Dirk Lamoen en Bart Partoens zeggen dat de komst van de Vlaamse supercomputer hen in staat heeft gesteld om studies uit te voeren die voordien onmogelijk waren.
Hieronder enkele resultaten verkregen door rekenen op de VSC Tier 1.



3500 nodedagen van de Tier 1 waren nodig voor de berekeningen bij het werken op Bi - Sb - Te - Se verbindingen die de bouwstenen bieden voor bekende topologische isolatoren. De figuur links toont de bandstructuur voor een Bi-dubbellaag bovenop een plaat van vijf QLS Bi_2Se_3.

Ander werk richt zich op zonnecel absorbeerlagen waarvoor de ladingsdrager concentratie wordt berekend op basis van de “first principles”.
In de onderstaande figuur links wordt de netto vrije ladingsdrager concentratie getoond voor $CuInSe_2$ (kristalstructuur in onderstaande figuur rechts) bij een temperatuur van T = 300 K als een functie van de chemische potentialen van Cu en In. Positieve waarden vertegenwoordigen een netto concentratie van gaten (p-type) en negatieve waarden een netto concentratie van elektronen (n-type). Het gebruik van hybride functionalen voor supercellen vereist de Tier-1 om de berekeningen uit te voeren, een totaal van 4000 nodedagen was nodig.





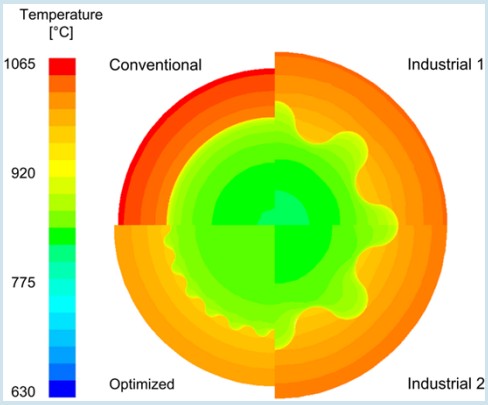
Cu atoms : blue, In atoms :: pink and Se atoms : green.

Results of using the VSC Tier 1 to solve big problems

Carl Schietekat is a PhD fellow at the Laboratory for Chemical Technology (LCT) at Ghent University (promotors: prof. dr. ir. Guy B. Marin, prof. dr. ir. Kevin M. Van Geem). The research at the LCT is focused on the design of new and the optimization of existing industrial processes in the field of transport fuels, energy carriers and functional materials. Carl's research is in the field of Computational Fluid Dynamics simulations of steam cracking reactors. Steam cracking of hydrocarbons is the predominant commercial process for producing many platform chemicals such as light olefins. These platform chemicals are the building blocks for most polymers and the starting molecules for the production of many additives, solvents and other high-value chemicals.

A major factor for the steam cracking process energy efficiency is the formation of a carbonaceous coke layer on the inner wall of the tubular reactors. Therefore the application of three-dimensional reactor configurations to decrease the coking rate is investigated. By means of improved heat transfer, lower temperatures at the process gas-coke interface and thus lower coking rates are obtained compared to conventional tubular reactors. On the downside, the higher pressure drop of these reactors results in a loss of selectivity towards the process main product, i.e. ethylene. As experimental quantification of this selectivity loss is difficult, the performance of different reactor geometries is evaluated using Computational Fluid Dynamics (CFD) simulations accounting for the gas-phase chemistry and coke formation.

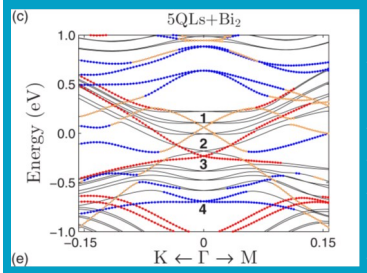
The incorporation of detailed chemistry within complex flow simulations requires extremely long CPU times, but thanks to parallelization on the Tier 1 of the Flemish Supercomputer Center (VSC), it is possible to complete the simulations in a timely manner. A study on finned reactor tubes resulted in an optimal design, denoted 'SmallFins'.



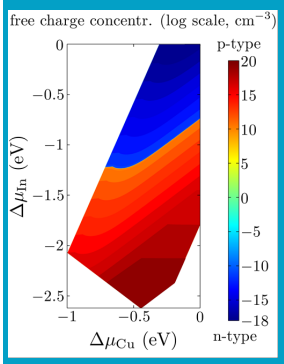
As shown in the figure, the metal temperature in the SmallFins reactor is lower than in the conventional bare tube and two industrially applied designs, resulting in the lowest coking rate.

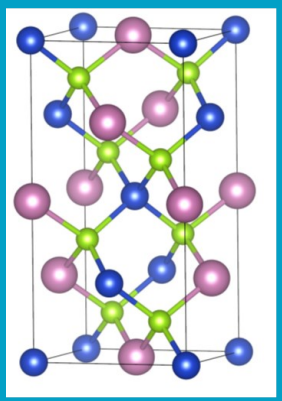
The research groups Electron Microscopy for Materials Science (EMAT) and Condensed Matter Theory (CMT) of University of Antwerp are collaborating closely on a range of projects focusing on the computation of material properties that directly depend on the electronic structure of solid compounds. Many of these compounds are promising innovative materials for applications such as photovoltaics, photocatalysis, spintronics, quantum computers, plasma based deposition techniques. Dirk Lamoen and Bart Partoens acknowledge that the advent of the Flemish supercomputer has enabled them to perform studies that were previously impossible.

Some examples of the research enabled by the Tier 1:
3500 node-days of the Tier 1 were necessary for the calculations when working on Bi – Sb – Te – Se compounds that provide the building blocks for well–known topological insulators. The figure at the left shows the band structure for a Bi -bilayer on top of a slab of five QLs Bi_2Se_3



Other work focuses on solar cell absorber layers for which the charge carrier concentration is calculated from first principles.
In the figure below left the net free charge carrier concentration is shown for $CuInSe_2$ (crystal structure shown in the figure below right) at a temperature of T = 300 K as a function of the chemical potentials of Cu and In. Positive values represent a net concentration of holes (p-type) and negative values a net concentration of electrons (n-type). The use of hybrid functionals for supercells required the Tier-1 facility to perform the calculations, which needed 4000 node-days.





Cu atoms : blue, In atoms : pink and Se atoms : green.

Opleidingen — Courses

VSC organiseert een reeks opleidingen in de eerste helft van 2015. Gedetailleerde en actuele informatie over deze activiteiten is beschikbaar op https://vscentrum.be/en/events/events.
De opleidingen worden in het Engels gegeven en daarom wordt onderstaande informatie niet in het Nederlands vermeld.

The VSC organizes a number of training events for its users in the first half of 2015. Details and up-to-date information on these events is available at: https://vscentrum.be/en/events/events

January 2015

Linux introduction, introductory
January 13, 9h-17h, ICTS opleidingscentrum D, W. de Croylaan 52a, 3001 Heverlee
Python introduction (part I) , introductory
January 20 and 21, 9h-13h, ICTS opleidingscentrum D, W. de Croylaan 52a, 3001 Heverlee
Introduction to HPC @ UGent, introductory
January 30, 10h-17h, multimediazaal of Campus de Sterre (S9), Universiteit Gent

February 2015

HPC introduction, introductory
February 11, 9h-17h, ICTS opleidingscentrum A, W. de Croylaan 52a, 3001 Heverlee
Linux introduction, introductory
February 12, 9h-17h, EuroDemo room, VUB, Triomflaan Toegang 6, 1050 Brussel
Python introduction (part II) , introductory
February 24 and 25, 9h-13h, ICTS opleidingscentrum D, W. de Croylaan 52a, 3001 Heverlee
HPC introduction, introductory
February 19, 9h-17h, EuroDemo room, VUB, Triomflaan Toegang 6, 1050 Brussel
Linux introduction (part I), introductory
February 26, 9.30-12.30, Middelheimlaan 1, 2020 Antwerpen

March 2015

Linux introduction (part II), introductory
March 5 and 12, 9.30-12.30, Middelheimlaan 1, 2020 Antwerpen

April 2015

Node level performance optimization, advanced
April 9 and 10, 9h-17h30, ICTS opleidingscentrum D, W. de Croylaan 52a, 3001 Heverlee
Spring School on Computational Tools for Materials Scientists, specialist workshop
April 13-17, 9h-17h, auditoria A2 and A3 of Campus de Sterre (S9), Universiteit Gent
Introduction to MPI, intermediate
April 22, 9H-17h, multimediazaal of Campus de Sterre (S9), Universiteit Gent
Introduction to R: an open-source statistical toolbox,introductory
April 23-24, 13h-17h, Campus Pleinlaan, Vrije Unversiteit Brussel

May 2015

Migrating old to modern Fortran, specialist workshop
May 20, 9h-17h, ICTS opleidingscentrum D, W. de Croylaan 52a, 3001 Heverlee
Introduction to multithreading and OpenMP, intermediate
May 21-22, 9h-17h, multimediazaal of Campus de Sterre (S9), Universiteit Gent

Events marked as *introductory* do not require prior knowledge, while i*ntermediate* indicates that prerequisites should be checked. The subjects in the *advanced* track are more specialized, and are presented by experts in their field.

Aankondiging Gebruikersdag

Datum : **dinsdag 5 mei 2015**

Plaats: Brussel, The International Auditorium

Voorlopig programma:

- voormiddag: workshops

- namiddag: plenaire sessie met presentaties

- afsluitende netwerkreceptie

Reserveer alvast de datum in je agenda! Meer informatie over het programma volgt.

Announcement Users Day

Date : **Tuesday 5 May 2015**

Place Brussels, The International Auditorium

Tentative programme:

- morning: workshops

- afternoon: plenary session with presentations

- network reception

Block already this date in your agenda! More information will follow.

KU LEUVEN

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Vrije Universiteit Brussel

VSC Vlaams Supercomputer Centrum

Vlaams Supercomputer Centrum

Tuesday 27 januari 2015, Technopolis (Mechelen)

Next-generation supercomputing in Flanders: value creation for your business!

13:00—13:30	**Welcome and registration**	
13.30 - 13.35	Welcome and introduction	Prof. Dr Colin Whitehouse (chair)
13.35 - 13.45	The importance of High Performance Computing for future science, technology and economic growth	Prof. Dr Bart De Moor, Herculesstichting
13.45 - 14.05	The 4 Forces of Change for Supercomputing	Cliff Brereton, Director Hartree Centre (UK)
14.05 - 14.25	The virtual Engineering Centre and its multisector virtual prototyping activities	Dr Gillian Murray, Director UK virtual engineering centre (UK)
14.25 - 14.45	How SMEs can benefit from High-Performance-Computing	Dr Andreas Wierse, SICOS BW GmbH (D)
14:45—15:15	**Coffee break**	
15.15 - 15.35	European landscape – its initiatives towards supporting innovation and its regional perspectives	Serge Bogaerts, HPC & Infrastructure Manager, CENAERO (B), Belgian delegate to the PRACE Council
15.35 - 15.55	Big data and Big Compute for Drug Discovery & Development of the future	Dr Pieter Peeters, Senior Director Computational Biology, Janssen R&D (B)
15.55 - 16.15	HPC key enabler for R&D innovation @ Bayer CropScience	Filip Nollet, Computation Life Science Platform Architect Bayer Cropscience (B)
16.15 - 16.35	How becoming involved in VSC: mechanisms for HPC industrial newcomers	Dr Marc Luwel, Herculesstichting
16.35 - 17.05	Q&A discussion	Panel/chair
17.05 - 17.15	Closing	Philippe Muyters, Flemish Minister of Economics and Innovation
17:15—18:15	**Network reception**	

How to reach Technopolis http://www.technopolis.be/nl/index.php?n=2&e=37

Admission is free but registration is needed before 16 January 2015 via https://vscentrum.be/industry-day-2015

More information about the presentations

Welcome by Prof. Dr. Colin Whitehouse

Prof. Dr. Colin Whitehouse is a current member of the Hercules Science Commission. His personal field of research relates to semiconductor-based nanoscience and nanotechnology, the design and implementation of next-generation semiconductor materials and device structures. This research activity has included the use of HPC modelling to investigate interface formation in semiconductor quantum-well, -wire and –dot device structures, and also the dominant strain-relaxation mechanisms involved in "strained-layer" device structures.

Colin has spent career periods in the semiconductor industry, in senior positions in the UK University sector and also in key UK Government Laboratories. Most recently he was Deputy Chief Executive of STFC, the UK Research Council responsible for the operation of very large-scale international-class science facilities and was also Director of the STFC Daresbury Laboratory in Cheshire,UK where he was very closely involved with the formation of the major new Hartree High Performance Computing Centre, in collaboration with IBM and Intel.

Colin is an elected Fellow of the Royal Academy of Engineering, the Institute of Physics and the Institute of Metals, Mining and Materials. He has published in excess of 300 journal papers and conference presentations, including many invited papers. He was also, until very recently, the Chair of the UK R&D Society which organises high-level policy debates regarding the role of science and technology in innovation and economic growth. In that capacity, he chaired a major discussion event at the Royal Society in London in 2012 relating specifically to HPC, a meeting that involved key UK and international speakers and also the UK Minister for Science and the Universities.

The 4 Forces of Change for Intense-Computing by Cliff Brereton

Cliff Brereton, Director of the UK Hartree Center

Cliff leads the Hartree Centre created to deliver economic impact to UK Industry and commerce, through the use of advanced simulation and modelling in product design and R&D. The use of modelling and simulation in product design, enables better products and services to be developed as well as doing this faster and cheaper, reducing the time to value. The Hartree Centre was opened by the Chancellor of the Exchequer on February 1st 2013 and is a division within the Science and Technology Facilities Council. The Hartree Centre uses High Performance Computing, Big Data Analytics and Visualisation to provide its clients with better product design outcomes. Prior to Cliff commencing his role at the Hartree Centre, he spent 19 years with IBM in a range of sales and management roles, delivering value to IBM clients either through Enterprise or Scientific products or services.

A number of external forces are driving how supercomputing systems will be used and in fact designed in the future. These are: wider Industrial use and engagement, Power, Big-Data and Democratisation.
In his presentation the Director of the Hartree Centre will discuss these 4 forces' and how the Hartree Centre is harnessing these to deliver new value and insights to its customers, in a data driven world.

More information about the presentations

The Virtual Engineering Centre and its multisector virtual prototyping activities by Dr. Gillian Murray

Dr Gillian Murray – Director – Virtual Engineering Centre, University of Liverpool

Dr Gillian Murray has over twenty years' experience working in new product development, business model formulation and the exploitation of science and technology.

Her experience has incorporated roles in both industry and academia, including working at a strategic level in the development of models for industry engagement and the creation of industry-academia partnerships leading to the commercialisation of intellectual property and knowledge transfer.

Instrumental in the formation and development of the Virtual Engineering Centre (VEC) into a leading UK technology innovation centre for engineering development, Gillian's role as Director of the VEC includes the establishment of a new model for business and R&D collaboration between SMEs, large corporates and academia. Working within sectors such as Aerospace, Automotive, Energy and FMCG, the VEC innovation 'sandpit' engagement model, brings together business and academia working on industry challenges and has developed a strong profile and interest for adoption at both regionally and nationally level.

The presentation will demonstrate the VEC's unique model of engagement and collaboration with industry with an emphasis on the strategy employed for developing a unique ecosystem of innovative SMEs. Gillian will highlight how this methodology supports the widely accepted theme of the need for a collaborative and multi-disciplinary approach to address some of industry's key challenges.

How SMEs can benefit from High Performance Computing by Dr. Andreas Wierse

Dr. Andreas Wierse—SICOS BW Gmbh

Andreas Wierse obtained degrees at the universities of Bonn and Stuttgart specialising in the visualisation of numerical simulations. After spending eight years at the University of Stuttgart for the development of virtualisation software he started the spin-off company VirCinity GmbH for the commercial development of the COVISE software for the visualisation of numerical simulation results, initially developed at the University of Stuttgart. This spin-off evolved to Visenso GmbH managed by Dr. Wierse till the end of 2011. In 2011 and 2014 respectively he became managing director of SICOS BW GmbH and HWW GmbH, two companies that offer consultancy services including consultancy about high performance computing.

The presentation will explain how HLRS Stuttgart and SCC at the Karlsruhe Institute for Technology address small and medium sized enterprises (SME) in order to support them in the uptake of high performance computing and large scale data technology. SICOS BW has been founded with the support of the Ministry for Science, Research and Art in Baden-Württemberg. Its focus is on one side the support of these SMEs, on the other side it helps the computing centres to organize their offer and their structure to be able to handle industrial users as well as their research users. Different aspects of these activities will be presented and discussed.

European Landscape—its initiatives towards supporting innovation and its regional perspectives by Serge Bogaerts

Serge Bogaerts graduated in 1992 as Mechanical and Electrical Engineer at the Free University of Brussels (ULB). Researcher in numerical fluid mechanics at the von Karman Institute, then study engineer in nuclear safety at Tractebel Engineering and, in 2003, researcher in CFD-Multiphysics at Cenaero, Serge knows the challenges of numerical simulation. Manager of the operations of Cenaero supercomputers since 2006, he has a confirmed experience in leading projects of procurement and operation of HPC infrastructures. Since October 2012, he has been appointed Belgian Delegate to the PRACE Council.

The key role of Computational Science in supporting innovation has been recognized worldwide for years and the implementation of persistent High Performance Computing (HPC) infrastructure is considered strategic for many countries. PRACE, Partnership for Advanced Computing in Europe, is the framework providing such an infrastructure to European researchers. Targeting the support of scientific excellence, through high standard peer review process, the organization is also devoting efforts and resources to the support of European competitiveness through the development of programs targeting industrial research. This relatively recent trend is aligned with the need to further develop the competitiveness of European industry. On the same line, a number of initiatives aim at enlarging the range of companies that benefit from HPC trying to decline the success of the early adopters, mostly large manufacturing or oil & gas companies, towards small and medium sized enterprises (SME) with high potential for innovation. We will give an overview of the corresponding landscape and sketch some perspectives at a regional level.

HPC key enabler for R&D innovation at Bayer CropScience by Filip Nollet

Filip Nollet—Computational Life Science Platform Architect Bayer CropScience

CLS platform architect for Bayer CropScience CLS (2009-today)
System engineer for University College Ghent (2003-2009)
Bachelor Degree Multimedia and Communication Technology (PIH, Kortrijk, 2002)

In 2010, Bayer CropScience introduced ‘High Performance Computing’ into its Seeds & Traits Research and Development department. This new model of computation was built to cope with different types of challenges: the exponential growth of data; a new analysis platform; higher throughput; and the increasing shift from wet to dry lab research. Centralizing the bioinformatics tools and generated data, allowed both the wet lab scientists and the bioinformatics experts to reduce drastically time spent on regular or complicated types of analysis. Today, complex pipelines can run and finalize in a highly reduced timeframe, thereby speeding up our decision making processes.

Vlaams Supercomputer Centrum

More information about the presentations

Big data and Big Compute for Drug Discovery & Development of the future by Dr. Pieter Peeters

Pieter J. Peeters, PhD
Senior Director Computational Biology, Discovery Sciences
Janssen Research & Development

Pieter Peeters is heading the European computational biology team in Discovery Sciences at Janssen Research & Development. His group is aiding the drug discovery and development teams in Janssen R&D in their search for novel safe and effective drugs by applying both computational as well as wet lab 'omics approaches, including chemogenomics, functional genomics and chemical genomics.
He joined Johnson & Johnson in 1999 working on enteric nervous system diseases.
Pieter obtained his Ph.D. in Applied Biological Sciences (medical molecular biology) at the Center for Human Genetics from the Catholic University Leuven, Belgium and graduated as a bioengineer (gene and cell technology and interface chemistry) at the same university.
Currently, he is the Janssen lead for the ExaScience life lab, a collaborative effort between Intel, IMEC and Janssen with the aim of expediting R&D in healthcare by applying high performance computing approaches. In addition he is the Janssen lead for the Innovative Medicine Initiative project on the application of inducible pluripotent stem cells in drug discovery and drug safety testing (StemBANCC).

The life science industries can only envy the predictive prowess of the physical sciences that is embodied in computer assisted engineering. Nevertheless, pharmaceutical industries including Janssen and regulatory authorities show a renewed interest in co-opting computational simulation, often referred to as Quantitative Systems Pharmacology, for the evaluation of benefits and risks of therapeutic approaches. It still remains a bottleneck that the characteristics of biological components are far less well understood than those of their mechanical counterparts. Theoretical derivation of these is still solidly beyond our reach. However, advances in miniaturization and parallelization of an expanding arsenal of biological readout technologies are beginning to enable the acquisition of sufficient data to learn, generalize and emulate the behavior of biological subsystems. Scaled up Machine Learning approaches are proving instrumental in this endeavor, and are deployed in Janssen to learn and predict the biochemical impact of compounds based on their chemical structure or phenotypic effects, or the sensitivities to compounds dictated by a given genetic makeup.

The explosion of primary data processing needs for high volume data sources like massively parallel sequencing and high content imaging, and the leap in scale of Machine Learning approaches and Quantitative Systems Pharmacology translate to increased needs in computational performance. To rise these challenges, Intel and the micro and nanoelectronics research center IMEC, have teamed up with Janssen and the five universities in Flanders, Belgium to found the ExaScience Life Lab, which states the creation of novel supercomputer solutions for applied life sciences as its mission. In addition we recently acquired access to the Flemish Supercomputer Infrastructure to enable computational biology and chemistry.

Industrial users of the VSC Tier 1

HPC at Janssen Pharmaceutica

Jörg Wegner, Senior Scientist at Janssen Pharmaceutica

The Research&Discovery (R&D) organization of Janssen Pharmaceutica NV is facing the same exponential data growth as all other scientific and business operations in a global competitive environment. As an example it is easy to count duplicated rows in an Excel file of 10000 lines, but duplication removal in files with a 100 million entries becomes a much more challenging question. Of course, within R&D much more complex tasks are required. Because of this large-scale, computing becomes critical since most computation tasks do not scale linearly but quadratically, cubic, or even exponential with the growing amount of data. Thus, a doubling in the amount of data does not increase the computational requirements by a factor of two, but by a factor of 4 (quadratic), 9 (cubic), >>10 (exponential). Finally, this will require a careful analysis and change in the way the data is processed by using the expertise of large-scale computing experts.

Three examples that are done in collaboration with multiple partners like the VSC (Flemish Supercomputer Centre), IMEC (Interuniversity Microelectronics Centre), Intel and multiple academic partners are large-scale next generation sequencing (NGS) analysis, high-content imaging (HCI) analysis, and large-scale machine learning (ML).

The progress in sequencing is producing TB amounts of NGS and high-content screening (HCS) data. Both of them will help Janssen to understand biological details of patients and complex biological phenotypic systems much better than single enzymatic (and somewhat artificial biological) systems. For being able to judge the relevance and impact of such data sets for R&D, novel large-scale machine learning approaches can be utilized for understanding and supporting novel experimental designs and especially their risk estimations.

We might wonder why this is relevant? A simple example is the attrition rate of drugs in the clinic Phase II, which everyone in the Pharma industry is facing.

The HPC efforts with the VSC are aiming at reducing the risks of progressing lead compounds to drugs and patient/disease disease sequencing data by understanding and analysing such large data sets. Janssen is aiming at reducing the failure rate in the clinic II by utilizing large-scale computations on the data being available and produced by Janssen and all of its collaboration partners, who also might not have the compute or analytics capacity on their own to do this strategically. Finally, of course, besides of reducing the risk of existing drug pipelines Janssen is also aiming at unraveling new paths for unmet medical needs of patients for whom no treatment options might exist at this point in time.

Jörg Wegner

Industrial users of the VSC Tier 1

HPC at 3E

Rory Donnelly, Programme Manager Wind Simulations at 3E

3E NV is a Belgian renewable energy consultancy firm, delivering advisory services and software solutions for sustainable energy project developments and operations worldwide. Several (research) projects are ongoing in which supercomputing plays an indispensable role. One prominent example concerns 3E's wind energy branch.

Rory Donnelly, Programme Manager Wind Simulations at 3E, says:

"3E utilize the meso-scale Weather Research and Forecasting (WRF) modeling software to simulate atmospheric conditions over areas such as the Belgian onshore and offshore region for a period of several decades. These simulations yield a representation of the long-term wind resource, which we can use in power generation predictions for the benefit of wind park development studies. By assessing the risk profile and viability of wind farms in this way, developers and owners can increase performance and returns on their projects, and can attract and inform investors."

"Over the last few years, 3E has been able to rely on the (human) resources of the Flemish Supercomputer Center (VSC). This has allowed us to streamline our procedure and deliver mesoscale assessments in a cost-effective way, both in terms of FTEs and computer time. Access to the vast and reliable HPC infrastructure of the VSC – first at Ghent University, then on Flanders' own Tier1 supercomputer – has been an absolute advantage and has helped us considerably to make a difference in a competitive market. The availability and the expertise of the dedicated helpdesk has also been a great asset."