Newsletter Issue No. 6
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Welcome

Prof. Peter V Coveney
Principal Investigator & Comp-BioMed Coordinator

I would like to wish all our readers a very happy and successful 2019 and welcome you to the first Newsletter of the year. We are excited to be able to announce the CompBioMed Conference that will take place later this year, 2019, in London (see article below and on the back page). We plan to make this conference a bi-annual event in which we attract people from all over the world to discuss and share the work that we are doing and hear about work of other groups and projects that align with our own. This will broaden our partnership and set us on the path for even greater collaborations.

We are also pleased to be able to describe the work of LifeTec Group, an SME in the Nertherlands and partner in CompBioMed that is looking into numerical models for planning surgical procedures. They are making important steps to allow personalised medicine to be used in the clinic.

In November we ran our Birds of a Feather session at SC18 in Dallas. This was a great opportunity to meet with like-minded people to discuss the latest research. As part of CompBioMed Visitor Programme UCL has welcomed visitor with funding through the HPC-Europa3 Transnational Access Scheme. Maryam Lotfi has been working on binding affinity calculations in collaboration with EPCC, using time on the ARCHER supercomputer. UCL has also been awarded 25,000 Summit node hours, as part of the INSPIRE DOE INCITE project. More details can be found in the article on page 2.

We are also attracting further Associate Partners, and are pleased to introduce AstraZeneca, Université Libre de Bruxelles and the IT'IS foundation. We are always interested in working with new institutions, and therefore welcome anyone who is interested to join as an Associate Member to contact us.

In addition to our Conference, we also have other training events and meetings planned. We will again be at the BSC Winter School, presenting a training session on HPC-based computational biomedicine. CompBioMed research is working with ever greater frequency with containers as we investigate cloud computing along with HPC. We are therefore organising a workshop at SURFsara to give more detail on containers and how to use them. Finally we are planning our AHM at the end of April in the beautiful city of Oxford.

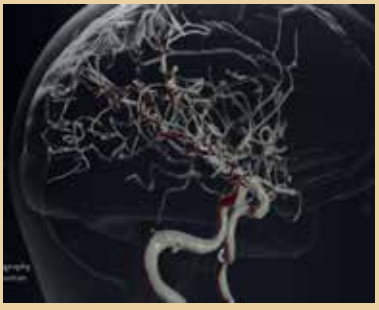
CompBioMed Conference

The conference will address all aspects of the rapidly burgeoning domain of computational biomedicine, from genomics through various organ systems to whole human and population levels, embracing data driven techniques, mechanistic modelling and simulation, machine learning or combinations thereof. We welcome contributions from academic, clinical and industrial participants alike.

Following review by the organising committee, selected papers will be invited for submission to a theme issue of the *Journal of the Royal Society Interface Focus*, due for publication in March 2020.

The conference will take place on 25-27 September 2019 at the Institute of Engineering and Technology (IET) London: Savoy Place. The CompBioMed Conference 2019 will combine a venue with innovative catering and spectacular views of the River Thames with an exciting programme of relevant symposia and world-renowned plenary and invited speakers, proposed and secured by our International Organising Committee. Confirmed plenary speakers:

- *Andrew Hopkins*
- *William J. Lorgensen*
- *Amanda Randles*
- *Anne M. Robertson*
- *Oliver Röhrle*



More information can be found on page 4 (back page)

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News and Events Highlights

Summit Award for UCL

The Centre for Computational Science has been awarded an allocation of 25,000 Summit node hours through 31 July 2019. This is the equivalent to about 15 million core hours on Titan, the former number one in the Top 500 list of supercomputers, which we have been working on for over a year. The access is given inter alia to extend the INSPIRE DOE INCITE project, which is designed to help determine drugs to administer to cancer patients whose target proteins have developed resistance to the first level drugs they have been treated with.

Summit is the current number one in the Top 500 list of supercomputers, and operates at a peak of ca 200 pflops. Meanwhile, the UK flagship supercomputer, ARCHER, has a peak performance of 2.55 pflops.

EU Centre of Excellence CompBioMed2 funding is focused on the transition to the exascale, and Summit brings us substantially closer at 200 pflops. This is over 170 flops faster than any previous machine we have worked on.

On the path to the exascale, much work remains to be done to ensure we can extract maximum performance from this new generation of computers.

With this and other work, the CCS plans to be active in co-design of codes and workflows with US-based Argonne National Laboratory (ANL) / Department of Energy (DoE) in the race to the exascale. ANL expects to have their own Intel machine, Aurora, in production at some stage in 2021.

Birds of a Feather at SC18

Peter Coveney, along with Hugo Falter of ParTec, Mariano Vazquez of BSC-CNS, and Cristin Merritt of Alces Flight held a Birds of a Feather in Personalised Medicine at SC18 in Dallas, TX. With an audience attendee group hailing from around the world we discussed the latest research, highlighted resources, and the heard about the newest spin-off from BSC-CNS: ELEM Biotech.

Peter led the proceedings on the latest research coming from the Centre of Excellence, with a focus on the significant growing levels of projects and collaborations in play. Leading on from Peter, Hugo discussed European HPC that can now begin to enable the medical field at nearly all levels – from research to clinical settings. Mariano described the aspirations of the biotechnical possibilities with HPC resources and their aims for progressing the idea of a Virtual Human through replications and modelling of human physiology with ELEM Biotech. Cristin then took the stage to discuss what pathways were emerging with cloud HPC technology, focusing on the use of containers as a potential outreach point for collaboration and mass data collection.

After the presentations the group held an informal discussion concerning the aspirations for this field in the coming years. This discussion continued after the event, opening up further liaisons with the USA by the CompBioMed Team and allowing us to reach out to the international community expanding our insights for the future.

CompBioMed Visitor Programme

Maryam Lotfi has joined Peter Coveney at UCL over the last 3 months as part of the CompBioMed Visitor Programme, funded by the HPC-Europa3 scheme, operated within UK by EPCC (Edinburgh). She has been working on a research project looking at the rapid, accurate and reliable calculation of binding free energies of diverse sets of protein targets and ligands using two fast computational approaches called ESMACS and TIES which have been developed in this group. The accurate prediction of binding affinities of ligand to protein is a principal objective of drug discovery and personalized medicine.

Coming from Iran, Maryam had little previous experience with high performance computing for solving advanced problems and performing research activities through computer modeling, simulation and analysis in drug discovery, however, shortly after her arrival at UCL, she visited Edinburgh and attended an introductory course on HPC at EPCC.

As part of her Transnational Access from HPC Europa3, she was awarded 100,000 core hours on ARCHER. Having used this she was then able to use the same amount again through additional allocations availalbe to the CompBioMed Centre of Excellence. The work has been so successful that she is already working on a publication from the research.

Commenting on her stay at UCL, she commented that " working at UCL was a very positive experience for me and I learned a vast amount from being embedded at the Centre for Computational Science." In addition, this is her first time to the UK, and she has enjoyed exploring London and the rest of the UK during her short stay.

Université Libre de Bruxelles

The Laboratory of Experimental Medicine (LME) at Université Libre de Bruxelles (ULB) handles all biological tests suitable for (pre)-clinical practice and has long experience in fundamental medical research. They produce recombinant myeloperoxidase, monoclonal antibody: material instrumental for the study of atherosclerosis (test bench for arteries, device for fibrinolysis).

Karim Zouaoui Boudjeltia, Karim.Zouaoui.Boudjeltia@ulb.ac.be, is the Director of the LME.

AngioSupport - Numerical Simulations in the assessment of Coronary Artery Disease

Tim Van Den Boom, MSc
R&D Engineer, LifeTec Group
Bettine Van Willigen, MSc
R&D Engineer, LifeTec Group
Dr Marco Stijnen,
Head of MedTech Innovation, LifeTec Group

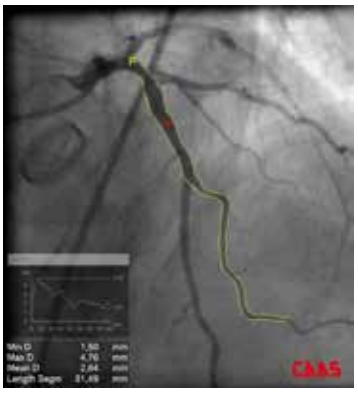
The cardiac team at the Catharina Hospital Eindhoven have a meeting every day to assess the severity of coronary artery disease from approximately 15 patients based on their coronary angiogram and Fractional Flow Reserve (FFR). The FFR is the ratio between the pressure distal (P_d) to the stenosis and the aortic pressure (P_a) ($FFR=P_d/P_a$). As a rule of thumb, an FFR < 0.8 is assumed to lead to ischemia in the myocardial tissue downstream of the stenosis and an intervention should then be performed. The cardiac team decides on a treatment plan for these patients which may consist of Percutaneous Coronary Intervention (PCI) or Coronary Artery Bypass Graft (CABG). For patients with multiple stenoses, a complex coronary geometry or diffuse coronary artery disease, it is hard to predict the outcome of the different treatments. Therefore, defining a treatment plan for these patients is challenging.

This is a typical example of where computer simulations may assist clinicians in their daily work, and in this particular case it was the origin of a collaboration between the cardiac team and LifeTec Group. Within the scope of CompBioMed, LifeTec is developing an interactive tool - called AngioSupport - to support coronary interventions by predicting the FFR after the intervention (post-FFR).

AngioSupport is a toolchain comprising of a segmentation tool and a 1D wave propagation model. The patient geometry is captured from a bi-planar angiogram by segmentation (Coronary Angiographic Analysis Systems, Pie Medical Imaging). An existing 1D wave propagation model of the human vascular system was simplified and extended with the coronary system, as developed at the Eindhoven University of Technology. To simulate the pressure and flow propagation, by feeding the model with patient specific clinical measures such as patient length, weight, heart rate and aortic blood pressure, the pre-op FFR is calculated throughout the patients system. Subsequently the clinician can select standard stent sizes and deploy them in the area they deem affected by disease. Alternatively, they can simulate the CABG option by selecting the location of the anastomosis on the coronary tree.

In practice, the clinician will only have to load the coronary angiogram and, subsequently, perform multiple interventions. The post-FFR is computed in real-time and can be compared between the different interventions. This allows AngioSupport to be used during the cardiac team meetings, where patient treatment plans are determined in a short time span. By allowing clinicians access to the numerical models through the straight-forward AngioSupport user interface, clinicians will have an extra tool to support this difficult but vital decision.

Besides coronary applications, the individual tools are also valuable in other areas. 1D models are also employed in hemodynamic simulations of the vasculature in the brain, as part of CompBioMed research at the Sheffield University, where they are developing OpenBF. This shows the flexibility of 1D modelling for describing complex vasculatures. Moreover, 1D models of the whole human vascular system can serve to provide essential boundary conditions for localized 3D simulations of hemodynamics in and around cardiac or vascular devices. The challenge for CompBioMed to bring simulation support to the community is on!



CompBioMed Welcomes New Associate Partners

AstraZeneca

AstraZeneca is a global, innovation-driven biopharmaceutical business that focuses on the discovery, development and commercialisation of prescription medicines, primarily for the treatment of cardiovascular, metabolic, respiratory, inflammation, autoimmune, oncology, infection and neuroscience diseases. AstraZeneca operates in over 100 countries. The innovative portfolio of medicines of AstraZeneca are used by millions of patients worldwide.

Ola Engkvist, Ola.Engkvist@astrazeneca.com, is Team Leader/Associate Director working in Cheminformatics, Machine Learning, Bioinformatics and Data Mining and is the contact point for CompBioMed activities.

IT'IS Foundation

The Foundation for Research on Information Technologies in Society (IT'IS) is an independent, non-profit research foundation dedicated to improving and advancing the quality of people's lives by enhancing the safety and quality of emerging electromagnetic technologies. IT'IS have currently signed an NDA with the Centre for Computational Science at UCL and they are now working on their first virtual human simulation. There is more information about the Mission of the Foundation and in particular about their research initiative IT'IS for Health on the website https://itis.swiss/itis-for-health/. Dr Esra Neufeld, neufeld@itis.swiss, is the project leader for computational life sciences.

Upcoming Events

CompBioMed Training: Winter School, 2019,

BSC, Barcelona
13-15 February 2019

Short course on HPC-based Computational Biomedicine.

The objective of this course is to give a panorama on the use of HPC-based computational mechanics in Engineering and Environment through the projects BSC is carrying out. The programme will include the basics of what is behind the main tools: computational mechanics and parallelization. A number of travel grants will be offered to participants to assist them with their travelling expenses. More information can be found: https://bit.ly/2RPIKAt

Container Technology for HPC and Cloud Computing,

SURFsara, Amsterdam,
28-29 March 2019

In this meeting we will gather computational services developers together with users from academia, industry and healthcare sectors to discuss the most recent advances in container technology, cybersecurity and related services. We will focus on the use of these technologies in computational modelling and their integration within HPC and cloud computing infrastructures, data mangement and security. The meeting will involve presentations of diverse applications and services arising in academic, industrial and clinical contexts. To register and for more information visit: https://bit.ly/2Db7gUq

CompBioMed All-Hands Meeting,

University of Oxford, UK
29 Apr - 1 May 2019

Our All-Hands Meeting for 2019 will take place at University of Oxford. We will be inviting Core and Associate Partners and drawing up plans for the final months of our current project.
We are looking forward to updating our partners on the work that we have been doing and the progress that we are making towards our goals. We also will hold our 3rd Innovation Advisory Board meeting at this time, discussing the future of CompBioMed as we work towards the start of CompBioMed2

CompBioMed Conference 2019

For the conference we have brought together people from within our Core and Associate Partners and beyond to make up an impressive International Organising Committee (https://www.compbiomed-conference.org/international-organising-committee/). The Committee is comprised of many distinguished researchers in their fields of study, who will help to attract the highest calibre of invited speakers and make our conference truly exciting.

We are planning fifteen symposia under 3 general themes:

- **Biomedical Applications (including)**
  - Organs
  - Molecular Medicine
- **Methodology (including)**
  - Uncertainty Quantification
  - Multiscale Modelling
- **Technology & Outreach (including)**
  - Education, Training & Public Awareness
  - Regulatory Science and *in silcio* Clinical Trials

More information on these symposia can be found at https://www.compbiomed-conference.org/symposia/.

Early Bird registration is now open: https://www.compbiomed-conference.org/registration/.

Call for papers: deadline for abstract submission is 15th May 2019, template and more information: https://www.compbiomed-conference.org/call-for-papers/

Find CompBioMed online

Our website (www.compbiomed.eu) is full of all the latest news and information about CompBioMed, including further information on our Partners and Associate Partners, past and future events. We have an active and growing following on Twitter (@bio_comp), a user-forum on LinkedIn (CompBioMed) and we have our own YouTube channel (Computational Biomedicine), where you can watch live streaming of events and presentations at previous events and webinars, as well as our Virtual Humans film.

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