CompBioMed

Newsletter Issue No. 1
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# Welcome

Prof. Peter V Coveney
*Principal Investigator & CompBioMed Coordinator*

It is my pleasure to welcome you to CompBioMed's first Newsletter. Its publication after the first six months of the Centre's existence provides the opportunity to look back at what has been accomplished so far as well as where we are heading to in the next six months and beyond.

The initial period of our existence has been a very busy and exciting one. Our kick-off meeting at the University of London in early October attracted over 60 participants and we have been on the go ever since. Aside from a very good mix of academic, industrial, and clinical partners, we have grown from the start an equally diverse set of Associate Partners, who now outnumber the original ones. Indeed, we continue to enjoy expansion in this respect, and our Associate Partners are fully engaged in both exploiting our capabilities as well as adding to them.

Our presence is visible in many areas already, by dint of our leadership in numerous domains and our participation in a large number of diverse activities. Among these, I might mention that in our biomedical research we are making use of a large number of European supercomputers, from within the CompBioMed partnership and beyond, while deploying our most demanding, compute and data intensive applications — for blood flow, cardiac modelling, drug discovery and targeting — on some of the largest machines available in the pre-exascale era.

We actively participate in collaborations with other H2020 funded Centres of Excellence, perhaps most closely with (www.bioexcel.eu). We have participated in and organised a number of meetings, the latest of which is a jointly organised conference with Bioexcel on Free Energy Calculations from Molecular Simulation: Applications in Life and Medical Sciences at UCL on 31st May 2017 (preceded by closed informal scientific and technical discussions on 30th May). A recent meeting, convened to discuss the convergence of cloud and high performance computing technologies, attracted around 80 participants. The culmination of our public activities will be an evening on the Virtual Human, to be held at the IMAX theatre in the London Science Museum on 27th September 2017, for which publicity will soon be getting underway.

I hope you will enjoy reading this Newsletter and I encourage you to get in touch with us about topics of interest and your possible active participation in our Centre of Excellence.

# Recent Events

The **European HPC Summit Week 2017 in Barcelona Supercomputing Centre (15th – 18th May 2017)** began with the EXDCI workshop and an engaging series of presentations on the Petascale to Exascale transition, exploring both the nature of the transition and what is required to achieve Exascale performance. Important considerations included how to deal with data, where to compute/store/analyse and how to generate future talent. These are exciting times and we are looking forward to contributing the experiences and insights from our academic, industrial and clinical partners in CompBioMed to see the Exascale transition successfully achieved.

Attendees gathering at the European HPC Summit week 2017

CompBioMed was allocated a dedicated session on 16th May, where we held talks and workshops focused on our Centre of Excellence. The event was held under the motto "HPC for Innovation: When Science meets Industry", which brought together experts from academia and industry, who presented their recent advances in HPC-supported science and engineering. Giovanni Erbacci (Cineca Supercomputing Centre) demonstrated advances in brain research in his talk about developments in the Human Brain Project, while Hector Martinez-Navarro (Oxford University) presented HPC simulations of the human heart for arrhythmia risk stratification. The session concluded with our plans for innovations in training, led by Andrea Townsend-Nicholson (UCL), with topics on opportunities and challenges faced in computational biomedicine, such as achieving gender balance, diversity and innovation and sustainability.

# Milestones

Our latest achievements are all publicly available and include:

- Publication of 10 papers since our project started, with an 11th accepted for publication last week
- Publication of an exciting and innovative training programme (D3.3) and Innovation Activities (D4.1)
- An informative website that provides information and resources about all aspects of our project (D3.1), including our management (D1.1-D1.3) and outreach activities (D3.2)
- The public availability of our community software repository on the CompBioMed website (D5.1)

# General Assembly News

The All-Hands Meeting (AHM) in Barcelona this April marked the General Assembly's second meeting. The members of the Innovation Advisory Board were agreed upon, alongside the date of its initial meeting, which will coincide with the Free-Energy Workshop in London (30th May), where many of the initial 10 members will attend. With our 9-month review coming up in July, we took the opportunity to ensure that we are up to date with our Key Performance Indicators, among other items. There was a discussion around the possibility of our participation in the 2018 Centre of Excellence call. Finally, we discussed the location of our next AHM, which has now been set for Amsterdam in March 2018.

CompBioMed researchers chewing the fat at the AHM dinner

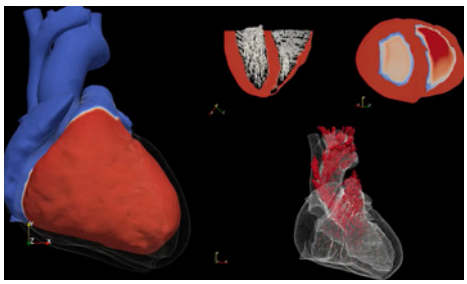
Peter Coveney's research group, Andrea Townsend-Nicholson and host Mariano Vázquez

# Towards The Computational Human: HPC-based Simulations For The Cardiovascular System


## Dr Mariano Vázquez

*Applications Manager & Leader of Work Package on Biomedical Research Activities for CompBioMed*


Computational scientists, physiologists and medical doctors are working together towards the aim of building a computational human thanks to supercomputers. A virtual "doppelganger" will allow us to better understand how the human body works. Among the goals are improving diagnosis, treatment and prevention of diseases; optimizing medical devices of all kinds and studying drug delivery and action. Within CompBioMed, Barcelona Supercomputing Centre (BSC) and the University of Oxford we focus on the heart.



From a physicist's point of view, a heart is a fully coupled, massively complex system. An electrical activation impulse rapidly propagates through the cardiac muscle, in a rhythmic and coordinated way. This electrical wave drives the muscular contraction which, acting upon the blood, produces the heart's pumping action. A clever disposition of tendons, muscular fibres and valves harmonically regulate inflow and outflow of blood, filling and emptying ventricles and atria. In CompBioMed and based on BSC's simulation software Alya, we are developing the most comprehensive cardiac computational model. The sheer complexity of the problem has several origins. First, such a tightly coupled multiphysics system needs novel algorithms, both accurate and robust. The computational requirements of such a problem are vast, not only in terms of hardware (i.e. massively parallel computers are required) but also in terms of software (i.e. a highly efficiently implemented code to exploit that computational power). Next, the proposed physiological models are difficult to implement and validate, given experimental evidence is both relatively scarce and indirect. Finally, as Nature is not an engineer's product, we have no access to Nature's masterplan that would precisely describe the basis for our simulation, so we must set up the simulation scenarios relying on a combination of medical mages, medical intuition and numerous simplifications.

To pursue such objectives, the University of Oxford and BSC are working together in a highly complementary way. Oxford has expertise in the use of cardiac simulations to address concrete clinical problems, particularly on the electrophysioligical side. Additionally, its scientists have a strong background in image processing to prepare the simulation scenarios. On the other hand, BSC's computational scientists are experts in programming parallel codes to simulate multiphysics. BSC's main code is Alya, which is capable of simulating the full fluid-electro-mechanical cardiac problem on high-end supercomputers. Together, Oxford and BSC are running complex cardiac simulations targeting diseases such as hypertrophic cardiomyopathy, strokes or arrhythmias.


Further reading/references: Coupled electromechanical model of the heart: parallel finite element formulation. P. Lafortune, R. Arís, M. Vázquez and G. Houzeaux. International journal for numerical methods in biomedical engineering, 28, 1. 2012.


## Aix-Marseille University

The Laboratory of Mechanics, Modelling and Clean Processes (M2P2) at the University of Aix Marseilles works in the fields of Digital Fluid Mechanics and Process Engineering. This research is associated with the methodological development of high performance codes for blood flow. The contact for M2P2 is Julien Favier (julien.favier@univ-amu.fr).

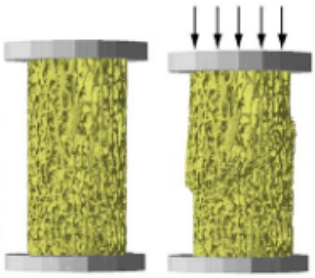
## Universidad Católica de Murcia

The Structural Bioinformatics and High Performance Computing Research Group (BIO-HPC) is based at the Catholic University of Murcia (UCAM, South East Spain). They work in the exploitation of High Performance Computing Architectures (Supercomputers, GPUs) for the development, acceleration and application of bioinformatics applications. The principal point of contact is Dr Horacio Sanchez (hperez@ucam.edu).

# Bone DVC Service And Pulse Wave Analysis For Cerebral Vasospasm Detection

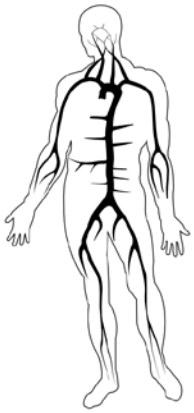

## Dr Alessandro Melis

*Research Associate at INSIGNEO, Institute for in silico medicine, University of Sheffield*

The measurement of strains induced by loading on bone micro-structure is of fundamental importance in musculoskeletal research. However, the accurate direct quantification of bone tissue displacement is an open challenge. The Digital Volume Correlation (DVC) method consists in imaging a specimen of bone tissue under compression while inside a microCT system. Two stacks of images are acquired: one in rest configuration without any load applied, and the second in loading configuration. The BoneDVC is a computational workflow aimed at the analysis of these microCT images. The workflow compares the two datasets and employs an elastic registration algorithm to compute the linear displacement field mapping the loaded volume to the reference one. Finally, by means of differentiation, the computed displacement field is used to calculate the strains in the compressed specimen. The BoneDVC implementation is known to be more accurate than any commercially available alternative, and it is now being made available through CompBioMed to the research community. Two papers describing the BoneDVC service and its deployment on HPC facilities are in preparation [1,2]. The poster "3D full field strain distribution in the mouse tibia under loading measured by digital volume correlation" by Dr M. Giorgi won the first prize in the poster competition at the latest Insigneo Showcase (Sheffield, UK).

A branch of cardiovascular research is focused on the development of 1D models of pulse wave propagation. These models accurately predict the transmission and reflection of waveforms in the arterial tree. The waveform shape depends on the network's mechanical properties, and the study of waveform features is a rich source of information for diagnostic purposes. A drawback of these models resides in the large number of parameters to be set in patient-specific scenarios. The 1D model developed at University of Sheffield includes all the main large systemic arteries and has been used in combination with statistical emulation methods to perform a computationally efficient dimensionality reduction through sensitivity analysis. The same computational workflow was also applied to a condition of brain circulation, known as the cerebral vasospasm. This is the progressive narrowing of intracranial arteries due to the rupture of an aneurysm and ensuing haemorrhage. The 1D model was used to highlight the inefficacy of currently used biomechanical markers and to identify new ones. Dimensionality reduction through statistical emulator work has been recently published [3]. The work on cerebral vasospasm was presented at the Insigneo Showcase in a poster "In silico identification of cerebral vasospasm biomarkers" by Melis et al., and has been submitted for publication. This 1D model has been selected in CompBioMed as a cardiovascular application to demonstrate the benefits of performing Monte Carlo-type analysis using HPC and cloud systems.




[1] P. Bhattacharya, E. Dall'Ara, W. Griffiths, M. Giorgi, A. Melis, M. Viceconti, A digital volume correlation service for the full field quantification of displacement and strain in bone tissue biomechanics (in preparation).
[2] A. Melis, E. Dall'Ara, A. Marzo, M. Vazquez, G. Pringle, M. Viceconti, and CompBioMed Consortium, HPC for the rest of us: porting real-world research applications to an HPC environment (in preparation).
[3] Melis A, Clayton RH, Marzo A. Bayesian sensitivity analysis of a 1D vascular model with Gaussian process emulators. Int J Numer Meth Biomed Engng. 2017;e2882. https://doi.org/10.1002/cnm.2882.


# CompBioMed Welcomes New Associate Partners

## KINDI – Centre for Computing Research

KINDI works closely with Qatar and the Qatar University community by promoting quality research programs in the vital area of computer and information sciences and engineering. Prof. Abbes Amira (abbes.amira@qu.edu.qa) has a background in Computer Engineering with a focus on embedded systems and HPC in connection with health applications. KINDI Director, and alternative contact is Dr Noora Fetais (n.almarri@qu.edu.qa).

## Oxford NIHR Biomedical Research Centre

The Oxford NIHR Biomedical Research Centre is a partnership between the University of Oxford and the Oxford University Hospitals NHS Foundation Trust. The main contact is Dr Philip Fowler (philip.fowler@ndm.ox.ac.uk) who is a Senior Researcher based at the John Radcliffe Hospital in Oxford.

## Alces Flight

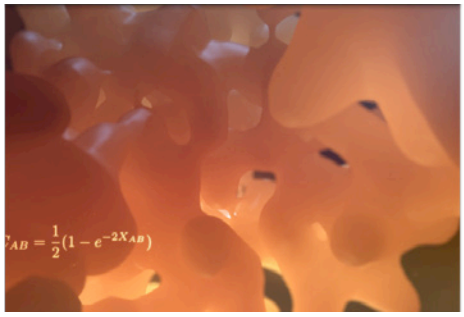
Alces Flight is an arm of Alces Software formed in 2008 by a group of IT professionals with the aim of simplifying software configuration and management for Linux-powered high performance compute cluster and storage systems. Cristin Merritt (cristin.merritt@alces-software.com) is the Partner Manager for Alces Flight.

# Upcoming Events

CompBioMed & Bioexcel
Free-energy Workshop
UCL, London
31 May 2017

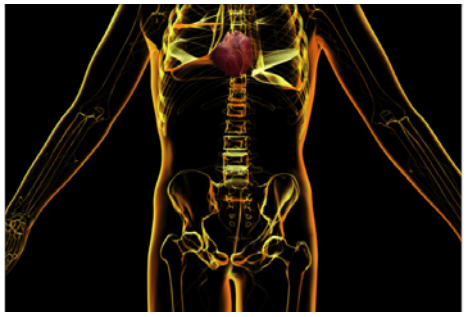
Calculating free energies of various binding processes between compounds and proteins is now possible with high levels of accuracy and precision, as well as speed and reliability. This meeting will assess the state of the art, through the participation of leading practitioners from academia and industry by extensive discussion and justification of methods, applications and experimental validation.

CompBioMed & OpenMulitMed
Workshop at EPMA 2017
Valletta, Malta
14-17 September 2017



In combination with The European Association for Predictive, Preventative & Personalised Medicine (EPMA) World Congress in Malta, CompBioMed has teamed up with the COST action, OpenMultiMed, to arrange a 4 hour workshop to address the important overlapping aspects of the two projects.

The Virtual Human
IMAX event
Science Museum, London
27 September 2017



CompBioMed will feature at the London Science Museum IMAX theatre as part of the Science Museum Lates series of events. We will presentan hour-long evening event describing the Virtual Human, including stunning simulations on aspects of computational biomedicine using supercomputers, starting at 19.30 on Thursday 27th September 2017.

# Recent Events

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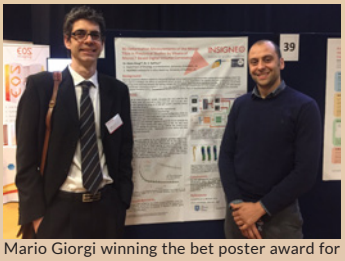

Mario Giorgi winning the bet poster award for CompBioMed research on BoneDVC at Insigneo's Showcase 2017

The CompBioMed project was represented with a display stand at the annual **Insigneo Showcase at Sheffield University (11th May 2017)** where Insigneo's researchers, high profile attendees from healthcare research, clinical practice, funders and industry convened for a day of discussion, networking and presentations. All CompBioMed activities were promoted and the winner of the best poster, Mario Giorgi presented the BoneDVC and openBF services. The Showcase attracted a significant industrial presence and the event received major press attention for CompBioMed.

Kenji Takeda from Microsoft Azure Research speaking at the Cloud & HPC in biomedicine Summit 2017

Eighty researchers working in academia, industry and the healthcare sector travelled from across Europe to attend the **CompBioMed Cloud & High Performance Computing in Biomedicine Summit held at UCL (27th April 2017)**, sponsored by Microsoft. The event, the first of its kind, provided a forum for software developers and scientists to meet with cloud and high performance computing providers. The speakers addressed key challenges faced when computing beyond the desktop in biomedical research and personalised healthcare. The day concluded with a panel discussion focused on the level of security provided when computing on the cloud.

Panel discussion at the Cloud & HPC in Biomedicine Summit 2017

# 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 Associates and past events. We have an active and growing following on Twitter (@bio_comp), a user-forum on LinkedIn (user-forum) and we have recently made our own YouTube channel (Computational Biomedicine), where you can watch live streaming of events and presentations at previous events.

CompBioMed Coordinator:
Peter V. Coveney (p.v.coveney@ucl.ac.uk)

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