

## Newsletter Issue No. 8 September 2019

### Prof. Peter V Coveney

Principal Investigator & Comp-**BioMed Coordinator** 

Welcome ers for their continued support and interest in our work. As we come to the

end of the first phase of CompBioMed, we take this opportunity to focus on some of the activites that our Centre of Excellence has enabled.

We are, of course, looking forward to the CompBioMed Conference which is happening this month. and we are anticipating hosting some 200 people in London for an exciting programme of talks, posters and discussions. The aim of this conference is to include the diverse topics that CompBioMed covers in a format that will appeal to all of our target user communities

The continuation of CompBioMed is also now guaranteed and we are working towards the start of CompBioMed2 in October 2019. We will be holding our Kick-Off meeting at the LRZ site in Garching, Munich. LRZ is a new Core Partner in CompBioMed2 and we are pleased that they have kindly volunteered to organise this event. We will be focussing on the new topics that are introduced in CompBIoMed2 including Machine Learning applications and Data Analytics, in addition to continuing to push the boundaries in terms of planning for the exascale.

We would like to thank all our read- feature the toolkit offering from the FETHPC project VECMA. As we progress with CompBioMed the application of Validation, Verification and Uncertainty Quantification will become increasingly important, and we will be working closely with VECMA to utilitse their toolkit.

> Prof Marco Viceconti worked closely with us at the University of Sheffield and when he moved to University of Bologna, we ensured that we could continue this collaboration. He has recently instigated the In Silico World Community of Practice, which we feature in this Newsletter. The aim of this is to find a secure space to discuss the advance of and issues within this technology.

> We also feature a new video arising from a collaboration between University of Sheffield, Medtronic (an Associate Partner) and University Hospital Tours. With the expertise of Barcelona Supercomputing Center to render the video, this is another beautiful example of the real-world applications of the work done by Comp-**BioMed**.

> We also have news about the spin-out company ELEM Biotech, the HemeLB website and the event held at the UK parliament.

In this issue of the Newsletter, you will see that we

We hope you enjoy this edition, and continue your support for us to CompBioMed2

# Chaus ab Chao: Floating Point Pathology

### A new pathology in the simulation of chaotic dynamical systems on digital computers

The IEEE floating-point representation of real numbers has been standardized since the 1950s. While it is undoubtedly one of the great success stories of numerical



computation, it also has known pathologies, such as roundoff error and loss of precision. In his new article, Prof Peter Coveney describes a new pathology that manifests itself when floating-point numbers are used to

represent the statistical properties of chaotic dynamical systems. The authors show that, even for very simple chaotic systems, floating-point arithmetic can lead to errors that are not obvious, are not small, and do not go away as the precision of the floating-point numbers is increased.

This pathology is hitherto completely unknown and its ramifications are likely to be substantial. They may have an impact on climate modelling, other forms of fluid dynamics research (such as turbulence and fusion energy), astrophysics, as well as numerous areas of physics, chemistry, life / medical sciences, and machine learning/Al research. For the last named, where it has become guite fashionable to train "deep learning" networks on simulations of systems exhibiting chaotic dynamics, AI is liable to be learning behaviours which are not correct.



## HemeLB website

HemeLB is a high performance lattice-Boltzmann solver optimized for simulating blood flow through sparse geometries, such as those found in the human vasculature. It is routinely deployed on powerful supercomputers, scaling to hundreds of thousands of cores even for complex geometries.

HemeLB has traditionally been used to model cerebral bloodflow and vascular remodelling in retinas, but is now being applied to simulating the fully coupled entire human arterial and venous trees.

On the newly created website (hemelb.org) you can download the software and find comprehensive tutorials for installing and running HemeLB on your local machine. The list of relevant papers located there will help you understand the capabilities of the code as well as a link to videos of presentations related to HemeLB.



## CompBioMed's Virtual Human is on the move

#### Prof Andrea Townsend-Nicholson Professor of Biochemistry and Molecular Biology, University College London

It's been an exciting time for CompBiomed with the Virtual Human making public appearances in

the UK and beyond. On Wednesday 26th June 2019, a team from CompBiomed led by Professor Andrea Townsend-Nicholson and in collaboration with UCL and the UK Biochemical Society, introduced the Virtual Human to a cross party group of MPs, and Lords at the UK's Houses of Parliament. The purpose of this visit was to explain to parliamentarians how a virtual human uses digital evidence - from the 'letters' in the human genetic code to medical imaging of the heart - to seek real improvements to healthcare by delivering truly personalised medicine. The event was part of Evidence Week, which is organised by Sense About Science (https://senseaboutscience.org/ evidenceweek/) and aims to help politicians make sense of an increasing range of issues amid an explosion of scientific research and data. The team used a special tablet loaned by Dassault Systèmes, an Associate Partner of CompBioMed to show a 3D version of the virtual heart in action. The virtual digital 'Macarena-dancing' skeleton drew attention as the team demonstrated to MPs and Lords how the most fundamental aspects of living processes and cells are being reproduced by scientists to simulate tissues and organs.

Following the trip to Parliament, the Virtual Human next made an appearance on 27 August in ITU News, the United Nation's specialised agency for Information and Communications Technology (https://news.itu.int/meet-your-virtual-avatar-the-future-of-personalized-healthcare/). This was a great opportunity as ITU News showcases emergent technologies and ICT innovations that will impact on sustainable development worldwide. The news article highlighted the rapid and growing need for technology-enabled healthcare, pointing out that there will be a shortage of 12.9 million healthcare workers by 2035. Also highlighted was the fact that an important aspect of CompBioMed is educating the next generation of healthcare workers in the use of high performance com-

puting. As Prof Townsend-Nicholson savs. ""The research is fabulous," she "but said. the thing I've been particularly interested in, is training the next generation of scientist and clinicians to get them to become familiar with this tal natives so that June 2019

they are as anx-



technology, to get Booklets from the Evidence Week event them to be digi- that took place at the UK Parliament in

ious to see it come through as we are to give it to them.".

As part of the CompBiomed training and education programme, the Virtual Humans film has been shown to over 850 prospective students and their accompanying friends and relatives during Open Days at UCL in the last 2 years. There has been huge interest from these audiences who want to know more about the Virtual Human and when their own personal avatars will be coming on line. During one of these presentations, the editor of the Healthy Food Guide magazine (www.healthyfood.co.uk) was in the audience and was keen that the Virtual Human be brought to a much wider audience. In the September 2019 issue of the Healthy Food Guide, which has 90,000 unique subscribers per month, Prof Townsend-Nicholson published a Talking Point article on "The body double that could improve your health". Prof Townsend-Nicholson and the Virtual Human have enjoyed their summer travels and are currently putting their (real and virtual) feet up to write this blog before hitting the road again!



Panorama of the Sense about Science Evidence Week in the Uk Parliament



rcelona biotech fights

### **ELEM Biotech**

ELEM Biotech is a spin-out company from Barcelona Supercomputer Center. It creates models of the human body from patient scans to replicate how they work. These models evolve into virtual populations mirroring the diversity and pathologies of society. Biomedical companies use Virtual Humans to develop better treatments with unparalleled medical insights.

Their partner in Cloud Computing, Oracle has recently named them within their "History of Possibilities" section on the home page of their website. We are proud to be so closely associated with ELEM Biotech, and hope to support them further as their company grows.

For more information on the company and the possibilities for you and your research, visit their website: http://www.elem.bio



# The effect of aneurysm treatment on cerebral blood flow: an illustrative video powered by patient-specific modelling.

At this year's LINNC (Live Interventional Neuroradiology & Neurosurgery Course), which took place 3-5 June at the Louvre, Paris, Associate Partner and IAB member, Medtronic showcased a 3D video (https://www.youtube.com/watch?v=Pn1\_bD4r1cg) based on the research of Dr Alberto Marzo from the Insigneo Institute for *in silico* Medicine which explores the effect of deploying a flow diverter stent on blood flow in a patient-specific model.

The video was sponsored by Medtronic, in the Comp-BioMEd IAB, and the clinical supervision was provid-



ed by Dr Ana Paula N a r a ta, also a CompBioMed IAB member and Consultant Neuroradiologist

from Tours, France. It shows the effect of a specific flow diverter stent, the Pipeline Embolization Device by Medtronic, over the blood flow inside an artery. The first part shows visualizations of a Computational Fluid Dynamics (CFD) simulation inside an intracranial artery containing an aneurysm, without the stent. The second part is an accurate recreation of the stent delivery process. The final part shows visualizations of a CFD simulation of the blood, after stent implantation.

Patients suffering from brain aneurysms (abnormal bulging of a blood vessel) are often treated with a procedure (stenting) that sometimes leads to the dangerous obstruction of arteries. Dr Marzo, in collaboration with the University Hospital of Tours, France, led a

[1] A. P. Narata et al., "The Role of Hemodynamics in Intracranial Bifurcation Arteries after Aneurysm Treatment with Flow-Diverter Stents," Am. J. Neuroradiol., vol. 39, no. 2, 2018.

### In silico World Community of Practice

In Silico Medicine technologies are based on the idea of using computer models to predict quantities that are difficult or impossible to measure directly, but that are important to support a medical decision – in the case of choosing the best course of action for that specific patient – or to reduce, refine, and partially replace animal/human experimentation required to assess the safety and the efficacy of new medical products (In Silico Trials technologies).

Some of these disruptively innovative technologies have now left the research labs and are being translated into commercial products; but there is a series of barriers slowing down the adoption of *in silico* medicine technologies, one being that this field is still too young to have established industrial best practices.

To fill this gap, Prof Marco Viceconti's research team at the University of Bologna is launching an online Community of Practice that meets the need for a safe pre-competitive space where experts from academia, industry, and regulatory agencies can request and exchange advice on the technical details about these sophisticated technologies, and their regulatory qualification. The community is called *In Silico* World and is based on the Slack platform, that allow for dynamical manage-

team of researchers to investigate whether this was related to the way blood flows in vessels of a certain anatomy or geometry. They used their computer models to mim-

### Dr Alberto Marzo

Senior Lecturer, Insigneo Institute University of Sheffield

### Dr Ana-Paula Narata

Interventional Neuroradiology, University Hospital Tours

ic blood flow in arteries and through stents, and found that there might be a flow-related reason for the occasional failure of flow-diverting stent treatment in some vascular geometries, linked to alterations in blood flow [1].

The study identified important cause-effect mechanisms and significant associations with blood vessel anatomy which can guide treatment, reduce risk and extend use of a minimally invasive procedure that, before this study, was associated with the possibility of complications.

This research was supported by the Newton Collaboration Programme of the Royal Academy of Engineering and carried out through a collaboration with a Consultant Neuroradiologist from Tours (France), Dr Ana Paula Narata, a Lecturer from Universidade Federal do ABC (Sao Paulo, Brazil), Dr. Fernando Moura, a Lecturer from Argentina, Dr. Nacho Larrabide. The video was sponsored by Medtronic.

The prestigious LINNC Paris event provides an op-

portunity to discuss the latest techniques and issues in Interventional NeuroRadiology and Neuro-Surgery, and to meet a vibrant community of neuroradiologists and neurosurgeons dedicated to ad-



vance their practice and to achieve the best clinical outcomes for their patients.

ment of as many communication channels as necessary, each with its specified access list, its managers, its goals etc.

Here people with different backgrounds, ideas and know-how can work in a collaborative and supportive way to gain knowledge on a common interest or to achieve shared goals.



The community aims at fostering brainstorm-

ing and discussions in open channels as well as more technical and targeted work in private channels, dedicated to specific topics, groups, organizations or companies interested in *in silico* medicine. In collaboration with the Avicenna Alliance, the VPH Institute, and CompBioMed, we will organise and deliver technical webinars from world-class specialists and structured consensus processes aimed at establishing some widely accepted Good Modelling Practices, which can then be promoted with regulators and the editorial boards of scientific journals.

The access to the Community of Practice is by invitation only. If you are interested please send your expression of interest with evidence that you are a practitioner of *in silico* medicine or a decision-maker, by email to the Community Manager, Roberta De Michele (roberta.demichele2@unibo.it) to receive an invitation to participate.

### CompBioMed Conference 2019:

Institute of Engineering and Technology, London, UK 25-27 September 2019



The conference has 15 symposia, 4 keynote speakers, and over 50 invited speakers in addition to a large number of talks selected from submitted abstracts. The parallel programme takes place over 3 days and will cover all aspects of this burgeoning field, from genome through organ to whole human and population levels, embracing data driven, mechanistic modelling and simulation, machine learning and combinations thereof.

Registration is still open: https://www. compbiomed-conference.org/registration/

## Upcoming Events The Future of Quantum Com-

puting Science Museum, London, UK,

25 September 2019



Quantum computing represents a paradigm shift in computing technology. Answers that lie beyond the reach of current 'classical' computers may soon be within our grasp. Quantum technologies should offer the ability to process information in a way that allows us to model complex chemical processes, such as the way that drugs work in the body. What do they mean for storing and encrypting medical data, simulating the body and for AI?

The Science Museum has joined forces with CompBioMed to assemble a panel of experts to explore the future of this exciting forward-looking technology.



Now) and user-developers (FabSim3 and



CompBioMed2 KO Meeting

Leibniz Rechenzentrum, Munich.

Germany

21-23 October 2019

As we near the end of CompBioMed1,

we are already looking to the new as-

pects that will be explored in CompBi-

oMed2. During our Kick-Off meeting at

LRZ, our new Core Partner, we will look

at the Machine Learning aspects of the

research and the soon to arrive exascale.

We are looking forward to welcoming

our Associate Partners and introducing

them to these new aspects of the project

in addition to continuing the high-quality work that we started in CompBioMed1.

We hope that you will continue to sup-

port us through the second phase of this

(CINE Indiana.

ECMA*tk* 

The full public release of the VECMAtk, took place in June. It aims to facilitate Verification, Validation and Uncer-

tainty Quantification (VVUQ) for complex single- and multi-scale applications. This was the first of three annual releases planned over the duration of the VECMA project (http://www. vecma.eu/). The Toolkit release contains a suite of components, providing tools to:

- create VVUQ procedures (EasyVVUQ),
- automate the complex workflows emerging from these procedures (FabSim3),
- enable the efficient execution of large numbers of jobs on computational resources (QCG Pilot Job Manager),
- facilitates access to HPC resources for users (QCG-



QCG-Client)

The software toolkit

has been developed to enable automated VVUQ, and provide support for software applications regardless of the domain of interest. VECMA has established a collection of readily working algorithms for uncertainty quantification within existing multiscale computing tools. Tutorials are provided in four application areas as part of this release.

project.

For all the information and links to the tutorials and applications, please visit the VECMA toolkit website: https://www. vecma-toolkit.eu



# 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 (in CompBioMed) and we have our own YouTube channel (D Computational Biomedicine), where you can watch live streaming of events and presentations at previous events and webinars, as well as our Virtual Humans film ( https://youtu.be/1FvRSJ9W734).

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