

HORIZON
2020

A Centre of Excellence in Computational Biomedicine

Berichterstattung

Projektinformationen

CompBioMed

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[Projektwebsite](#)

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[10.3030/675451](https://doi.org/10.3030/675451)

Projekt abgeschlossen

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Periodic Reporting for period 2 - CompBioMed (A Centre of Excellence in Computational Biomedicine)

Berichtszeitraum: 2018-04-01 bis 2019-09-30

Zusammenfassung vom Kontext und den Gesamtzielen des Projekts

Computer based modelling and simulation is well established in the physical sciences and engineering, where the use of high performance computing (HPC) is now routine. Computational methods, based on human biology, are now reaching maturity in the biomedical domain, rendering

predictive models of health and disease increasingly relevant to clinical practice by providing a personalised aspect to treatment. Increasingly, these models are also being combined with machine learning and artificial intelligence.

A main purpose of our Centre of Excellence was to promote and foster the use of HPC as a fundamental cornerstone of computationally assisted biomedical research and help translate this into medical and clinical practice. We have, therefore, invested in community building to spread knowledge, tools and best practice to students, researchers and decision makers across the domain. HPC is now enhancing industries in the healthcare sector including pharmaceuticals and medical device manufacturers, and underpinning a range of emerging sectors, such as those concerned with e-health and personalised medicine. The innovative modelling and simulation techniques we developed and promoted within this Centre have proven to be of great interest and relevance to industrial researchers, HPC manufacturers and independent software vendors as well as with clinical practitioners and medical device manufacturers.

Arbeit, die ab Beginn des Projekts bis zum Ende des durch den Bericht erfassten Berichtszeitraums geleistet wurde, und die wichtigsten bis dahin erzielten Ergebnisse ▼

We have deployed several application codes across HPC centres, made possible through major allocations awarded to CompBioMed. Selected codes from our partners have been run on the largest supercomputers in the world and we have been working with the computer centres and collaborating with other EU Centres of Excellence to evolve our codes to run on emergent exascale machines. Cardiovascular applications have modelled the full vascular tree, investigated the effect on blood flow when plaques are formed and how the insertion of a stent, and conducting a bypass graft, can affect a patient's prognosis. Heart models have been used at multiple scales from a single cell to medical device trials on whole human hearts. In molecular medicine, collaborations have investigated novel drug interactions with potential targets in the body. Drug discovery tools based on state-of-the-art 3D-convolutional neural networks, have been developed, applying machine learning algorithms to speed up some calculations. Bone modelling software developed within our CoE in collaboration with imaging measurements performed at Sheffield Teaching Hospital is being used to determine how the angle of a fall can influence the nature of bone fractures.

Our most high-profile dissemination activity has been the production and screening of an IMAX film called "The Virtual Human" (<https://youtu.be/1FvRSJ9W734>) constructed from simulations from our Core and Associate Partners, with animations composited on the MareNostrum Supercomputer at Barcelona Supercomputer Centre (BSC). We organised a large-scale conference over 3 days with 200 participants, industrial sponsors and multiple parallel sessions. 83 scientific papers have been published by our partners who have also participated in over 230 major conferences and workshops and organised 20 workshops. We have established two courses for UCL's medical degree programme and biomedical students that have been attended by 245 students in total and will shortly be rolled out in other European centres across EU. Many of our training events and webinars have been recorded and are available on our YouTube channel, enjoying over 16,000 views across the whole channel.

We have established an Innovation Advisory Board (IAB), increasing and diversifying its initial membership in numerous ways. We have held three face-to-face meetings with the IAB where we have been able to implement many of their suggestions. Our Innovation Exchange Programme has enabled nearly 40 visits across our Core and Associate Partners. This has been aided through a memorandum of understanding between CompBioMed and HPC-Europa3, with their Transnational Access programme.

The current mechanisms for accessing services offered by HPC centres and cloud providers have been analysed, together with the requirements of CompBioMed users for non-conventional access (such as advanced reservations, on-demand access etc), resulting in a feasibility study for implementing such mechanisms by the HPC providers. We have enabled CompBioMed partners to deploy their applications on cloud and HPC architectures for diverse biomedical applications and have pushed the boundaries on several of the largest supercomputers in the world. CompBioMed has worked to promote the use of application container solutions in order to facilitate more efficient, reliable and portable application deployment, opening the possibility of using them in a clinical setting. We have updated and enhanced our software hub, detailing software applications from our Core Partners and Associate Partners

We have undertaken an extensive analysis and identification of solutions available within the consortium and analysed in detail the taxonomy of end-users that can benefit from the services offered by the CoE. Data storage and transfer technologies have been investigated, resulting in a deployment of the EUDAT B2SHARE service to support our data archive. Work has been conducted with two synchrotron facilities (European Synchrotron Radiation Facility and Diamond Light Source) to optimise the transfer of large datasets generated on site to remotely located HPC facilities. Individual partners have improved existing and widely used codes and have coupled them to extend the biomedical scenarios that can be investigated. We have introduced a number of our codes to clinicians who are now using them in some cases and planning their use others.

Fortschritte, die über den aktuellen Stand der Technik hinausgehen und voraussichtliche potenzielle Auswirkungen (einschließlich der bis dato erzielten sozioökonomischen Auswirkungen und weiter gefassten gesellschaftlichen Auswirkungen des Projekts)

The work we have conducted with HPC and cloud providers, merged through the use of container technology, has enabled us to investigate more widely the use of our applications in clinical settings and in industry. Some of our codes will benefit from the looming exascale and we are developing them in this direction; for clinical uptake at this time, we must provide applications that run in real time on lower end and cloud infrastructure.

The publication of over 80 scientific papers in leading international journals shows that we have are operating at the forefront of this field. We will continue to work on these applications, and apply our

methods in new fields of medicine where a combination of our capabilities plus market demand will see the greatest uptake within the broader healthcare sector.

In our training we are focussing on the core principles of biomedical research, and we are reaching out not only to computational scientists but targeting a new generation of students who will be demanding access to our methods within the clinical domain. We have integrated a course into medical curriculum at UCL, which teaches medical students how to work with supercomputers to solve specific problems which has proved successful for 2 years now and will be integrated into other partners' institutions.

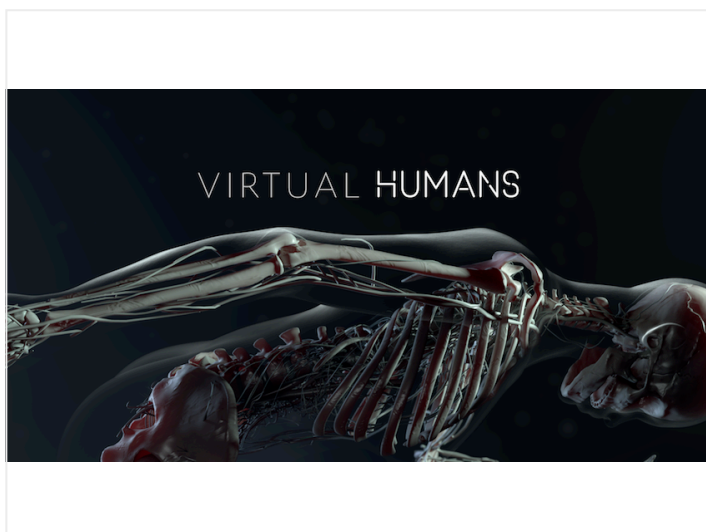
Our outreach activities have encompassed the general public, with an award-winning IMAX film, multiple TV and radio appearances, and several major public events which have drawn thousands of people to hear of our work and the importance of supercomputing in medicine over the first three years of our CoE.



CompBioMed logo



Amalgamation of images from IMAX film



Virtual Human promo picture

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