Grant agreement no. 675451

CompBioMed

Research and Innovation Action
H2020-EINFRA-2015-1
Topic: Centres of Excellence for Computing Applications

D1.4 Final Public Report

Work Package: 1

Due date of deliverable: Month 36

Actual submission date: September 30, 2019

Start date of project: October 01, 2016 Duration: 36 months

Lead beneficiary for this deliverable: *CBK*
Contributors: *UCL, BSC, UvA, UEDIN, SARA, USFD*

Project co-funded by the European Commission within the H2020 Programme (2014-2020)		
Dissemination Level		
PU	Public	YES
CO	Confidential, only for members of the consortium (including the Commission Services)	
CI	Classified, as referred to in Commission Decision 2001/844/EC	

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1. Version Log

Version	Date	Released by	Nature of Change
V0.1	16/08/2019	Emily Lumley	First Draft to WPLs to check
V0.2	28/08/2019	Emily Lumley	Input from WPLs incorporated
V0.3	18/09/2019	Emily Lumley	Revision from reviewers' comments
V1.0	27/09/2019	Emily Lumley	Final version for submission

2. Contributors

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3. Definitions and Acronyms

Acronyms	Definitions
1D	1 Dimension
BAC	Binding Affinity Calculator
BoF	Birds of a Feather
BSC	Barcelona Supercomputing Centre
CIR	Central Incubation Register
CoE	Centre of Excellence
cPPP	Contractual Private Public Partnership
CT2S	Computer Tomography to Strength
EC	European Commission
ESMAC	Enhanced Sampling of Molecular Dynamic with Approximation of Continuum Solvent
ETP4HPC	European Technology Platform for High Performance Computing
EUDAT CDI	EUDAT Collaborative Data Initative
FDA	United States Food and Drug Administration
FET	Future and Emerging Technologies
GPCR	G-Protein Coupled Receptor
GPU	Graphics Processing Unit
HPC	High Performance Computer
IAB	Innovation Advisory Board
IEP	Innovation Exchange Programme
IP	Intellectual Property
ISC	International Supercomputing Conference
LB	Lattice Boltzmann
LTG	LifeTec Group
MPI	Message Passing Interface
NMSK	Neuro-musculoskeletal
OAI-PMH	The Open Archives Initiative Protocol for Metadata Harvesting
openBF	Open BloodFlow
SC	Supercomputing Conference
ShIRT	Sheffield Imaging Registration Toolkit

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SME	Small or Medium Enterprises
SOP	Sustainability Operating Procedure
TB	Terabyte
TIES	Thermodynamic Integration with Enhanced Sampling
UCL	University College London
UK	United Kingdom
UNIGE	University of Geneva
UOXF	University of Oxford
UPF	Universitat Pompeu Fabra
US	United States
USFD	University of Sheffield
UvA	University of Amsterdam
VVUQ	Verification, Validation and Uncertainty Quantification
WMS	Workflow Management System
WP	Work Package

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4. Executive Summary

In D1.4: *Final Public Report*, we are examining the objectives set out for CompBioMed and the work that we have conducted in the last three years to achieve these objectives. The introduction will look at the over-arching objectives, with short examples of how we have achieved them and pointing to other deliverables that can show more details. This will be followed by a look at the Work Packages (WPs) and the tasks associated with them, explaining how we have achieved the goals that we set out at the proposal stage.

The objective of this deliverable is to give a non-confidential summary of the final status of the project and is aimed at a public audience with some knowledge of the field. For more in depth analysis of the various tasks and objectives, the final deliverables within each WP will give more detailed descriptions of the work carried out.

5. Introduction

The CompBioMed project determined six high-level objectives, which we have worked towards throughout the lifetime of the project.

> *The first objective of our user-driven Centre of Excellence in Computational Biomedicine is to coalesce the burgeoning HPC user community within the field and build on it to extend computational methods to a wide range of biomedical research areas. This will facilitate the uptake of high fidelity simulation and analysis in support of medicine and clinical practice. We will do this through several disease case exemplar themes, together with dissemination, training and community engagement activities that lie at the core of our proposed Centre.*

We have achieved this objective through the collaboration of many of our partners, the introduction of over 40 Associate Partners with which we closely collaborate. As an example, the work done at LifeTec Group with University of Eindhoven has introduced a simulation that is being used by cardiologists at the local hospital for determining the best treatment option for aneurysms. This is one of many applications, more of which can be found in D2.4: *Report on the Impact of Modelling and Simulation within Biomedical Research as enabled by CompBioMed* [1], which will be available at the end of the project.

> *The second objective of our Centre of Excellence (CoE) will be to promote innovation in the field of computational biomedical modelling and simulation. We will do this by identifying and supporting key priorities for three disease cases that will inform the tools and techniques that we investigate (cardio-vascular/respiratory, infection/immunity and neuro-musculoskeletal), as well as engaging with new clinical targets as the project evolves.*

Our Innovation Advisory Board (IAB) includes members from industry as well as clinicians to help us promote innovation in the most appropriate direction for our current disease use cases and helping to identify other potentials. As proof of our innovation strategy we have supported a spin-off and a start-up company (ELEM Biotech and EnsembleMD) within the project and we have monitored our partners Intellectual Property (IP) to identify the best chances for commercialisation for them. More

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information on these activities can be found in D4.5: *Report on Pre-commercial Activities* [2], which will be available at the end of the project.

> *The third objective of our Centre of Excellence is to train future generations of scientists within the field of computational biomedicine, by running training courses on topics such as High Performance Computer (HPC) use, software engineering and algorithm design, as well as training medical practitioners in the basic medical and clinical contexts of HPC simulation, at events with maximum community exposure such as community workshops and leading international conferences.*

We have organised and participated in a large number of training and workshop events (D3.6: *Final training and dissemination report* [3]) throughout the lifetime of the project. Our partners also participated in a large number of related conferences, spreading the work of the CompBioMed CoE. Our flagship video, “Virtual Humans” has been watched thousands of time on YouTube, and our partners have utilised it in outreach activities to the general public. Our recent translation of the video into French and German will also enable these activities to expand in CompBioMed2.

> *The fourth objective of our Centre will be to use best practice Software Carpentry tools and techniques, adopted from and in conjunction with industry and relevant institutes, to develop existing community codes to the extent that they become sustainable and widely used software packages throughout computational biomedicine research and its applications in healthcare, industry and medical practice.*

Working closely with the HPC centres in our consortium (EPCC, SURFsara and BSC) we have established best-use practices which are available on our website. We have strengthened these practices by working closely with a new FETHPC project (VECMA, project code: 800925) which focuses on Validation, Verification and Uncertainty Quantification (VVUQ). Our codes and applications are regularly featured in our Webinar series to show how they are used and to provide use cases for them. These are then published on our website and on YouTube for reference.

> *The fifth objective of our Centre of Excellence will be to engage with a range of industries across the entire healthcare value chain, from healthcare providers to pharmaceutical and medical device manufacturers, as well as ISVs and HPC system providers, to further the direction, uptake and exploitation of high performance computing within commercial organisations that are only now beginning to grasp the potential of high fidelity simulation and analysis for their healthcare-related businesses. We will do this by working in synergy with industrial partners, including SMEs and HPC providers within our consortium, to support appropriate high-end computing access mechanisms, convening an innovation board to help industrial users set the direction of our Centre and to benefit from the software tools and techniques developed.*

Our many and varied Associate Partners include industries across the entire healthcare value chain [4]. In addition to working with them to provide high fidelity simulations and analysis we have enabled them to develop their own work and introduce them to the possibilities opened through the use of High Performance Computing which can be evidenced in D5.6: *Report on Efficient HPC usage by the Biomedicine community* [5], which will be available at the end of the project

> *The sixth objective of our Centre will be to engage closely with medical professionals through our partner hospitals and the wider community of stakeholders, to promote (i) the tools, techniques as well as access mechanisms developed within our Centre; (ii) the wider field of computational*

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biomedicine; (iii) the importance of computational modelling as an integral part of the decision making process within specific clinical fields.

This objective has been reached and can be evidenced through the two Key Performance Indicators for the number of hospitals accessing HPC services and the number of patients analysed with patient specific workflows. With 6 hospitals having either mediated or direct access to HPC services and over 400 patient specific workflows having been analysed we are showing the advantages associated with the work of our CoE to the wider community.

6. Activities Carried Out

In this section we will outline the progress made per work package (WP). While we start with Work Package 1 for completeness, WPs 2-6 contribute the most relevant research and outreach activities within the project. Each WP will describe its objectives and a general overview of progress towards those objectives throughout the project followed by a more detailed update of progress per task. We will then conclude by summarising the most relevant results from the WP.

6.1. Work Package 1: Management

Work Package Objectives

To ensure the timely and high quality achievements of the project results and deliverables through quality control and risk management of the project as a whole. To provide timely and efficient administrative and financial coordination of the project and the compliance with contractual commitments.

Work Towards Objectives

This work package has ensured that CompBioMed has achieved its management objectives throughout the project. Coordination and management of the consortium have ensured support to the research, training and dissemination activities. All partners have participated in teleconferences and project meetings as well as through their contributions of work.

Work completed per Task

Task 1.1: Legal and Contractual Management [M1-M36] has coordinated amendments to the Grant Agreement for the addition of Evotec UK in place of EVOTEC AG, alterations in the financial management of the project in addition to updating the Consortium Agreement which was finalised shortly after the first reporting period.

Task 1.2: Financial Management [M1-M36] has been managed by UCL and has ensured the timely payment of the partners and the periodic and final financial reports.

Task 1.3: Consortium Coordination [M1-M36] included the publication of the Project Handbook [6] and Data Management Plan [7] on time. The Executive Board had regular teleconferences to ensure that the project ran to schedule. During the time of project there has been a Kick-off meeting and three All-Hands meetings during each of which we have held General Assemblies and meetings of the

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Innovation Advisory Board. We have dealt with the correspondence with the European Commission. Further to this we have interacted with external stakeholders to incorporate them into the project as Associate Partners of which we currently have over 40. [4]

Task 1.4: Periodic Reporting [M1-M36] has produced the 9-month report, the first periodic reports and will coordinate and put together the final periodic reports. The recording and analysis of the project KPIs has also taken place throughout the project.

Task 1.5: Project Quality Control [M1-M36] has overseen the quality control and timely delivery of the project's many reports and deliverables. We have submitted most deliverables on time using the Quality Control procedure outlined in the Quality Assurance Plan [8]. Those that were not on time were within 1 month of the submission deadline and in coordination with the Project Officer to ensure the quality we required.

Significant Results

1. Kick-off meeting and three All-Hands Meeting
2. Four General Assembly Meetings in line with the above meetings
3. Overall management and timely submission of deliverables
4. Executive Board participation
5. Work Package Leader meetings coordination and participation
6. Incorporation of over 40 Associate Partners

6.2. Work Package 2: Biomedical Applications

Work Package Objectives

The objectives of WP2 were the development and advance of the start-of-the-art in biomedical modelling and simulation from the desktop to the most powerful High Performance Computing (HPC) (Tier-0) systems. We have placed a special focus on the use of multi-petaflop HPC environments, putting several of our codes on the road to the exascale (another three orders of magnitude greater than the petascale that they were originally functioning at). WP2 has developed strategies, including new algorithms, to ensure that current and future high fidelity biomedical codes will perform optimally on emerging exascale machines and other novel architectures. Due to the innate multiscale character of computational biomedicine (patient, organ, cell, molecule), CompBioMed's WP2 worked to establish layered pipelines of simulation and data analysis codes, with the goal of mapping them to large-scale computational resources in an efficient way. In these ways we have guaranteed extensive reach for the biomedical researchers from academia, industry and the medical clinic.

Work Towards Objectives

This work package, led by Barcelona Supercomputing Center (BSC), has ensured that CompBioMed has achieved its simulation research objectives within the project, with important contributions from all participating partners. This is reflected in the number and quality of the journal and conference papers produced [9]. The papers show also the high intensity of the collaboration strategy in WP2. Additionally, WP2 has been very successful in connecting to other WP's activities. More detailed and scientifically specific examples of the research and progress can be found in the deliverables for WP2, most specifically, D2.4 which will be submitted at the same time as this deliverable. [1]

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Work completed per Task

Task 2.1: Deploy and Utilise Application Ready Environments [M1-M12]. This task was completed at the end of the first year and all the required codes were deployed on CompBioMed supercomputers. Further details can be found in D2.1: *Application Software Readiness and Fast Track Exploitation* [10]. Additionally, some of the codes (Alya, HemeLB, BAC) have been deployed and tested on other platforms (the Swiss PizDaint, the American Mira, Titan and Blue Waters, the Japanese K-computer), including a cloud provider system (Alya in Oracle Cloud, BAC on AWS, DNAnexus and Azure).

Task 2.2: Cardiovascular Exemplar Research [M1-M36]. This task has produced research within three different areas: cardiac (BSC, UOXF), vascular for the full arterial system (USFD, UCL) and vascular for small vessels (UNIGE, UvA, UCL, LTG). Each area has been addressed with different strategies which enabled the possibility of coupling them.

Cardiac

In addition to their individual projects with cardiac modelling, BSC and University of Oxford have collaborated on using the advanced code (Alya) from BSC in various scenarios from models of single cells through to investigations of possible medical devices.

Vascular for the full arterial system

University of Sheffield (USFD) has worked with a 1D model that facilitates the diagnosis of Cerebral vasospasm (a possibly fatal complication often experienced after a stroke). University College London (UCL) has initiated work on an ambitious task of modelling the whole human arterial and venous tree, using their HemeLB code for modelling blood flow.

Vascular for small vessels

University of Geneva (UNIGE) have developed a highly advanced blood flow modeller that can investigate multiple aspects of blood cells and platelets which has the potential to be used in determining the optimal position for a stent to be placed.

University of Amsterdam (UvA) have further developed their open source HemoCell simulation code extending its use and making it more robust, allowing them to investigate further possibilities and applications.

LifeTec Group (LTG) have developed a simulation tool, implementing a 1D model similar to the model by USFD mentioned above, that can help in the real-time determination of the best treatment strategy (stent or bypass) for coronary disease cases. This has been trialled in the hospital by clinicians to evaluate the usability, trust in the results and usefulness of the technology, all of which have been given positive feedback.

Task 2.3: Molecularly-based Medicine Exemplar Research [M1-M36] has enabled multiple collaborations with the academic research groups and both our small and large industry partners.

Universitat Pompeu Fabra (UPF), Acellera and Janssen have collaborated in a project which has looked at possible drug targets (ligands) and how they react with active sites and sites of interest for various diseases. They have also started work on Machine Learning within this environment.

Janssen and UCL used molecular simulation to predict the how effectively drug molecules might attach to protein targets (binding affinity) associated with diseases, including PDE2, BRD4 and several kinases. The novelty of this work is in the ability to account for the inherent changes in the targets.

UCL have examined the binding affinities of ligands for GPCR systems using two different strategies: ESMACS (enhanced sampling of molecular dynamics with approximation of continuum solvent) and TIES (thermodynamic integration with enhanced sampling), which allows a more rapid and accurate examination of the process.

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Evotec and UCL have established a close collaboration to investigate and develop computational methodologies for structural exploration and drug discovery which has led to a number of publications in various applications.
In addition to these specific cases, UPF, Acellera, Janssen and UCL are working on other projects within this field. More information on this can be found within Deliverable D2.4: *Report on the Impact of Modelling and Simulation within Biomedical Research as enabled by CompBioMed* [1]
Task 2.4: Neuro-musculoskeletal (NMSK) Exemplar Research [M1-M36]. USFD has been working on image registration and bone modelling, also coupling its bone modelling software to several others from UOXF and UNIGE. The Computer Tomography to Strength (CT2S) model has been tested on over 110 patients and is being trialled in the local hospital where it is being used to determine the bone strength and the risk of hip fracture of the patients.

Task 2.5: Post-processing and Error Analysis [M12 – 36]. This task started in M12 and was led by BSC where they compiled a VVUQ strategy (Validation, Verification and Uncertainty Quantification) for electro-mechanical coupling in collaboration with the University of Minnesota, Medtronic (Associate Partner) and the FDA. The VVUQ analysis goal was to increase the confidence of simulation by thoroughly testing the software, from the mathematical models up to programming issues. Being so complex, this is a framework or global strategy that must be adapted to each domain. This framework is supposed to be established by regulatory agencies, user communities, developers or experimental scientists. BSC and other CompBioMed partners are involved in the development of such ideas. This is being aided by a close collaboration with the VECMA project (800925) [11] under FET HPC initiative as part of EC H2020 programme which started in June 2018.

Task 2.6. Develop Plans for and Implement the Upscaling of CompBioMed Production Applications for Future HPC Platforms, Including those Heading Toward the Exascale [M12 - 36]. As added value, we produced a crib sheet on how to augment and adapt a code to be prepared to exploit different, future exascale architectures which can be found in D2.2: *Report on Deployment of Deep Track Tools and Services to Improve Efficiency of Research and Facilitating Access to CoE Capabilities* [12].
Within each Research Exemplar progress has been made towards future HPC platforms. This has included extensive work with container technology for facilitating the move of codes from cloud computers to HPC systems and ensuring compatibility between the two. Various codes are working towards more efficient upscaling to ensure that they will make full use of the forthcoming exascale machines which are expected from the US or China, with Japan and various European countries striving towards this too. Through the preliminary work conducted and in close collaboration with the US funding agencies that are in line to develop these machines, we are in a good position to provide strong feedback on the infrastructure needed in such machines, thereby contributing actively to the co-design process.

*Task 2.7: Develop and Implement Multiscale and Workflow Interfaces [M6-M30] (*This task is strongly linked to WP6, see Section 6.6 below) BSC is working on the improvement of coupling strategies through multi-point MPI communications in Alya. Our next steps will be on cardiac electrophysiology – mechanics coupling, using different mesh sizes for each problem and continuing to the particle tracking for the respiratory system (also applied to cardiovascular).

Significant Results

1. Deployment of codes in the HPC centres.
2. 83 papers published in international journals and presented at conferences
3. Code improvements, with new functionalities, in all three exemplars.
4. Progressing codes for exascale machines

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5. Close collaborations through Core and Associate Partners
6. Crib Sheet to guide code owners to prepare their codes for future exascale systems

6.3. Work Package 3: Training and Dissemination

Work Package Objectives

CompBioMed's Centre of Excellence is distributed in nature, so this work package aimed at providing a focal point for the collaboration within the project, and also with external stakeholders, by developing and coordinating the training (led by UvA) and dissemination (led by CBK) activities that enable it to engage external stakeholders in academia, healthcare and industry with the activities of the project.

In particular, the WP's specific objectives were to:

- Disseminate project outcomes online and through conferences/workshops and meetings.
- Develop training courses and online training materials in collaboration with project software developers and HPC experts.
- Grow existing and identify and build new end-user communities in computational biomedical research.
- Provide tailored training to academic and industrial researchers and clinical users.
- Run hands on training courses.
- Raise awareness about the challenges and opportunities of HPC in the field of Computational Biomedicine with all stakeholders.

Work Towards Objectives

WP3 has stayed on track with deliverables, milestones, and in regard to the attainment of its specific objectives. There has been a substantial amount of training and dissemination activity throughout the project, reported in detail in deliverables D3.4 [13], D3.5 [14] and D3.6 [3]. What is outlined below are highlights and specific cases that help to highlight this work.

Work completed per Task

Task 3.1: Production of a Dissemination Action Plan [M1 – M3] A detailed dissemination action plan (D3.2 [15]) was produced on schedule with a clear description of tools, tasks, target audiences and deliverables.

Task 3.2: Maintaining the CompBioMed Online Presence [M1 – M36]
CompBioMed's online presence is being constantly maintained and strengthened, as described in detail in D3.4 [13], D3.5 [14] and D3.6 [3].
The project's stakeholders are primarily targeted through the following channels:

- CompBioMed website (D3.1 [16]): www.compbiomed.eu
- CompBioMed Twitter account: @bio_comp
- CompBioMed YouTube channel "Computational Biomedicine"
- Scientific Events (conferences, workshops, seminars etc.)
- Scientific Journals

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- The mailing lists, websites, and social media channels of our core partners, associate partners, and related projects

At the time of writing, the key statistics for the website include:
- 202,539 visits
- 129 website pages
- 91 news/events posts

Key statistics for the CompBioMed Twitter account include:
- 804 Tweets
- 787 Followers
- 876 Likes
- 327,120 Twitter Impressions from our own account
- Over 1 million Twitter Impressions from other accounts

Key statistics for the CompBioMed YouTube page include:
- 82 videos uploaded
- 215 subscribers
- 14,429 views in total

Task 3.3: Produce Dissemination Materials [M1 – M36]
Project stakeholders have been targeted using the following dissemination materials:
- 2 leaflet distributed hundreds of times
- 48 poster presentatins
- 8 quarterly newsletters
- 11 monthly e-newsletters
- 83 scientific papers
- 11 popularised publications
- Theme issue of Frontiers in Physiology
- Theme issue of *Journal of the Royal Society Interface Focus* for the CompBioMed Conference (in preparation)

Across the full project, the CompBioMed consortium has co-organised or fully organised:
- 2 Conferences
- 8 Workshops
- 4 Sessions within external events
- 6 booths

Task 3.4: Develop the Training Plan [M1-M6]
The Training Plan (D3.3 [17]) was produced and submitted according to schedule (month 6). The plan described in detail the training activities that would be carried out during the project, as well as the approach to be used.

Task 3.5: Training Co-ordination, Development, and Delivery (M1-M36)
The Training Plan (D3.3 [17]) has been implemented throughout the project. In particular, CompBioMed training activities comprised 10 webinars, 3 face-to-face training events, university education courses, and other training activities, **for a total of more than 600 live participants and 5,000 YouTube views**, as described in detail in D3.4 [13], D3.5 [14] and D3.6 [3] and highlighted below:

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CompBioMed webinar series

The series started in November 2017 and ran until the end of the project. It comprised 10 webinars, each one focussing on a different topic and delivered by a different partner, **for a total of ±250 live participants, ±1.500 YouTube views in over 32 different countries:**

1) The first webinar titled "HPC simulations of cardiac electrophysiology using patient specific models of the heart (using CHASTE and Alya)" took place on 22 November 2017. The speakers belonged to UOXF. 76 people actually participated. Furthermore, by the time of writing, the webinar's recording has been viewed 332 times on CompBioMed's YouTube channel.
2) The second webinar was titled "Introduction to cloud computing for the VPH" and it took place on 30 January 2018. It was delivered by SURFsara and USFD. 21 people attended and, by the time of writing, the recording has been viewed 73 times.
3) The third webinar titled "Lattice Boltzmann method for CompBioMed (incl. Palabos)" was held on 19 March 2018. It was delivered by UNIGE. 24 people attended. Moreover, by the time of writing, the recording has been viewed 655 times.
4) Webinar #4 titled "Introduction to Biomedical Applications on High Performance Computers" was broadcast live on 07 June 2018. The speakers belonged to EPCC and UvA. 19 participants were connected, and 233 YouTube views are recorded up to now.
5) The fifth webinar, "High Throughput Molecular Dynamics for Drug Discovery", was held on 25 October 2018 and delivered by UPF. 12 people participated live and 101 people viewed the recording online.
6) CompBioMed webinar #6 was titled "CompBioMed: Innovations on medical student training", took place on 5 December 2018" and the speaker belonged to UCL. It was followed live by 14 participants and the recording was viewed 35 times up to today.
7) Webinar #7 ("Sensitivity analysis of a strongly coupled cardiac electro-mechanical model") was broadcast on 20 March 2019. The delivering partner was again UOXF. The webinar registered an attendance by 45 participants and was viewed 86 times on YouTube.
8) The eighth webinar titled "The EOSC Digital Innovation Hub: open data services for biomedicine and business" took place on 28 May 2019 and was delivered by EOSC-Hub. The webinar registered 9 live participants and 37 YouTube views.
9) CompBioMed webinar #9, "EUDAT Services for FAIR Data Management", was held on 27 June 2019 and delivered again by Surfsara. 13 people participated and, by the time of writing, the webinar's recording has been viewed 12 times on CompBioMed's YouTube channel.
10) CompBioMed last webinar (#10) was titled "HemeLB – Simulation of cardiovascular flow on high performance computers" and broadcast on 9 September 2019. The speaker belonged again to UCL. 10 people attended and, at the time of writing, the recording has been viewed 22 times.

UvA was in charge of the planning, organisation, hosting and facilitation of the series, in collaboration with the VPH Institute [18].

Training events

3 training events were organised within the CompBioMed project, **for a total of more than 70 live participants and ±4,000 YouTube views**:

1) CompBioMed Winter school 2018 took place at BSC in Barcelona "HPC-based simulations, Engineering and Environment with applications in Bioengineering" on 14-16 February 2018. Depending on the day, between 26-30 PhD students, master students and engineers attended the Winter School. Six CompBioMed travel grants were awarded to the most promising applicants for covering part of their travelling expenses. The recordings of the sessions have been viewed 3,583 times in total on CompBioMed's YouTube channel. BSC was in charge of hosting the event and its organisation in collaboration with PRACE, and speakers belonged to BSC, SURFsara, UvA, USFD, Microsoft, Evotec, UCL, UPF, Accelera.

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2) CompBioMed second training event was held in connection with the VPH2018 bi-annual conference in Zaragoza on 4 September 2018 and was titled "High Performance Computing for the VPH". 17 people participated and the YouTube recordings were viewed 291 times. UvA was in charge of its organization and speakers belonged to SURFsara, UCL and UvA.
3) CompBioMed Winter school 2019 ("Short course on HPC-based Computational Bio-Medicine") took place in Barcelona, at BSC on 13-15 February 2019. 25 people participated and the recordings were viewed 109 times. 5 travel grants were given to a selected number of participants for covering part of their travelling expenses. BSC was in charge of its organisation in collaboration with PRACE, and speakers came from BSC, UvA, UPF, Accelera, Bull, USFD, Evotec, UCL and SURFsara.

University Education courses

1) CompBioMed in medical curriculum at UCL: The Student Selected Component (SSC) of UCL's Medical School Curriculum provided an opportunity to educate medical students in Years 1, 2 and 6. This was an entirely novel training element introduced in CompBioMed, albeit not originally planned. **60 students in total** (20 each from years 1 and 2 in 2017-2018 and 20 from year 1 in 2018-2019) have successfully completed the course. The course was delivered by UCL and the HPC workshop was run by EPCC.
2) CompBioMed in science and engineering curriculum at UCL: The undergraduate research project course Advanced Practical in Molecular Biology has been designed to give Year 3 biomedical science and biotechnology students experience in experimental and computational aspects of metagenomic analysis on environmental soil samples collected from London parks. **185 students in total** (85 in 2017-2018 and 100 students in 2018-2019) took this course as part of their degree programme studies (BSc Biochemistry, BSc Molecular Biology, BSc Biotechnology and MSci Biochemistry). The course was delivered by UCL and the HPC workshop was run by EPCC.

Other training activities

1) Two CompBioMed sessions were held within the PATC Course: "HPC-based simulations, Engineering and Environment" organised by BSC (Barcelona, 14-16 February 2017), attended by approximately 40 participants.
2) The BioExcel & CompBioMed joint workshop on "Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences" [19] was held at UCL, London on 30 May 2017. The workshop was attended by 25 participants, mainly coming from the two CoEs.
3) The 3rd edition of the VPH Summer School series took place in Barcelona on 18-22 June 2018 and focussed on data integration, model verification and validation. CompBioMed gave its contribution with a talk and the organisation of a hands-on session by UPF and BSC.

Furthermore, the Training Portal [20] and Training Repository have been developed, populated and continuously updated. The Portal aims to be a sustainable open access educational and training resource for Computational Biomedicine, including HPC.

All the resources on the Training Portal will be advertised and disseminated as one unique consistent Training Package. A flyer has been prepared to allow its promotion and dissemination.

Task 3.6: Conference/Workshop Planning (M1-M36)

The CompBioMed workshops and events have been designed to promote the Centre of Excellence, as well as the project's results and success stories, as described in detail in D3.4 [13], D3.5 [14] and D3.6 [3]:

1) The first workshop was the Cloud & High Performance Computing in Biomedicine workshop [21] (UCL, London, 27 April 2017). This meeting was attended by 70 participants.

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2) The dedicated CompBioMed conference session [22] was held at PRACEDays 2017, the central event of the European HPC Summit Week held at BSC over four days (15 – 18 May 2017).
3) The BioExcel & CompBioMed joint workshop (UCL, London, 31 May 2017) on "Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences" [19] was attended by 92 participants.
4) On 15 September 2017, CompBioMed and OpenMultiMed held a Joint Session on "Multiscale Computing in Medicine: Clouds on the Horizon?" at the EPMA 2017 (The European Association for Predictive, Preventative & Personalised Medicine) World Congress in Malta and was attended by 25 participants.
5) On 27 September 2017, CompBioMed helped Alces Flight, a CompBioMed Associate Partner, to set up a workshop based around the Galaxy application which was attended by 15 people.
6) The CompBioMed "The Virtual Human" IMAX event on 27 September 2017 was part of the London Science Museum Lates series. The hour-long event described recreating a human being in silico and included an IMAX film composited on BSC's MareNostrum supercomputer. The performance took place in front of a sell-out audience of 400 members of the general public, along with invited attendees from academia, industry, the clinic, the UK government, and the media.

We ran a strong dissemination campaign for this event, including postings on Science Museum twitter account (boasting 667k followers) which generated over a million twitter impressions.

7) The "Cardiac Modelling, Fluid-solid Interactions and Biomedical Flows" workshop was held in Amsterdam on 28 March 2018. This was a collaborative effort between CompBioMed and the Spanish Network of Excellence 'The Virtual Heart' (VHeart). This event was attended by 35 members of the two projects.
8) The "Container Technology in Cloud and High Performance Computing Research and Commercial Applications" workshop was held in Amsterdam, Netherlands on 29-30 March 2019
9) On 29-30 May 2019, a meeting on "HemeLB: cardiovascular modelling and simulation in UKCOMES" was held in collaboration with UKCOMES project in London.
10) The CompBioMed Conference 2019 was held on 25-27 September 2019 in London with 3 parallel sessions over 3 days.

Furthermore, CompBioMed partners have participated to date in 176 dissemination events. Listed in D3.4 (section 6.2.2), D3.5 (section 7.2.2) and D3.6 (section 7.3.2)

The WP held teleconferences on a monthly basis to plan the work, share information on the different tasks and update each other on the different activities that are simultaneously taking place within – and in some cases beyond - the WP.

Significant Results

1. The IMAX event 2017 was attended by 400 members of the general public
2. The London Science Museum Lates event 2019 was attended by over 400 members of the general public
3. "The Virtual Humans" film release, with over 11,600 film views
4. Publication of 83 scientific papers
5. Our training events attended by more than 600 people globally and their recordings viewed 5,000 times
6. 245 medical and life science students educated
7. Participation in 170+ major conferences and workshops
8. Over 700 followers of CompBioMed Twitter account and over 1 million Twitter impressions

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9. A total of 14,400 views from CompBioMed YouTube page
10. 200 delegates attended the CompBioMed Conference 2019

6.4. Work Package 4: Innovation and Sustainability

Work Package Objectives

The objective of this work package was to establish our Centre of Excellence's relationship with wider industrial stakeholders, clinical and commercial, but also public sector/academia. The main objective was to ensure that the Centre of Excellence created and implemented both a strong sense of innovation and sustained its leadership in the use of HPC for biomedical research. Other objectives included creating our Innovation Plan [23] and our Sustainability Plan, coordinating the Centre's incubation activities and Innovation Exchange Programme, and establishing links between the Centre and European Technology Platform for High Performance Computing [24] (ETP4HPC) contractual Public-Private Partnership (cPPP) in HPC.

Work Towards Objectives

CompBioMed has always had innovation at the core of its research, and WP4 ensured that the results stemming from this research were regularly assessed (D4.2 [25] and D4.4 [26]) to determine their future prospects in the field. After writing the Innovation Plan (D4.1 [23]), this was implemented within T4.4, which included but was not limited to capturing both the Results (Foreground) and the Background IP resulting from the project and through regular reports at all the WP teleconferences. WP4 coordinated the incubation activities and interaction with the ETP4HPC. The Sustainability Plan (D4.3) was produced in M30 of the project but is not currently available publicly, it outlined how innovation will lead us forward in the centre

Work completed per Task

Task 4.1: Innovation Plan Development [M1-M6]
The Innovation Plan was delivered and is publicly available via the CompBioMed website [23]. It was presented to the Innovation Advisory Board (see below). Whilst this Task is complete, we have maintained the Innovation Plan, keeping it up to date, so that it was both used and useful. This included introducing the Innovation Panel at all WP meetings and dedicated meetings to discuss possible updates. Recently, the Results IP, monitored within our IP Registry, were used to contact the IP owners directly, regarding the shaping of our Innovation Plan.

Task 4.2: Incubator Co-ordination [M1-M36]
This task aimed to foster academic and industry partner collaboration to exploit HPC and associated e-infrastructure by raising awareness in industry, especially in SMEs, making available and providing support for the use of cutting edge HPC facilities. To this end we established a "Central Incubator Register" (CIR) as a point of contact for SMEs within the biomedical field. Our CIR presents an overview of existing incubators both internal and external to the project partners and is publicly available via our website [27]. There are currently both start-up and spin-off companies that have stemmed directly from work produced within CompBioMed: BSC's Dr Mariano Vazquez has formed ELEM Biotech as a BSC spin-off company [28] and EnsembleMD has been established by Prof Peter Coveney.

Task 4.3: cPPP Engagement [M1-M36]
This task created links to the ETP4HPC [24], an organisation representing the HPC contractual Public-Private Partnership (cPPP) and established a forum and mechanism for the HPC industry to interact with computational biomedicine community, whether in academia, hospitals or SMEs. A member of

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CompBioMed attended all ETP4HPC Board meetings to ensure that we were kept up to date with all the activities within this realm. To further facilitate this interaction, CompBioMed and ETP4HPC co-presented two Birds-of-a-Feather (BoF) sessions at ISC in 2018 and 2019 and another at SC19.

Task 4.4: Sustainability Plan Development [M1-M36]

Within this task, the Sustainability Operations Procedure (SOP) was developed, to ensure minimisation of damage through poor service. The SOP aimed to perpetuate the Centre beyond the initial 3 funded years. The additional 4 years of funding that the centre has now received will enable us to further these operations. We will facilitate biomedical users' access to supercomputers and Cloud computing systems, fulfil the needs of these users for data management and long-term data stewardship keeping up to date with the latest requirements of security and privacy in our data.

We have and will continue to support both closed and open software source models offering suggestions for possible licensing opportunites. This is done through management of the IP Register to follow the progress of our partners IP. We included our Innovation Capture Process tool, to help determine the status of any new IP, any associated information that is missing, and what the next steps are to achieve exploitation with its possible revenue streams.

As part of this task, the Innovation Advisory Board (IAB), was created, maintained and managed. After the first meeting, the membership was expanded to include medics as well as industry members. We have convened in-person meetings on three occasions and found that the suggestions were particularly useful, and we have acted on these, strengthening our SOP. More information on these suggestions and how we enacted them can be found in D4.5 [2].

Task 4.5: Pre-commercial Activities [M24-M36]

This task started in month 24 and conducted a study involving CompBioMed Core Partner users, Associate Partner and IAB members in order to determine the benefits of using HPC in the commercialisation pathways of computational biomedicine applications which can be seen in D4.5 [2]. We have undertaken a study to identify key functionalities where commercialisation is viable, or even favourable, over adopting academia-driven solutions and illustrated at which stages along this path use of HPC is being adopted in the area of computational medicine. We have formulated a set of commercialisation exemplars in collaboration with our industrial partners which are set out in D4.5 [2].

Task 4.6: Coordinate the Innovation Exchange Programme (1M-36M)

This task has established the Innovation Exchange Programme (IEP), which has recently been rebranded the Visitor Programme to make it more appealing to those outside the project. The IEP acts as a focus for technology transfer between academia, healthcare and industry in the field of biomedical computing. Since the start of our CoE, we have enabled forty exchange visits and these visits are noted and displayed on our website [29]. We have undertaken a Memorandum of Understanding with HPC-Europa3 to facilitate more exchanges through their Transnational Access scheme. We have also added value to enable both potential hosts and potential visitors to post their wishes on the website, so that they can locate suitable matches. Further, this will also be a key part of the start of CompBioMed2 in which we have enabled more funds for this service.

Significant Results

1. Three Innovation Advisory Board meetings
2. IAB membership increased from 10 to 17, including 5 clinicians.
3. Joint CompBioMed and ETP4HPC BoF sessions at ISC18, SC19 and ISC19
4. Forty visits enabled by our Innovation Exchange Programme
5. The creation of our Central Incubator Register, which was made public

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6. The implementation of our Innovation Plan, including the Innovation Capture Process
7. The creation and implementation of our CoE's Sustainability Operations Procedure.

6.5. Work Package 5: Resource and Infrastructure Support

Work Package Objectives

This WP facilitated the Fast Track developments in the project by deploying services to support our initial application scenarios by developing an understanding of the immediate, medium and long-term requirements of the applications in the biomedical research community. The needs included facilities for computation, data services, as well as (wide area) connectivity and appropriate security. We related application requirements to characteristics of current computational and storage architectures and established best practice recommendations for efficiently mapping biomedical applications to production resources. We worked to increase the number of biomedical applications deployed and used on leading HPC resources in Europe and ensured that leading HPC providers were well informed about future application needs in the biomedical community. Finally, we worked to streamline and strengthen the data infrastructure used by the biomedical applications on large-scale resources.

Work Towards Objectives

The Work Package had regular monthly meetings, with regular and active participation by the partners involved. It investigated the characteristics of the CompBioMed Fast Track applications and produced a set of requirements and best practice guidelines to run biomedical simulations efficiently on HPC and Cloud computing resources.
The partners involved in the WP worked to provide an exhaustive description of the computational characteristics of the different tools and simulation codes used by the community.
WP5 also created and maintained, the CompBioMed Software Hub [30] (see D5.1 [31]) a service offered to the computational biomedicine research community to facilitate access to the resources developed, centralised, and coordinated by the CompBioMed project. The Software hub was substantially enhanced halfway through the project in terms of its content and ease of use.

Work completed per Task

Task 5.1: Characterizing Biomedicine Community Application Requirements [M1-M6]
This task, concluded in month 6, worked to identify the compute, data service and connectivity requirements for the software that were primarily employed within the three research areas of CompBioMed: cardiovascular, molecularly-based and neuro-musculoskeletal medicine. The deliverable D5.2 *Report on computing and data needs of the biomedical community* [32] reports on the results of the work done in this task.

Task 5.2: Access Mechanisms for Computing and Data Resources [M7-M12]
In Task 5.2, we provided a technical analysis of the main mechanisms adopted to access the services offered by HPC centres and cloud providers. We analysed the requirements of CompBioMed users in terms of infrastructure usage to provide the basis for a more detailed study of the needs for non-conventional access models (such as advance reservations, on-demand access) and investigated the feasibility of implementing such mechanisms on the side of the HPC providers. The results of this study into alternative access models are reported in D5.3 *Report on access mechanisms to HPC systems* [33].

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The results of task 5.2 have been used to establish improved understanding of the technical requirements and possible limitations of new access mechanisms to HPC resources, and to identify the types of application that would benefit from higher quality of service and on-demand access.

Task 5.3: Efficient Infrastructure Usage by Community Codes (M1-M36)
In this task we focused on the deployment and performance analysis of CompBioMed applications on cloud and HPC resources the results of which can be found in D5.6: *Report on Efficient HPC Usage by the Biomedicine Community* [5]. Through the compute time allocations on the infrastructure made available through CompBioMed, all research partners have deployed and/or profiled their codes on the various architectures (including GPUs, clouds) for real biomedical applications. CompBioMed applications such as Alya, HemeLB, HemoCell and BAC, which are able to operate at the scale of many hundreds of thousands of cores, have also been deployed and tested on several of the largest supercomputers in the world such as Summit, Titan and Blue Waters.
This WP is working to promote the use of container application solutions for efficient and portable deployment of CompBioMed applications. We organised a meeting of Container providers and users at SURFsara this year which was very well received. SURFsara and USFD have collaborated on the deployment of the openBF cardiovascular software on SURFsara's Cloud and HPC system using Singularity containers while other partners are working with this technology for their simulation codes (e.g., UCL with Docker and BAC, UvA with Singularity and Hemocell, BSC with Singularity and Alya).

Task 5.4: Increasing Uptake of Existing e-infrastructures and Alignment with International Projects [M1-M36]
We worked with the scientific user community of the CoE to identify usage and application requirements which could make use of the various computing resources within Europe and beyond.
Target partners have been identified as points of contact within the European projects PRACE [34] (SARA, BSC, UEDIN), EUDAT [35] (SARA, UCL) and EOSC-hub [36] (SARA, UCL) with the purpose to assess and improve the applicability of these European infrastructure projects to biomedical applications and bring them to the CompBioMed community by promoting services and solutions to the consortium.
UOXF and BSC were awarded 54.60 million core hours on MareNostrum over 12 months (first of a 2-year allocation) for their project "In silico drug trials in the beating ischaemic human heart". Additionally, UCL is lead partner in a number of awards of time on the following International platforms:

- The BlueWaters machine at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, comprising 80M core hours, an NSF funded award with Associate Partner, Rutgers.
- The Titan machine at Oak Ridge National Laboratory (ORNL) in Tennessee, comprising 85M core hours.
- The Summit machine at ORNL, Tennessee, within and outside the initial award to Titan
- A project wide PRACE allocation, available on the MareNostrum machine at Barcelona Supercomputing Centre, comprising 400,000 core hours.
- A project wide PRACE allocation, available on Piz Daint at the Swiss National Supercomputing Centre (CSCS) of 7100 node hours.
- The SuperMUC machine at Leibniz Rechenzentrum (LRZ) part of the Bavarian Academy of Science, Germany, comprising 32M core hours.
- Early access (unrestricted) to SuperMUC-NG since January 2019
- The Theta machine at Argonne National Laboratory (ANL)

The US-based access is from US-based DOE INCITE awards with Prof Coveney as PI

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Task 5.5 Integrating Compute and Data Infrastructures [M1-M36]

We have supported the biomedical community, enabling existing data infrastructures to better work with large-scale computing and data service resources. The analysis conducted for the preparation of D1.3 *Data Management Plan* [7] and of D5.2 *Report on computing and data needs of the biomedical community* [32] was used to identify the data formats adopted by different CompBioMed partners, characterize the software required for the pre- and post-processing of simulation data and the tools and policies needed to access, move and categorize the input and output data files created and used during the simulation. EUDAT services were identified as the key data services within the consortium and we have worked to formulate and undertake a set of technical tasks to improve the working of our data management tools and storage services with large scale resources.

We have worked with key biomedical applications to determine suitable data transfer and storage mechanism for pre- and post-execution of the applications, including long term storage with suitable access control mechanisms. We have built on the knowledge acquired in that study to improve the service and to extend its applicability to different centres and will continue this work into CompBioMed2. The deliverable D5.5: *Preparing data infrastructure for large-scale resources: report on the optimization activities* [37] contains a summary of the work done in this task.

Task 5.6: Create [M1-3] and Maintain [M4-M36] a Community Software Repository

This task focused on the creation and maintenance of a centralized repository infrastructure, the CompBioMed Software Hub [30], for the applications made available through CompBioMed. The repository allows for easy access to the resources developed, centralised, and coordinated by the CompBioMed project. It should be noted that the hub does not host any software itself. This decision was taken because popular software repositories like GitHub offer all of the desired functionality for such purposes. There is therefore no need to replicate a similar infrastructure. In addition, linking to the projects, instead of hosting a copy, guarantees up-to-date version control and avoids redundancy that would be confusing to potential users.

The hub contains descriptions, information about HPC usage, links to relevant websites and media in the form of webinars or training videos, for 17 computational biomedicine services and end-user solutions developed by our Core and Associate Partners.

The repository is currently being updated to include the results obtained in Task 5.3 and Task 5.5 for the definition of best practices for e-infrastructure application usage (D5.4 [38] and MS16) which contains information about the usage of the software, including deployment on specific platforms, and the usage of the project's Application Pipelines. It is currently available for the Alya software with a plan to complete this before the end of the project.

The Hub also provides a centralised assistance web page connecting CompBioMed users and partners. This deliverable results from the work of all the partners involved in this task, namely UNIGE, SARA and BSC, but it was also discussed in a larger group, including UCL, UvA and CBK. In successive stages of CompBioMed, the CompBioMed Hub will be populated with further software.

Significant Results

1. Characterisation of CompBioMed applications computational requirements and infrastructure usage.
    - D5.2 Report of computing and data needs of the biomedical community [32]
    - D5.3 Report on access mechanism to HPC systems [33]
    - D5.5 Preparing data infrastructures for large-scale resources: report on the optimisation activities [37]
    - D5.6 Report on Efficient HPC usage by the Biomedicine community [5]
2. CompBioMed Software Hub [30]
    - D5.1 Release of Community Software Repository [31]

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- D5.4 Report on best practices for e-infrastructure application usage [38]

6.6. Work Package 6: Empowering Biomedical Applications

Work Package Objectives

The objectives of WP6 were to expose and publish existing end-user solutions to facilitate their uptake to a wider range of biomedical applications. For those already existing and widely used, it extended their usability and value for existing and new biomedical applications on HPC and data service infrastructures. This required them to be well tuned to HPC infrastructure in performance, reliability and security.
This WP promoted automation, particularly in the industrial and clinical application domains by establishing scalable and easy-to-use workflow facilities.

Work Towards Objectives

New end-user solutions were identified and published in a report that was available online and has been extended through the software hub reported in WP5. Existing solutions were extended from USFD, UPF, UCL, BSC and UNIGE through collaborations with both internal and external partners. USFD, UvA, BSC and UCL worked on tuning their solutions to HPC environments with increasing compute power in aiming for forthcoming exascale machines.
Partners have collaborated greatly throughout the project to extend and adapt their solutions for use with our industrial partners to exploit their commercial capabilities. Through the project, ELEM Biotech has been established, providing software-as-a-service to biomedical industries. EnsembleMD is another spin-off company from the work conducted at UCL.
USFD and BSC developed workflows that can be automated and used to enable data to flow from one site to another, including one workflow (CT2S described in deliverable D6.6 [2]) where one of the sites is a UK hospital.

Work completed per Task

Task 6.1: Expose and Publish Existing Solutions (M1-M18)
All 11 planned fast track solutions were deployed followed, in some cases, by a deep track development (e.g. the rewriting of ShIRT and coupling between existing solutions such as openBF/HemeLB/Alya). D6.1 *Report on existing solutions in support of biomedical applications* [39] was produced at M12 as planned; in addition, the aforementioned report on end-user solutions was released at M15.

Task 6.2: Emerging Use Cases for Existing Solutions (M12-M36)
Task 6.2 started as planned at the end of M12, and was informed by the end-user report which was updated in D6.4 [40] (M24) and D6.6 [2] (M36) ensuring it was current throughout the life of the project.
Our end-users are incredibly diverse, resulting in one-solution-fits-all not being a possible model for our CoE. We have therefore worked with individual use cases to determine where they fit most appropriately with other workflows within the project. For example; work conducted at USFD was used to inform a similar workflow at BSC. Also models used at Eindhoven University of Technology are being used to support tools developed by LifeTec Group. A detailed report on how end-users have influenced and supported the development of each CompBioiMed application will be included in D6.6 *Final report on the end-user solutions* [2].

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Task 6.3: Adaptation to Commodity HPC Infrastructures (M12-M36)

Throughout the project a number of our partners have worked with commodity HPC infrastructures. The use of GPUs has proven to be a useful method for enhancing various codes including those used by Acellera. More information on all the activities in this area can be found in D6.5 [41] which was published in M24.

In addition to this the use of Cloud computers or Cloud HPC infrastructures is being extended by a number of partners (Associate and Core Partners). EnsembleMD's flagship product is a cloud-based application designed to facilitate the calculation of drug binding affinities to aid in drug development activities. Their products are heavily dependent on containerization technologies to allow portability across cloud platforms.

BSC is improving cloud-deployment of Alya. In particular tests have been conducted on Oracle Cloud, with very good results.

Task 6.4: Develop and Deploy an Informatics Platform which will Store all the Data Collected and Processed within CompBioMed (M1-M12)

Originally, the task had planned to lead to the deployment of an instance of the p-medicine informatics platform [42] to allow biomedical researchers to analyse their data, perform queries and extract content to initiate their modelling and simulation activities. All data within the data warehouse that reside at the core of this informatics platform are fully anonymised. However, this activity was subject to change based on the user needs analysis conducted by work packages 2, 5 and 6 to assess the data requirements of the project researchers and associate partners. The resulting system arising from task 6.4 was designed to meet the detailed requirements outlined in deliverable D1.3: *Data Management Plan* [7].

CompBioMed has four separate tasks/deliverables that depend on understanding the project's data requirements. To understand the requirements of the project, a data working group was formed to survey the requirements of the consortium. A summary of the results of this survey can be found in D6.2: *Deployment of Project Informatics Platform* [43].

The requirements gathered through this activity pointed to a system capable of storing arbitrary data in many different file formats, which can be shared with other users and preserved for the long term. It is beyond the scope of the CompBioMed project to develop such a system from scratch, but fortunately it is also unnecessary. The EUDAT [35] project, started in 2011, aims to provide Europe's scientific and research communities with a sustainable pan-European infrastructure for improved access to scientific data. EUDAT, therefore, exists to work with projects such as CompBioMed, and provides an attractive means for such projects to meet their data management and preservation obligations. Within CompBioMed there are a number of common partners with EUDAT namely, BSC, UEDIN, UCL, SARA.

The EUDAT B2SHARE service allows data to be shared openly or kept private. Regardless of whether deposited data are made open or kept private, metadata records submitted as part of a data deposit are made freely available for harvest via OAI-PMH protocols. Accessible data are made available directly to users of EUDAT CDI (Collaborative Data Infrastructure) [44] services through graphical user interfaces and application programming interfaces. We have deployed our own instance of the B2SHARE software, linked to the wider EUDAT infrastructure through the B2HANDLE and B2FIND services, to publish data for third-party use. An instance of the B2SHARE service has been deployed on resources at CompBioMed partner UCL, with 100TB of storage allocated to the project from UCL's resources.

This system is now available for CompBioMed researchers to store and share data, and we have developed metadata standards and conducted pilot projects that exploit this service as part of the end user's day to day workflow.

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Task 6.5: Workflow Infrastructure Deployment (M1-M36)
7 workflows have been deployed and profiled in the project HPC systems using different workflow management systems (WMS). The USFD workflow for the NMSK solution boneDVC has been profiled in Archer (UEDIN Tier-1) using the Taverna WMS. The in-stent restenosis model developed by UvA has been ported to the Lomonosov 2 supercomputer in Moscow using the MMSF and associated MUSCLE WMS for strongly coupled workflows. Partner UCL used the RADICAL WMS from the Associate Partner Rutgers University for the execution of large-scale hybrid application such as those of the BAC solutions for the prediction of binding affinities between molecules and target proteins. More details are available in deliverable D6.3 *Report on Workflow system provision* [45]. An update on workflow development, deployment and testing will be reported in deliverable D6.6: *Final report on the end-user solutions* [2].

Significant Results

1. Analysis and identification of end-user solutions within consortium
2. HPC end-user categorisation
3. Large-scale data transfer workflow
4. Development of workflow linking hospital and university infrastructures and dealing with management of patient-sensitive data
5. OpenBF deployed on SARA's Cloud and Cartesius HPC
6. Development of HemeLB and BAC to run on emerging exascale machines

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7. Conclusion

This deliverable gives a summary of the extensive work that has been done in the project over the last 3 years. Although the report has been written in terms of the individual work packages it is clear that there has been a lot of inter-WP collaboration to make the project successful and to achieve its goals. We have had wide and significant impact on the general public not least through our Virtual Humans film and the outreach activities related to that in addition to the second event at the Science Museum Lates events on Quantum Computing that coincided with the CompBioMed Conference. Our expansive list of Associate Partners also shows that we have had influence in industrial and academic institutions. Our clinical impact can be evidenced through our collaborations between Core Partners and local hospitals to the point of working directly with clinicians in the hospital to determine the applicability of models through to directly analysing patient data in our simulations. Furthermore, we are working with early career clinicians, in our teaching courses for biomedical and medical students and were pleased to welcome some of these to our conference in September 2019. This aspect will be furthered in CompBioMed2 as we roll it out in other European institutions. The research work that has taken place has involved both new and existing collaborations, enabling results that may have taken much more time on an individual level. The HPC centres have worked closely with us to ensure that compute time is readily available to enable our research to be run efficiently and effectively.

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