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CompBioMed2

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D6.1: Report on the Establishment of the Community Engagement

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1 Version Log

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3 Definition and Acronyms

Acronyms	Definitions
AHM	All Hands Meeting
BSC	Barcelona Super Computing
COCIR	European Coordination Committee of the Radiological, Electromedical and Healthcare IT Industry
CoE	Centre of Excellence
CPU	Core Processing Unit
CRO	Contract Research Organisation
DNA	Deoxynucleic Acid
DoA	Description of Action
EC	European Commission
EFPIA	European Federation of Pharmaceutical Industries and Associations
EU	European Union
GCP	Good Clinical Practices
GLP	Good Laboratory Practice
GPU	Graphics Processing Unit
GSP	Good Simulation Practices
HPC	High Performance Computing
HTA	Health Technology Assessment
ICH	International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use
IHI	Innovative Health Initiative
IMI	Innovative Medicines Initiative
ISW_CoP	InSilicoWorld Community of Practice
LRZ	Leibniz Supercomputing Centre
OECD	Organisation for Economic Co-operation and Development
OLA	Operational Level Agreement
SLA	Service Level Agreement
SSC	Student Selected Component
UCL	University College London

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UEDIN	University of Edinburgh
UNIBO	Alma Mater Studiorum – Università di Bologna
UPF	Universidad Pompeu Fabra
USFD	University of Sheffield
UvA	Universiteit van Amsterdam
VPH	Virtual Physiological Human

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4 Public Summary

Starting from a preliminary analysis of the engagement needs, it emerged that the computational biomedicine domain is transitioning from a pioneering to a more mature stage, where the role of stakeholders differentiates into a value chain that spans all the activities between fundamental research and socioeconomic impact.

For these reasons, the engagement activities have also been differentiated depending on the target groups, namely the research community, reached through the participation of the CompBioMed Centre of Excellence (CoE) in various workshop and conferences; the biomedical industry, for which we distinguish 'partnerships' and 'collaborations' between each Core Partner and an external body, and the general public.

Engagement activities also take the form of Service Provision, with the establishment of an Internal Helpdesk for end-users and the Visitor Programme, Training and Retraining initiatives in the fields of computational biomedicine and advanced HPC training.

Last but not least, the partners are using the In Silico World Community of Practice (ISW_CoP) as an engagement portal for different stakeholders. ISW_CoP is an online community based on Slack and operated by UNIBO to promote the development of a community in which all practitioners of *in silico* medicine working in academia, industry, consulting firms, governmental and non-governmental organisations can discuss, collaborate, and co-develop best practices in the field.

In particular, the community hosts High Performance Computing (HPC) support channels, that capitalise on the expertise and knowledge of HPC experts among the CompBioMed partners to offer free support to those who would like to improve the performance of their computational biomedicine solutions with high performance computers.

5 Introduction

The needs for stakeholder engagement within the CompBioMed2 CoE are to some extent specific but can also be incorporated into those of other initiatives. Partner UNIBO at the outset explored these needs with the collaboration of two not-for-profit international organisations that represent the computational biomedicine community: the VPH (Virtual Physiological Human) Institute[1], which represents primarily the academic and clinical stakeholders, and the Avicenna Alliance[2], which represents various industrial and commercial stakeholders.

This preliminary analysis, based on informal interviews with members of the two representative organisations, suggested that the computational biomedicine domain is

[1] https://www.vph-institute.org/
[2] https://avicenna-alliance.com/

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transitioning from a pioneering stage where the interactions are mostly pre-competitive, to a more mature stage where the role of stakeholders differentiate into a value chain that spans all the activities between fundamental research and socioeconomic impact.

The pioneering stage involves a number of actors small enough to be satisfied with the engagement provided by the membership in the two aforementioned associations, the networking within the consortia of the EU-funded projects, and a few specialised conferences, such as the biennial VPH conference. Furthermore, the EC previously funded some coordination and support actions in this domain (STEP, 2006-2007; VPH NoE, 2008-2013; VPH-FET, 2010-2011; ITFOM, 2011-2012; Discipulus, 2011-2013; PHS Foresight, 2012-2014; Avicenna, 2013-2015), which ensured considerable levels of networking.

As the domain transitioned to a stage with stakeholders operating across the entire value chain, the existing forms of engagement started to appear insufficient. The primary demand that emerged from the experts we informally interviewed was the need for a place where experts of all different backgrounds could exchange best practices. For this, we decided to develop a Community of Practice, defined as "a group of people who share a concern or a passion for something they do and learn how to do it better as they interact regularly".

Starting from this analysis, partner UNIBO designed an online Community of Practice called In Silico World (ISW-CoP). ISW-CoP is a private social network based on the Slack technology[3], and a twin website[4], that is used primarily for outreach and to share persistent content.

In approached the creation of the Users' Engagement Portal for CompBioMed2, as planned in the Description of Action (DoA), we felt compelled to develop synergies with other initiatives that were also converging toward the creation of such a Community of Practice.

Another factor that we had to consider in developing the engagement activities was of course the COVID-19 pandemic. From early 2020 all physical meetings and any other form of in-person networking became practically impossible, and all the engagement efforts had to be moved online. Our expectation was that the opportunity to combine our effort with that of other initiatives, could reduce the negative impact of such a situation. We have found in many aspects this shift to online working has benefited our networking, allowing more people to meet that wouldn't normally be able to travel. However, in other aspects it has reduced our effectiveness in direct networking. Both opportunities and threats related to the pandemic will be demonstrated throughout this document.

Considering all of this, and to reduce the amount of duplicated effort, it was decided not to create a separate Users' Engagement Portal but rather to develop our users' engagement strategy in collaboration with the In Silico World Community of Practice.

In the following we present the engagement activities separating general engagement of stakeholders, services to the community, and the development of the Community of Practice.

[3] https://insilicoworld.slack.com/
[4] http://insilico.world/

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6 The stakeholders

Computational Biomedicine solutions potentially affect a wide range of stakeholders. We use the term solution, instead of the generic term code, because in most cases a computational biomedicine solution requires a combination of codes, data, and standard operating procedures to be useful. These enable the solution to be used for the specific purpose they were intended, usually referred to as Context of Use.

The first group of stakeholders is represented by the Developers of Computational Biomedicine solutions. In addition to developing some important solutions, the CompBioMed Centre of Excellence provides a number of services to help other developers improve the scalability and the computational efficiency of their codes.

The second group are the users. Computational biomedicine solutions can be used for three main purposes: biomedical research (Research users), as decision-support systems in the clinical practice (Clinical users), and as tools for the development and the assessment of medical products (Industrial users). All these users require dedicated training, so we identify a fourth group of users as the educational users.

Around developers and providers, we can identify other stakeholders, along the specific value-chains. For the developers, beside the users, we can identify the manufacturers of HPC systems (HPC Manufacturers), with whom the developers should employ codesign activities for designing future and exascale HPC systems.

The clinical users are paid by the Payers (a variety of public or private entities that in each country are responsible for paying healthcare) and serve the Patients. The industrial users are authorised to sell their medical products by Regulators and sell their product to Healthcare Providers.

The educational users teach Students (mostly in medicine, biology, bioengineering, and biophysics degrees).

Lastly, we consider two horizontal stakeholders, the Policy Makers, regional, national, or at EU level, and the Public at large.

The tree below provides a hierarchy using just one example for each stakeholder group, or organisation representative of such group.

- Developers ➔ Partner UNIBO
    - HPC Manufacturers ➔ European Technology Platform for High Performance Computing
- Users
    - Research Users ➔ Centre for Metabolic Bone Diseases, University of Sheffield
    - Clinical Users ➔ Sheffield Teaching Hospitals Metabolic Bone Centre
        - Payers ➔ UK NHS England
        - Patients ➔ International Osteoporosis Foundation, patients' chapter

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- Industrial Users ➔ European Federation of Pharmaceutical Industries
  - Regulators ➔ European Medicine Agency
  - Healthcare providers ➔ European Health Management Association
- Educational Users ➔ UCL undergraduate degree programme in Biochemistry
  - Students ➔ all students in UCL biochemistry programme
- Policy Makers ➔ members of the EU Parliament Committee on Research (ITRE)
- Public at large

7 Engaging with Stakeholders

The engagement activities directed towards the various stakeholders (researchers, industrialist, public) have been differentiated depending on the target groups; the specific activities are described in the three sections below.

7.1 Engaging the Research Community

Working together with WP1, we are engaging with the research community through the participation of the CompBioMed consortium in various workshops and conferences where we promote CompBioMed results and success stories for interested audiences, to encourage the development of the Computational Biomedicine community and to raise awareness of the domain. D1.3: *Dissemination Action Plan* highlights some of the conferences we have or intend to participate in. As part of WP6 (Task 6.1: Engagement), and within the limits imposed by the COVID-19 pandemic, we will set up a booth during at least one selected international conference, where we will invite participants to join our community, exhibit available solutions and provide information on how to engage with CompBioMed. Initially, we planned to do this during ICT2020; however, this was postponed, so we aim to participate in this when it next takes place.

Other activities include the dissemination of relevant scientific papers from CompBioMed, our Associate Partners and the wider community on our website and social media platforms (LinkedIn, Twitter, YouTube). Currently (Mar 2021) we have 100 followers on our new (Aug 2020) LinkedIn company page, over 1150 followers of our Twitter account and over 600 followers on YouTube. This ensures that we are reaching a diverse range of stakeholders and the consistent increase over the lifetime of our use of these platforms shows our continued engagement. Our webinar series is recorded and made available on our YouTube channel and website, where we are able to answer any questions by the viewers. Finally, we plan to repeat the CompBioMed Conference in 2021 using a virtual platform to ensure maximum participation from a worldwide audience. A smaller fee for participants should encourage those within the EU13 and HPC-poor countries to attend and gain the knowledge of the cutting edge work on Computational Biomedicine. We will also aim to broaden the field to include experimental and clinical practitioners to investigate appropriate methods to integrate them into the computational field and determine areas in which we can further collaborate.

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7.2 Engaging with the Biomedical Industry

Our engagement strategy[5] toward the biomedical industry follows three parallel lines:

a) Engagement through the associate partnership programme
b) Engagement through the Avicenna Alliance
c) Engagement through the Innovative Health Initiative

To this end, under T4.5, UEDIN are maintaining a live document, for internal use only, which tracks Core Partners' active partnerships and collaborations. The aim is to both record all collaborations for input to CompBioMed deliverables and reviews, and to share this information between Core Partners to help create new collaborations and make full use of those that are already underway.

We differentiate between 'partnerships' and 'collaborations' between each Core Partner and the external body, as follows.

- Partnerships are where staff at each Core Partner are directly funded by the body, perhaps as PIs, WP Leaders, Task Leaders, and/or providing technology support (consultancy, data safe haven management, hardware, etc.).
- Collaborations are interactions creating synergies, between staff within the Core Partner and staff at the other body, where the collaborative effort may or may not be funded directly by CompBioMed2.
- Collaborations can also be simply potential collaborations: synergies with CompBioMed that you think may be beneficial.

Each body can be either an EU Project, a CompBioMed User Community, or 'Other', e.g., a US Project, or a Country-led Project.

7.2.1 CompBioMed Associate Partnership Programme

CompBioMed has always been user-focussed and from the start we have endeavoured to bring in institutions that will benefit from and be of benefit to our Centre of Excellence. The Associate Partner scheme allows these institutions to interact more proactively with us, and us with them. We have over 50 Associate Partners, which are listed on our Associate Partner page[5], and we are keen to continue growing. We aim to use our Centre of Excellence to meet and share ideas and resources worldwide.

To ensure the ease of joining as an Associate Partner, we do not require any paperwork. An agreement from the main contact point for a new Associate Partner is provided, and with this the institute is added to the website, along with the contact details of the main contact. They are also included in two mailing lists (compbiomed-all@ucl.ac.uk, compbiomed-associate@ucl.ac.uk) allowing updates to be communicated more easily. For example, they are

[5] https://www.compbiomed.eu/associate-partners/

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kept updated on all our news via the Newsletters and special announcements. New Associate Partners are given first refusal of a talk at the next All-Hands meeting (AHM), which enables them to meet (virtually during the pandemic) and be introduced to the consortium, along with a more in depth explanation of their work.

We currently have 5 Associate Partners from EU13 countries (Poland (4) and Bulgaria) , and a further 2 from countries that are HPC-poor (Portugal and Armenia). We are currently working to increase this from both sets of countries, and hope that the upcoming CompBioMed Conference 2021, will give us the opportunity to engage with a wider audience due to the online nature of the conference and the reduced fees that are enabled through lower overall costs associated with the online format.

7.2.2 The Avicenna Alliance

The Avicenna Alliance is an international not-for-profit organisation incorporated in Belgium, which represents the emerging industrial sector linked to computational biomedicine. Established as a direct result of the Avicenna Coordination and Support Action funded by the EC, since 2016 the alliance has been representing this industrial sector worldwide. The alliance engages with the academic community throughout the VPH Institute, a similar organisation that represents the academic community active in the field. Among the many activities of the Avicenna Alliance, one that is particularly relevant to CompBioMed is the GSP Task Force, described in more detail below.

In a number of fields, good practice standards (GxP) define the consensus, within a community of practice, on how to best conduct a mission-critical activity. In the biomedical field, some important GxP standards are the Good Laboratory Practice (GLP) produced by the Organisation for Economic Co-operation and Development (OECD), or the Good Clinical Practice (GCP), a quality standard for designing, recording and reporting trials that involve the participation of human subjects, produced by the International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH).

In the last few years within the Computational Biomedicine Community of Practice the idea has been growing that the development of a Good Simulation Practice (GSP) standard would help to increase the acceptance of these methods among practitioners, simplify their certification, and ensure better quality in the use of these methodologies. The development of a GSP standard is a long and complex process. To kick-start it, the Avicenna Alliance established, in collaboration with the VPH Institute, a GSP Task Force, a group of industrial and academic experts mandated with the development of a "Green Paper on future Good Simulation Practice standard". Green papers are preparatory documents aimed to stimulate discussion around a policy, published before the policy-making activity starts.

CompBioMed has considerable ties with the GSP Task Force, starting from the two co-chairs of the task force (Prof Marco Viceconti, UNIBO, and Dr Luca Emili, associate partner In Silico Trials). The #GoodSimulationPractice channel on the ISW_CoP sees the participation of various members of the CompBioMed CoE and offers an opportunity for engagement. Recently, Prof Viceconti circulated to this community of practice an open letter entitled "Positioning In Silico

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Medicine as a computationally-intensive science: a call to arms"[6] where he stressed the importance that HPC is going to play in the future development of computational biomedicine. We expect to continue these engagement activities in the near future in collaboration with the Avicenna Alliance and the VPH Institute, aimed to attract this community to the use of HPC methods on a regular basis.

7.2.3 The Innovative Health Initiative

The Innovative Medicines Initiative is one of the most successful public-private partnerships that the European Union has supported. The last incarnation of this initiative, which sees the collaboration of the EC with the European Federation of Pharmaceutical Industries and Associations (EFPIA), has a budget of €5.9bn, funding 166 projects involving more than 5,000 participants.

In connection with the preparation of Horizon Europe, a proposal was presented for a European Partnership under Horizon Europe for Health Innovation called Innovative Health Initiative (IHI). This new Joint Undertaking will see the participation of the EC, EFPIA, but also COCIR (European Coordination Committee of the Radiological, Electromedical and Healthcare IT Industry), MedTech Europe (European trade association representing the medical technology industries), and EuropaBio (European Association for Biotech Industries). This represents nearly the totality of the trade organisations active at the EU level on biomedical products. IHI scope will be much broader than that of the current initiative: the current focus on medicinal products will be extended to every biomedical product including medical devices, medical technologies, and advanced therapy medicinal products.

The CompBioMed consortium has established early contacts with IHI representatives, held on Nov 25th, 2020 where the potential synergies between our Centre of Excellence and IHI were discussed with Patrick Boisseau (MedTechEurope), Annika Eberstein (COCIR) and Magda Chlebus (EFPIA). Topics that were discussed include the participation of IHI consortia to the #Scalability channel of ISW_CoP managed by the CompBioMed consortium; training and retraining activities on HPC in Computational Biomedicine activities specifically targeted at biomedical industries; involvement of IHI in the long-term sustainability of CompBioMed. The Consortium will continue to explore these and other ideas, in order to maximise the engagement of the European biomedical industry in our Centre of Excellence.

7.3 Engaging the General Public

The CompBioMed website has separate sections for the General Public[7] and Clinical Users[8]; however, we see these as very closely linked in terms of our outreach and approach. Whilst Clinical users will have more specialised knowledge of the medical aspects of our work, the

[6] https://secret-viceconti.blogspot.com/2021/01/positioning-in-silico-medicine-as.html?m=1
[7] https://www.compbiomed.eu/general-public/
[8] https://www.compbiomed.eu/home/clinical-users/

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computational aspects will be somewhat unknown to many of them. Therefore, we have the obligation to inform them of all of our work and how it can affect their own research and medical practices, as well as informing the general public on the role that computational simulations could have in the future of their medical care. Traffic to the website is tracked for analysis of the impact of our engagement activities, and whilst the home page has had over 15,000 hits, the General Public page has had nearly 800 and the Clinical Users page over 500. We expect these numbers to increase, and we hope that our current activities outlined below will facilitate such growth.

Within the first 18 months of CompBioMed2, we have been severely restricted in terms of the in-person events that we can host. However, this has had the positive outcome that the research conducted in relation to COVID-19 has ensured the highest possible interest from the general public and resulted in numerous news features and articles. Presently we have appeared in around 7 news reports and 27 news articles and features. A full list with more details will be given in the dissemination deliverable D1.5: Report on Dissemination and Innovation due in M25.

In addition to these news events, we are also planning a follow up film to the Virtual Human, which we plan to premier to a public audience early in 2022, when we anticipate travel will be more accessible again. Although it is possible to host such an event online, we would like to replicate and surpass the success and interest that the event at the London Science Museum garnered in 2017. With the increase in technology around online events, it is possible that we could coordinate an in-person and virtual event to maximise exposure throughout Europe. We would aim to have this in a European country and hopefully within the EU13 or an HPC-poor country. Having learnt from the first film, we will ensure that the voice-over is on a separate audio file so that we can translate this into more languages and disseminate it more widely to these countries early on in the process.

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8 Service Provision

8.1 Internal Helpdesk

As the number of services offered increases, along with the associated demand from end-users, we have created the first instance of a light-weight helpdesk, for internal use only, which will track requests for service access. This will ensure that all end-user questions are dealt with in a timely manner, which will ensure all potential income streams are managed and tracked.

Within the activities of WP4, CompBioMed partner UEDIN, has created this internal helpdesk system using a simple, shared spreadsheet, which ensures that all CompBioMed services are supported fully.

The helpdesk lists every service and provides a contact expert. These experts are in the form of either a mailing list or a collection of email addresses, thus avoiding identifying only a single person, as this tends to constitute a single-point-of-failure.

The various service requests or general questions can be submitted via a Slack channel, the various, multiple CompBioMed contact email addresses, webforms, face-to-face contacts, etc. The helpdesk will be run by a named Helpdesk Operator who will monitor the status of the various, ongoing service requests and general questions. The Operator will provide a triage for the simpler requests and provide a customer-facing conduit to the more technically-minded experts. In general, the operator will be provided by UNIBO; however, the helpdesk is designed to permit multiple operators working concurrently and, as such, any service owner can view and progress their associated tickets as and when they wish.

Lastly, we are considering introducing a Service Level Agreement (SLA) (and associated Operational Level Agreement (OLA)) for each service to measure both progress and quality, and potentially apply these to both CompBioMed and third-party services. This would ensure planned processes and procedures are executed timely and effectively.

8.2 Visitor Programme

The Visitor Programme (originally termed the Innovation Exchange Programme), has been ongoing since CompBioMed1. With interest in the programme growing during the first iteration, we allocated funds in CompBioMed2 to encourage participation from more Partners (Core and Associate) that might not be able to find the funding for themselves. Due to this, we have made the criteria for applying somewhat stricter, with the requirement for a written proposal of work along with an estimate of costs for the travel. This is reviewed by two scientific partners (independent of the visit) to determine if the work assists us to fulfil our obligations and is of benefit to the Centre of Excellence. The funding proposal is reviewed by

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CBK Sci Con, who hold the funds for this. Once an agreement from all three reviewers is received, the host and visitor are notified, and they can commence with the visit.

Due to the outbreak of COVID-19 pandemic, this activity has had to be put on hold, as travel has become more difficult. However, with an increase in Associate Partners from EU13 and HPC-poor countries, we hope to engage with these partners to foster synergistic research projects and enable them to undertake training and use of HPC centres through this scheme in the remaining time of the CoE.

9 Training and Retraining

The training activities of CompBioMed are considered as important players in the engagement of communities and stakeholders, so that they can create awareness about developments and services. During CompBioMed1 there was an effort to provide visibility to a comprehensive set of courses and different activities organized by the partners: the outcomes have been reflected in the initial version of the CompBioMed training repository and the organization of regular webinars every year quarter. In order to provide further impact, CompBioMed2 training efforts have been defined in two separate tasks: training for computational biomedicine and advanced HPC training.

This specification of two training tasks provides the necessary focus to go beyond the existing activities and cover a wider range of topics, so that different communities are reached, and the gaps can be filled by the contents provided by different CompBioMed partners (and possibly the collaboration of external stakeholders). As a general rule, the goals are set to define new and/or improve existing training activities, which may be categorized as biomedical, computational or hybrid according to their contents. Training courses aim at providing specialized knowledge with eminently practical approaches, and as a complement for outreach, the regular series of webinars are kept as open windows to show the work and achievements of CompBioMed partners and collaborators.

9.1 Advanced Training Series

The initiative of advanced HPC training stresses the values of supercomputing and cloud systems as an essential support for large-scale biomedical research. As a general fact, regular HPC-related training within CompBioMed presents the use of these systems to the communities and stakeholders, so that they learn how to integrate them in their everyday activities. However, the scope of the advanced HPC training task 6.4 actually aims at building a comprehensive set of new and/or enhanced courses to teach the required skills to optimize the exploitation of HPC resources with contents on programming, debugging, machine learning, software engineering and/or data management.

As training is keeping a strong practical component, advanced HPC training also stays close to biomedical topics, which are always considered as main motivation and driving force for course developments. Some existing activities from CompBioMed1, such as the PRACE Short Course on HPC-Based Computational Biomedicine organized at BSC (with collaboration from a

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wide variety of partners), were already designed in a hybrid approach between biomedical and HPC content. In that sense, task 6.4 in CompBioMed2 will promote and increase the number of these types of training, using the initial level of expertise and biomedical background of the main target audience, and take learners to the advanced HPC topics.

As a starting point, an understanding of the interests of CompBioMed partners together with communities and stakeholders will define the future catalogue of advanced HPC training. Therefore, the initial efforts were put into the definition of a compact course on essentials of parallel programming, advanced Linux and mastering the use of supercomputers with applied computations: these topics were included in a first event called “Cluster Computing for Computational Science”, where it was possible to combine contributions from SURF, UvA and Acellera. Future activities will look for further collaboration between partners and more advanced topics with applications: in particular, machine learning and sensitive data management are acknowledged as important topics, and further developments may be covering these topics.

9.2 Student Training

A key objective enunciated in the CompBioMed1 proposal was to educate and train the next generation of computational biomedical researchers through new access mechanisms best suited to the community. This community of users is diverse and comes from academia, industry and clinical practice. Specific details of the training programme were described at the time of the original CompBioMed submission. These had an emphasis on the promotion of familiarization with and the sharing of best practice in specific computational elements of the CoE and were directed specifically towards two areas: 1) specialised workshops for researchers actively involved in the development of codes and 2) hands on training focused on simulation software specially designed for the user community. The proposed training programme was to be provided through three major training workshops to be delivered alongside a relevant conference or meeting.

Of especial note during the formulation of the training plan in the first few months of CompBioMed1 was the fact that this community of users have hitherto had a relatively small amount of relevant formal education. Also of note was the involvement of researchers in the CoE with significant roles in university education. As a result, a novel opportunity presented itself that enabled the development and provision of a unique and innovative training programme that twinned the research of the CoE with the educational delivery through taught courses embedded within the formal university curriculum. Whilst the three major training workshops originally proposed were successfully delivered as envisaged, a separate training strand was developed. This education strand comprised taught courses within the university curriculum and was delivered in parallel to medical students and to biomedical science students from academic year 2017-2018 in collaboration with CompBioMed partners EPCC and SURF.

Over the past four years, the CompBioMed Centre of Excellence has delivered training in HPC to the biomedical researchers of the future by integrating the research of the consortium with undergraduate teaching in universities. Training courses developed in this way have been

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delivered as part of the taught curriculum and have also been offered as PRACE training courses for HPC researchers wishing to engage with the field of biomedicine. To date, over 600 students have been trained as part of their taught programme of study, creating a new Community of Practice in Computational Biomedicine. The demographic of this cohort is ~50% female, improving diversity and inclusivity in HPC. In CompBioMed2, this education strand of training was formalised within WP6 as Task 6.2 *Expanding CompBioMed Medical Student Training Programme* and Task 6.3 *Training Computational Biomedicine Researchers*. In addition to the delivery of the courses described in 9.2.1 and 9.2.2, we are working to identify existing courses with computational biomedical content and applications that can be ported to HPC to add to CompBioMed's repertoire of education courses.

9.2.1 Medical Student Training (Task 6.2)

The Student Selected Component (SSC) of any medical school curriculum worldwide is a taught course that allows students to choose a specific topic in a medically-relevant area of interest to them. The SSC provides an ideal opportunity to formally integrate HPC into the medical curriculum and CompBioMed has delivered an HPC-based molecular medicine SSC at UCL every year since 2017-2018. From 2020-2021 CompBioMed has expanded and now offers this SSC to medical students at the University of Sheffield (USFD), in collaboration with UCL, USFD and associate partner Alces Flight. This work has been highlighted in a State of the Practice talk at SC20[9].

The SSC provides students with a theoretical understanding of the importance of the relationship between human microbiomes – the microorganisms present in and on the human body – and human health and provides them with the practical opportunity to use state of the art computational resources to run a metagenomics pipeline. These courses have run with students collecting their own microbiome data and performing experimental work to determine the microbial sequences that are analysed computationally. During the COVID-19 pandemic, microbiome data from databases were analysed computationally, meaning that we were still capable of running the course. Each year the courses are filled to capacity, showing the interest in and enthusiasm for this area of research. Work is currently being undertaken to 1) expand the SSC training beyond UCL and USFD to include the training of medical students at Universidad Pompeu Fabra (UPF), University of Amsterdam (UvA) and the University of Oxford and 2) to develop HPC-based SSCs in cardiovascular and in neuromusculoskeletal research. We are currently working with Associate Partner Dassault Systèmes, with USFD and with UPF to develop HPC-based cardiovascular SSCs for 2021-2022.

9.2.2 Biomedical Student Training (Task 6.3)

An expanded version of the metagenomics SSC has been used since 2017-2018 for a third year undergraduate research project for students taking Molecular Biosciences degrees (MSc/BSc Biochemistry and BSc Molecular Biology) at UCL, providing students with the opportunity to complete research that integrates both experimental and computational work, going from hypothesis generation to the writing of a research paper on their findings. With the shift to

[9] https://sc21.supercomputing.org/attend/newsletter-archive/

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purely computational work as a result of the pandemic, the medically-relevant microbiome DNA sequence data generated previously from this course was used to provide data sets for the SSC and this Molecular Biosciences course shifted its focus to obtaining sequence data from publicly-available DNA sequence repositories, adding an element of data science to the HPC work. The potential to adapt the cardiovascular SSC under development with Dassault Systèmes for delivery to MSc Bioengineering students is being pursued as a second biomedical student course exemplar.

10 Towards a Community of Practice

10.1 The In Silico World Community of Practice (ISW_CoP)

The In Silico World Community of Practice (ISW_CoP) is an online community based on the Slack technology operated by UNIBO to promote the development of a community of practice where all practitioners of *in silico* medicine working in academia, industry, consulting firms, governmental and non-governmental organisations can discuss, collaborate, and co-develop best practices in the field.

After a period of experimentation, the ISW-CoP started to operate in November 2019, through the support of four EU-funded projects: CompBioMed2, Strituvad, Primage, and the IMI project Mobilise-D. CompBioMed2-specific activities started in March 2020 (as planned in the Description of Action, T6.1).

The Slack platform allows a community-like environment where public central spaces for conversation coexist with private channels for teams to collaborate on specific tasks or projects. The community is invitation-only, in order to ensure that only people with a professional or educational interest in *in silico* medicine can gain access. The public web site provides forms to submit membership requests; in addition, ISW-CoP has been promoted among the consortia of the four supporting projects, and through the two domain-specific associations (VPH Institute and Avicenna Alliance). To date (Mar 2021) the community has around 380 members representing disparate organisations such as universities, research hospitals, CROs, software developers, regulatory agencies, medical device companies, pharma companies, patients' organisations, social and economy analysts, HTA agencies, payers, etc. The membership is growing steadily, as new initiatives are launched. To date ISW-CoP has 22 channels, of which 9 are public (e.g. accessible by all members). Besides the CompBioMed specific channels we discuss below, the #GoodSimulationPractices channel run by the GSP Task Force established by the Avicenna Alliance and the Medical Device Innovation Consortium, and the #Health4Trials, an IMI-endorsed channel established by the Mobilise-D project to share best practices on the use of advanced digital health technologies in regulatory drug trials are currently quite popular.

Several channels, both public and private, are specifically devoted to CompBioMed objectives:

- **#compbiomed-ahm:** public channel used as "virtual coffee break" during the CompBioMed All Hands Meeting of 15th-17th June 2020 and to be used in the upcoming second all-hands meeting on 23-25 June 2021;

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- **#compbiomed2, #compbiomed-wp3, #compbiomed-wp4, #data-publication and #compbiomed_ct2s_hpc** private channels for internal use of the project partners;
- **#scalability:** public channel for the engagement of the wider community around computational science or computational biomedicine.
- **#codesign:** public channel for the engagement of the codesign and wider exascale community.

10.2 The HPC Support Channels on ISW_CoP

These channels capitalise on the expertise and knowledge of HPC experts among the CompBioMed partners to offer free support to those who need to improve the performance of their computational biomedicine solutions with high performance computer. But they are also safe spaces where users share experiences and problems related to the computational efficiency and scalability of computational biomedicine solutions.

The channels are managed by UNIBO in tight collaboration with WP2 and WP4 partners and it is in particular tied to Task 2.4 ”Emergent Community Application Support” (initial point of contact for both external users and both Core and Associate Partners in their initial steps towards parallelisation of existing applications and deployment on HPC resources) and Task 4.3 ”Optimising Biomedical Application Usage of Current and emerging e-Infrastructures” (support in getting the application running on CompBioMed HPC resources through parallelisation, porting, optimising, and/or scaling).

10.2.1 The Scalability Channel

The core engagement activities of CompBioMed2 so far is represented by the #scalability channel.

The channel had a slow start: after we started it in May 2020, it was active in June 2020, but then it went quiet over the summer. Currently there are 85 experts subscribed to the channel, but the number of posts (20 posts) is quite limited in comparison. In order to improve the engagement, we have had a small number of editorialised posts that report the specific experiences we had so far in the CompBioMed Centre of Excellence. The calendar of editorialised posts is the following:

Marco Viceconti	UNIBO	Introduction	1-12-2020
Mariano Vazquez	BSC	Parallelisation of biomedical FEA: the Alya experience	7-12-2020
Jonas Latt	UNIGE	Parallelisation of biomedical CFD: the Palabos experience	14-12-2020
Mat Bieniek	UCL	Parallelisation of biomedical MD: the BAC Experience	21-12-2020
Jon McCullough	UCL	HemeLB	11-1-2021
Gabor Zavodszky	UvA	HemoCell	18-1-2021
Ivan Benemerito	USFD	OpenBF	25-1-2021
Vincenzo Carbone	InSilicoTrials	NuMRis - Numerical Magnetic Resonance Implant Safety	17-2-2021
X. Li, P. Bhattacharya	Sheffield	CT2S/ARF10	1-3-2021
Mat Bieniek	UCL	Computing Binding affinity with BAC	8-3-2021

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Roberto Fino	Acellera	Managing large scale MD studies with HTMD	15-3-2021
Enrico Dall'Ara	USFD	MouseTibia service	22-3-2021

After each expert contributes to the channel, we tweet about it on CompBioMed Twitter account. This allows to continuously promote the community and the channel itself, and to reach more researchers; indeed, we notice new requests for membership each time a tweet goes online.

10.2.2 The Parallelisation Channel

The Parallelisation Service, which is currently under development at the time of writing, will provide support to end users in their initial steps towards parallelising existing serial applications and deploying them on HPC resources.

The Service itself is preparing to launch, once the necessary Terms & Conditions, Data Policies and SLAs are agreed, completed, and published on our website.

End users may submit requests for their serial applications to be parallelised via the Parallelisation Channel within the CoP, or via the various, multiple CompBioMed contact email addresses, webforms, face-to-face contacts, etc.

Applicants will then be asked to complete a detailed application form, outlining the source code, the necessary input files and the expected output files, and any data security issues that may arise. This application form will also be available in a simpler form via a webform within our website.

New end users will be gathered via Task 2.4 "Emergent Community Application Support", which is the initial point of contact for all end users, i.e., both external users and both Core and Associate Partners, in their initial steps towards parallelisation of existing applications and deployment on HPC resources). Thereafter, the effort to parallelise these applications will be provided by T4.3 "Optimising Biomedical Application Usage of Current and emerging e-Infrastructures".

The main source of engaging with new users will be managed by Task 2.4. One platform of engagement will be the parallelisation channel within the CoP, following the process established by the scalability channel. Over the following months we plan to provide industrial-strength exemplars, outlining how medical applications have been empowered by exploiting HPC.

Other methods of engagement will involve contacting medics and hospital-based Core and Associate Partners, with a view to discuss their current application usage, particularly the more computationally intensive, if computation could be performed remotely at an HPC centre or if HPC resources are available on-site. We will also exploit the External Expert Advisory Board contacts, who are typically well connected to practicing medics with heavy computational requirements, to gather new end users. T4.5 is currently collating an extensive list of partnerships and collaborations (both active and potential) provided by each of the Core

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Partners, and this list presents a rich source of potential end users. Finally, T2.4 members will attend computational biomedical conferences, including our own CompBioMed conferences, and approach potential clients.

10.3 The Co-design Channel

This channel was recently (December 2020) created for first-level support to handle problems/requests about codesign in terms of hardware and/or software. We offer to benchmark the codes of any users on different hardware architectures which are available on the heterogeneous set of testing systems of the CompBioMed2 partners LRZ, BULL and SURF. We have prepared a living document containing the current hardware (CPU/GPU types, count, memory size, type and bandwidth as well as net bandwidth) available on the different testing systems so that our users can see the hardware that can be currently used.

The channel is intended to be used to engage the codesign and wider exascale community to discuss topics such as how our users can reach the exascale, to which architectures (e.g. accelerators/GPUs) they may port their codes (how/by which framework, programming language), how to deploy and benchmark software on the different architectures (e. g. compiler, flags, spack, easybuild, testing infrastructure etc.) as well as to discuss upcoming exascale systems, conferences and workshops.

10.4 The Scalability Webpage

The twin web presence to the #Scalability channel is the Scalability Support web page[10] on the In Silico World web site. While it is necessary to have a web presence for the CompBioMed-related activities in the community of practice, we need to be careful not cannibalise resources to the project's primary public web site[11]. Thus, for the time being this page will merely provide some information on the service we provide through the #Scalability channel in the ISW-CoP, plus relink useful resources published on the CoE's web site. On the other hand, the #Scalability channel is listed among the services the CoE provides on the CoE's web site[12].

11 Risk Management

The following possible sources of risks have been identified:

a) Because of the still scarce understanding from the biomedical research community of the opportunities provided by HPC, there is the risk that a limited number of external users access our scalability services.

[10] http://insilico.world/scalability-support-channel/
[11] https://www.compbiomed.eu/
[12] https://www.compbiomed.eu/compbiomed-scalability-channel/

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Probability	Medium
Impact	Low
Risk assessment	Medium
Mitigation	To mitigate this risk we could expand the educational activities, and also develop a targeted communication toward biomedical researchers that shows, using CompBioMed2 solutions, the benefits HPC can offer in this field.

b) The reviewers' recommendations to focus on applications that are exascale candidates could cause a narrowing of the scope of the project. This could make more it more difficult for CompBioMed to engage with a community that is still largely HPC-illiterate.

Probability	Medium
Impact	Medium
Risk assessment	Medium
Mitigation	If CompBioMed2 were asked to drop this core activity, it would be resisted as it undermines a central purpose of the CoE. To meet its objectives, the CoE would be forced to collaborate with external initiatives and projects to achieve the required level of engagement, which is clearly counterproductive.

12 Conclusions

The analysis on the Computational Biomedicine community led to the identification of two main groups of stakeholders for the solutions developed within the CompBioMed Centre of Excellence, the Developers of solutions and services, and the Users, further distinguished into research, clinical, industrial and educational users, policy makers and the public at large.

The stakeholder identification led to the implementation of different engagement strategies and activities that range from communication through digital outlets, such as the project website and social channels, that are very effective in reaching especially the public at large, to the organization of and participation to conferences and workshops, to the creation and management of discussion channels on the In Silico World Community of Practice, and the synergies with other organizations such as the VPHi, the Avicenna Alliance and the IHI.

Other initiatives directed towards internal or Associate Partners are the Internal Helpdesk, to track requests for service access, and the Visitor Program, to foster synergistic research projects between host and visitor partners, for the training on and use of HPC centres.

Other significant communities of researchers, biomedical and medical students are reached through the training activities organized by the partners, and that are each year very successful.

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All the activities detailed in this document and summarized in these Conclusions are aligned with the management and dissemination activities in WP1 and sustain each other – especially for what concerns the project online presence (T1.4) and the Conference/Workshop/Event planning (T1.6) resulting in a virtuous, self-sustaining cycle.

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