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D3.5 Report on Training and Dissemination

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Table of Contents

1	Vers	sion Log	4
2	Cont	tributors	4
3	Defi	nitions and Acronyms	5
4	Exec	cutive summary	6
5	Intro	oduction	6
6	Trair	ning	7
	6.1	CompBioMed presence in PATC Course at BSC (Barcelona, 14-16 Feb 2017))9
	6.2	BioExcel & CompBioMed joint workshop (London, 30 May 2017)	9
	6.3	CompBioMed webinar series	9
	6.3.1	1 Webinar #1	11
	6.3.2	2 Webinar #2	12
	6.3.3	3 Webinar #3	13
	6.4	CompBioMed in medical curriculum at UCL	14
	6.5	CompBioMed in science and engineering curriculum at UCL	15
	6.6	CompBioMed Winter School 2018 at BSC (Barcelona, 14-16 Feb 2018)	16
	6.6.1	1 Training evaluation	17
	6.7	CompBioMed's presence in VPH Summer School 2018 (Barcelona, 18-22 Ju	ine 2018)
		17	
	6.8	CompBioMed training event at VPH2018 (Zaragoza, 4 Sep 2018)	18
	6.9	Training Portal and Repository	18
	6.10	Key Performance Indicators	19
7	Disse	emination	20
	7.1	Dissemination Materials and Related Activity	21
	7.1.1	1 Project Newsletters	21
	7.1.2	2 Website	22
	7.1.3	3 Social Media	24
	7.1.4	4 Publications	25
	7.1.5	5 Activities with Related Projects	27
	7.1.6	6 Other	28
	7.2	Event Activity	28
	7.2.1	1 Organisation of Events	28
	7.2.2	2 Participation in Events	29
	7.3	Dissemination Network and Target Audiences	30
	7.3.1	1 The CompBioMed Network	30
	7.3.2	2 Targeting Academia, Industry, and the Clinic	32
	7 2 2		
	7.3.5	3 Targeting the General Public	32
	7.3.3	 Targeting the General Public Targeting HPC Poor Countries 	32 32
	7.3.3 7.3.4 7.4	 Targeting the General Public Targeting HPC Poor Countries Key Performance Indicators and Output Measurement 	32 32 33
	7.3.2 7.3.4 7.4 7.5	 Targeting the General Public Targeting HPC Poor Countries Key Performance Indicators and Output Measurement Plans for the Second Half of the Project 	32 32 33 35
8	7.3.4 7.4 7.5 Cond	 Targeting the General Public	

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List of Tables and Figures

Table 1 - Overview of CompBioMed training activities	8
Table 2 - CompBioMed webinar series 2017/2018 calendar	10
Figure 1 - Screenshot of Webinar #1	11
Figure 2 - Screenshot of Webinar #2	12
Figure 3 - Screenshot of Webinar #3	13
Figure 4- Picture taken during the "HPC for medics" workshop delivered by EPCC	15
Figure 5 - Picture taken during BSC Winter School 2018	16
Figure 6 - Replies to BSC Winter School feedback questionnaire's last question	17
Figure 7 - Training Portal filtering options	19
Figure 8 - CompBioMed Newsletter Third Edition, Front Page	21
Figure 9 - CompBioMed monthly e-newsletter	22
Figure 10 - CompBioMed Website Homepage	23
Figure 11 - CompBioMed Website Views	23
Figure 12 - CompBioMed Twitter Account	24
Figure 13 - CompBioMed YouTube Account	25
Table 3 - CompBioMed Consortium Website Activity	37
Table 4 - CompBioMed Consortium Social Media Activity	39
Table 5 - CompBioMed Consortium Non-Peer Reviewed Publications	40
Table 6 - CompBioMed Consortium Other Activities	40
Table 7 - CompBioMed Event Organisation Activity	41
Table 8 - Dissemination related to the CompBioMed-Science Museum "The Virtu	al Human"
Event	42
Table 9 - CompBioMed Consortium Event Participation Activity	44



1 Version Log

Version	Date	Released by	Nature of Change
V1.0	15/02/2018	Manuela Corsini (UvA)/Hugh Martin (CBK)	First draft, sent to internal reviewers
V1.1	01/03/2018	Manuela Corsini (UvA)/Hugh Martin (CBK)	Second draft, revised based on reviewers' comments
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3 Definitions and Acronyms

Acronyms	Definitions
BSC	Barcelona Supercomputing Center, partner of CompBioMed
СВК	CBK Sci Con Limited is a consultancy, partner of CompBioMed, leading the dissemination activities within WP3
CoE	Centre of Excellence
DNA	Deoxyribonucleic acid
DoA	Description of Action
EPCC	UK's supercomputing centre based at the University of Edinburgh, partner of CompBioMed
НРС	High Performance Computing
Insigneo	Institute for <i>in silico</i> Medicine
КРІ	Key Performance Indicator
NGS	Next-Generation Sequencing
PATC	PRACE Advanced Training Centre
PRACE	Partnership for Advanced Computing in Europe
rDNA	ribosomal DNA
RNA	Ribonucleic acid
SSC	Student Selected Component
SURFsara	The Dutch national high-performance computing and e-Science support centre, partner of CompBioMed
ТР	Training Plan
TR	Training Repository
UCL	University College London, coordinator of CompBioMed
UNIGE	University of Geneva, partner of CompBioMed
UOXF	University of Oxford, partner of CompBioMed
UPF	Universitat Pompeu Fabra, partner of CompBioMed
USFD	University of Sheffield, partner of CompBioMed
UvA	University of Amsterdam, partner of CompBioMed and WP3 leader
VPH	The Virtual Physiological Human
VPHi	The Virtual Physiological Human Institute
WP	Work Package



4 Executive summary

CompBioMed is undertaking, under work package 3 (WP3), the development and provision of a range of dissemination and training activities with associated supporting material, which are described in detail in previous WP3 deliverables (D3.2 Dissemination Action Plan, D3.3 Training Plan and D3.4 Report on Dissemination and Training Material).

The present WP3 deliverable, D3.5 Report on Training and Dissemination, aims at providing an overview of the dissemination and training activities carried out and the material developed in the first half of the CompBioMed project, as well as an update of the Dissemination and Training Plans for the coming 18 months.

Through the dissemination of CompBioMed research findings to academic, industrial, and clinical users, we will contribute to the strength and leadership of the EU in HPC technologies in Computational Biomedicine, also having an impact on emerging HPC markets. Through the building of networks between our community and the encouragement of collaboration activities, together with our training agenda, we will accelerate European excellence in Computational Biomedicine.

5 Introduction

Computational methods, based on human biology, are now reaching maturity in the biomedical domain, rendering predictive models of health and disease increasingly relevant to clinical practice by providing a personalized aspect to treatment. Computer based modelling and simulation is well established in the physical sciences and engineering, where the use of high performance computing (HPC) is now routine. CompBioMed is a user-driven Centre of Excellence (CoE) in Computational Biomedicine, designed to nurture and promote the uptake and exploitation of high performance computing within the biomedical modelling community. Our user communities come from academia, industry and clinical practice.

Work package 3, Training and Dissemination, aims 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 us to engage external stakeholders in academia, healthcare and industry with the activities of the project.

Within work package 3, four deliverables have already been completed:

- D3.1 Website Release (CBK) month 3 the project website provides a focal point for the dissemination activities of the project.
- D3.2 Dissemination Action Plan (UvA) month 3 A detailed and comprehensive report on the dissemination actions that will be carried out by the project.
- D3.3 Training Plan (UvA) month 6 A report with a detailed training plan, including both training events, means of delivery, and partners responsible for the training.
- D3.4 Report on dissemination and training material (UvA) month 12 Report on dissemination and training material as produced by the project and on delivered training and dissemination actions, as well as update to the training plan and dissemination action plan.

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The present deliverable aims at providing an overview of the training and dissemination activities carried out and the material developed so far within the CompBioMed project (months 1 to 18), as well as an update of the Dissemination and Training Plans for the next 18 months. The original deadline for D3.5 was month 24, but this was changed to month 18 to align with the 18-month review of CompBioMed by the European Commission.

6 Training

One of the key objectives 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 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.

The CompBioMed Training Plan (D3.3) aims to:

- bridge High Performance and Cloud Computing communities to biomedical communities
- offer a roadmap to access High Performance and Cloud Computing for Biomedicine
- assess High Performance and Cloud Computing code useful for Biomedicine and find exemplars for training
- reduce the complexity of Computational Biomedicine for novices
- cater for diverse user bases including trainers (and train the trainers)

These aims are targeted at the user groups that lie at the heart of CompBioMed: academic, industrial and clinical users.

The training is delivered by CompBioMed scientists alongside HPC experts within the project. The material is provided by those experts. Our approach is to add the biomedical context to the already existing HPC/cloud courses, re-using as much as possible the available material, thus keeping the development of new resources to an absolute minimum. The CompBioMed consortium relies fully on its partners to avoid duplication and exploit the already available training courses and material.

Table 1 shows an overview of the implementation status of CompBioMed training activities.



Title	Date, place and resp partner	Status and n. of participants	Section
CompBioMed presence in PATC Course "HPC-based simulations, Engineering and Environment" at BSC	14-16 Feb 2017, Barcelona (BSC)	Held (40 participants)	6.1
BioExcel & CompBioMed joint workshop "Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences"	30 May 2017, London (UCL)	Held (25 participants)	6.2
CompBioMed webinar series	Started in Nov 2017, every 2-3 months, online (UvA)	On-going, 3 held (121 participants in total)	6.3
CompBioMed in medical curriculum at UCL	Started in Nov 2017, London (UCL)	On-going (40 participants in first year)	6.4
CompBioMed in science and engineering curriculum at UCL	Started in Nov 2017, London (UCL)	On-going (85 participants in first session)	6.5
CompBioMed Winter school 2018 at BSC "HPC-based simulations, Engineering and Environment with applications in Bioengineering"	14-16 Feb 2018, Barcelona (BSC)	Held (30 participants)	6.6
CompBioMed's presence in VPH Summer School 2018	18-22 June 2018, Barcelona (UPF+BSC)	Currently being organised	6.7
CompBioMed training event at VPH2018 "High Performance Computing for the VPH"	4 Sep 2018, Zaragoza (UvA)	Currently being organised	6.8
CompBioMed Winter school 2018/2019 at BSC (tentative)	Winter 2018/2019, Barcelona (BSC) (tbc)	Tbc	-

After the implementation of the first training events (Winter school 2017/2018 at BSC, Training event at VPH2018, 4 webinars, UCL's medical curriculum-year 1), we will be able to update the training plan with more realistic data and updated information on the users' specific needs and challenges. This will be done on the basis of the feedback received by the training participants and collected through specific questionnaires on the occasion of each training/webinar.

All the available training recordings and materials are made publicly available on the CompBioMed Training Portal (section 6.9): this includes copies of the course slides, teaching



material, code examples and hands-on exercises, where available. This results in a sustainable open access educational and training resource for Computational Biomedicine.

CompBioMed is committed to meeting a list of Key Performance Indicators (KPIs). The two KPIs related to training are described in section 6.10.

The following sections provide the details of the training activities listed in Table 1, the Training Portal and the KPIs.

6.1 CompBioMed presence in PATC Course at BSC (Barcelona, 14-16 Feb 2017)

Two CompBioMed sessions were held within the <u>PATC Course: "HPC-based simulations,</u> <u>Engineering and Environment"</u> organised by BSC (https://www.bsc.es/education/training/patccourses/patc-course-hpc-based-simulations-engineering-and-environment-2/agenda) (Barcelona, 14-16 February 2017): an introductory session of the CompBioMed CoE on Day 1 and a session on Cardiac Computational Modelling on Day 3.

Approximately 40 participants attended the course, with basic to intermediate level knowledge of HPC. The students were mainly users of HPC applications and code developers.

6.2 BioExcel & CompBioMed joint workshop (London, 30 May 2017)

The BioExcel & CompBioMed joint workshop on "Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences" was held at UCL, London on 30 May 2017.

The workshop was attended by 25 participants, mainly coming from the two Centres of Excellence (CoEs), and focused on scientific and technical discussions pertaining to the theory, algorithms and their implementation on high performance architectures.

6.3 CompBioMed webinar series

The CompBioMed D3.3 Training Plan foresees the organisation, every 2-3 months, of regular webinars on a range of topics, for a range of audiences. To meet this the CompBioMed webinar series started in November 2017 and will run until the end of the project.

The University of Amsterdam (UvA) is in charge of the planning, organisation, hosting and facilitation of the series, although the speakers belong each time to a different partner.

All 2018 webinars have already been planned (see the calendar in Table 2) and announced on <u>CompBioMed's website</u> (http://www.compbiomed.eu/training-3/). In order to ensure that the webinar series maintains the CompBioMed flavour, the topics alternate between the 3 CompBioMed application fields (i.e. cardiovascular, molecularly-based and neuro-musculoskeletal medicine) and the HPC/Cloud perspective.

N.	Date	Title	Delivering Partner	Status
1	22-Nov-17	HPC simulations of cardiac electrophysiology using patient specific models of the heart (using CHASTE and Alya)	UOXF	Held (76 participants)
2	30-Jan-18	Introduction to cloud computing for the VPH	SURFsara + USFD	Held (21 participants)
3	19-Mar-18	Lattice Boltzmann method for CompBioMed (incl. Palabos)	UNIGE	Held (24 participants)
4	07-Jun-18	Introduction to Biomedical Applications on High Performance Computers	EPCC + UvA	Announced
5	25-Oct-18	High Throughput Molecular Dynamics for Drug Discovery	UPF	Announced
6	05-Dec-18	CompBioMed: Innovations on medical student training	UCL	To be announced

In order to avoid timetable clashes the webinar calendar takes into account the other training activities already planned: that is, the Winter School at BSC (14-16 February 2018, Barcelona); CompBioMed's presence in VPH Summer School 2018 (18-22 June 2018, Barcelona); the training event at VPH2018 (4 September 2018, Zaragoza).

The webinar series is advertised through the CompBioMed quarterly newsletter (this reaches over 200 people), the monthly e-newsletter (reaches 144 people), website, social media channels, the VPH Institute's newsletter (reaches approximately 7200 people), website, and social media channels, as well as the partners' relevant formal and informal networks. For each webinar, a flyer is produced to facilitate its dissemination, also offline at meetings and conferences.

Each webinar is recorded and these are uploaded a few hours after the event onto the <u>CompBioMed</u> YouTube channel (https://www.youtube.com/channel/UCUilfmesH_psiArXT3xcppA/featured) and website, as well as the VPH Institute's website. Webinar slides are also downloadable from the CompBioMed website.

At the end of each webinar, attendees are asked to fill in a feedback questionnaire that contains the following questions:

- 1. Which user group do you belong to? (Academic/Clinical/Industrial)
- 2. How would you rate the training in the overall? (1=poor; 5=excellent)
- 3. Did you find the training useful? (1=not at all; 5=extremely useful)
- 4. Did the training meet your expectations? (1=not at all; 5=perfectly)

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Page 10

Version 1.2



- 5. Did the training meet your experience level? (1=not at all; 5=perfectly)
- 6. Would you recommend it?
- 7. What did you best like of the training?
- 8. What did you like the least?
- 9. What did you feel was missing?
- 10. Any further remarks/suggestions for improvement?

After the responses are collected, four reports are produced for each webinar: registration, attendee, performance and survey. These reports are saved in the project's intranet and shared with the speakers and the whole consortium. They are particularly useful for those partners running subsequent webinars. Once the first four webinars have taken place, an overall evaluation of the feedback will be made. This takes into account the users' specific needs and challenges, and it will be used to plan the second year of the series.

The details of the first three webinars are reported in the following paragraphs.

6.3.1 Webinar #1

The first webinar titled "<u>HPC simulations of cardiac electrophysiology using patient specific</u> <u>models of the heart (using CHASTE and Alya)</u>" (http://www.compbiomed.eu/compbiomedwebinar-1/) took place on 22 November 2017. The speakers belonged to the Computational Cardiovascular Science team of the University of Oxford and provided an insight on the latest research on the topic, focussing on two HPC simulation softwares of cardiac electrophysiology: CHASTE (Cancer, Heart And Soft Tissue Environment) and the Alya System. The first has been developed by the Department of Computer Science at University of Oxford and the second is Barcelona Supercomputing Center's (BSC) simulation code for multi-physics.

Out of 111 registrations, 76 people actually participated. 65-70 people were connected throughout the whole duration of the webinar (1 hour) (63% attendance rate).



Figure 1 - Screenshot of Webinar #1

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Furthermore, by the time of writing, the webinar's recording has been viewed 122 times on the <u>CompBioMed YouTube channel</u>

(https://www.youtube.com/channel/UCUilfmesH_psiArXT3xcppA/featured).

The feedback collected was very positive: the overall score for the webinar was on overage 4.3 out of 5 ("How would you rate the training in the overall? 1=poor; 5=excellent") and 100% of the respondents stated they would recommend the webinar.

6.3.2 Webinar #2

The second webinar was titled "<u>Introduction to cloud computing for the VPH</u>" (http://www.compbiomed.eu/compbiomed-webinar-2/) and it took place on 30 January 2018. It was delivered by SURFsara and the INSIGNEO group from the University of Sheffield (USFD).

In this webinar, a Cloud computing environment was described as well as how it can help with scientific research. Participants learned how to set up and access a virtual machine, as well as to install software and run simulations. As an example, it was shown how to configure and run openBF, a computational library for 1D blood flow simulations in straight elastic arteries, and how to visualize the output produced by the code.

Out of 26 registrations, 21 people attended and this remained constant throughout the whole webinar duration (1 hour) (81% attendance rate).



Figure 2 - Screenshot of Webinar #2

Moreover, by the time of writing, the recording has been viewed 37 times on <u>CompBioMed's</u> <u>YouTube channel</u> (https://www.youtube.com/channel/UCUilfmesH_psiArXT3xcppA/featured).



The feedback collected was positive: the overall score for the webinar is on overage 3.8 out of 5 ("How would you rate the training in the overall? (1=poor; 5=excellent") and 89% of the respondents stated they would recommend the webinar.

6.3.3 Webinar #3

The third webinar titled "Lattice Boltzmann method for CompBioMed (incl. Palabos)" (http://www.compbiomed.eu/compbiomed-webinar-3/) was held on 19 March 2018. It was delivered by the University of Geneva (UNIGE).

The webinar provided a general introduction to the lattice Boltzmann method for computational fluid dynamics and showed how this tool is used efficiently for biomedical applications. The examples provided included a vertebroplasty and a hemodynamics solver, both based on the open-source library Palabos. The former simulates a cement injection process in vertebroplasty, and the latter the dynamics of blood flow after the insertion of a flow diverter in an artery with an aneurysm. Both tools work with patient-specific data and are intended as support tools for medical decision making.

Out of 34 registrations, 24 people attended and this remained constant throughout the whole webinar duration (1 hour) (71% attendance rate).



Figure 3 - Screenshot of Webinar #3

The feedback collected is very positive: the overall score for the webinar is on overage 4.6 out of 5 ("How would you rate the training in the overall? (1=poor; 5=excellent") and 100% of the respondents stated they would recommend the webinar.



6.4 CompBioMed in medical curriculum at UCL

The Student Selected Component (SSC) of UCL's Medical School Curriculum provides an opportunity to educate medical students in Years 1, 2 and 6. This is an ideal scenario for providing a training flow that can be used to support the establishment of new clinical specialisations centred around the use of big data and high-performance computing-based biomedical modelling. This is an entirely novel training element introduced in CompBioMed, albeit not originally planned.

The Skin Microbiome SSC is currently offered to Year 1 and to Year 2 Medical Students. This course provides medical students with the opportunity to use state of the art laboratory and computational resources to complete a metagenomics project in molecular medicine. Using conserved regions of ribosomal RNA gene sequences from the bacterial genome, the identity of the different bacterial species present in skin samples obtained from student volunteers will be determined. Under supervision, students design and carry out original experimental work, analyse data, compare results of their specific experiments with the group and write a report on the findings. A test of the theoretical aspects of the experimental techniques is taken. SSC activities include a combination of field work, wet laboratory-based experimental work, taught lectures, supervised workshops and small group tutorial sessions, as follows:

- 1) Introductory session during which the topic is introduced and the experimental protocols established.
- 2) Wet laboratory work (9 hours) involves the following workflows (3 sessions of 3 hours each): sample collection of skin microbes, purification of microbial genomic DNA, polymerase chain reaction amplification of the V4 region of the 16S rDNA gene, purification of the amplicon, quantification of the dsDNA and DNA sequencing on a Illumina MiSeq platform.
- 3) Computational work (12 hours) involves the following workshops:
 - a. understanding the command line and Next Generation Sequence analysis of 16S microbial sequences using Qiime, a software programme for investigating quantitative insights into microbial ecology, on a local cluster machine,
 - "HPC for Medics" an introduction to HPC and a workshop on obtaining accounts on the Cirrus HPC platform at Edinburgh Parallel Computing Centre including use of this resource to install Qiime for analysis of Next Generation Sequences obtained experimentally, and
 - c. at least two data analysis workshops.

40 students in total – 20 each from years 1 and 2 – enrolled on the Skin Microbiome SSC in 2017-2018, the first time this course ran (November 2017 - January 2018). The module was popular and oversubscribed with 14 and 7 students unable to enrol on it for the Year 1 and 2 cohorts, respectively. In future years, the course will be again offered to 20 students per year. The course was delivered by UCL and the HPC workshop was run by EPCC.



Figure 4- Picture taken during the "HPC for medics" workshop delivered by EPCC

All module resources are placed on GitHub and made available to students via the UCL institutional virtual learning environment, Moodle, and will also be published on the CompBioMed training portal.

The feedback is being collected through exit surveys. Once the last submissions are received, the feedback will be collated and analysed.

6.5 CompBioMed in science and engineering curriculum at UCL

UCL's undergraduate research project course BIOC3301 – 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. Students collect a soil sample and isolate the DNA of the soil's microbiome. Polymerase chain reaction is used to amplify part of the ribosomal 16S gene, which is then sequenced on an Illumina MiSeq platform. As part of the data analysis, students learn how to use a PC command line, basic Python programming and how to process the NGS raw data.

Following a workshop "Rough Guide to HPC for Bioscientists", they are given access to a highperformance computing clusters to analyse their data. 85 students have taken this course in 2017-2018 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.



6.6 CompBioMed Winter School 2018 at BSC (Barcelona, 14-16 Feb 2018)

The Barcelona Supercomputing Center's Winter School "<u>HPC-based simulations, Engineering</u> and <u>Environment with applications in Bioengineering</u>" (http://www.compbiomed.eu/events-2/compbiomed-training-winter-school-2018-at-bsc/) took place on 14-16 February 2018 in Barcelona, at the Campus of the Universitat Politècnica de Catalunya.



Figure 5 - Picture taken during BSC Winter School 2018

The objective of this 3-day course was to give a panorama on the use of HPC-based computational mechanics in Engineering and Environment through projects that CompBioMed partners are carrying out (Cardiac, Musculoskeletal and Molecular exemplars). This panorama included the basics of what is behind the main tools: computational mechanics and parallelization. The format included both theoretical and hands-on sessions.

The training was organised by BSC, in collaboration with the Partnership for Advanced Computing in Europe (PRACE), as BSC is a PRACE Advanced Training Centre (PATC). The trainers belonged to the following partners: BSC, SURFsara, UvA, USFD, Microsoft, Evotec, UCL, UPF and Acellera.

The event announcement was disseminated through the CompBioMed, PRACE and VPHi websites and newsletters as well as partners' websites, networks and social media.

40 students registered for the course. Depending on the day, between 26-30 students attended to the Winter School. The participants comprised PhD students, master students and engineers. Six CompBioMed travel grants were awarded to the most promising applicants for covering part of their travelling expenses. After the event, the grantees were asked to write an article on the Winter School, which can be found on the Winter School's webpage of CompBioMed's website, together with the full recording of the event.

The following paragraph describes the methodology and the main outcomes of the evaluation exercise carried out by BSC at the end of the training.

PU Page 16 Vers This project has received funding from the European Union's Horizon 2020 research and innova

Version 1.2



6.6.1 Training evaluation

The goal of the training evaluation at BSC is twofold: on the one hand, to capture the impact of the training program; on the other hand, to allow an insight of the attendees' personal progress. It also provides understanding on how to support them in implementing the learned methodologies/tools in their work.

BSC designed an exit questionnaire based on the well-established Kirkpatrick model of evaluation of professional training. The questionnaire is purposefully very concise (6 questions are posed) and focuses solely on the learning outcomes of the courses. Out of 30 attendees, 15 responded to the exit questionnaire. An overall analysis of the results is available upon request.

As shown in Figure 6, a clear majority (67%) responded "high" or "very high" to the last question ("How would you rate the overall value of this course?").



Figure 6 - Replies to BSC Winter School feedback questionnaire's last question

6.7 CompBioMed's presence in VPH Summer School 2018 (Barcelona, 18-22 June 2018)

The VPH Summer School series is co-organized by the Universitat Pompeu Fabra and by the Virtual Physiological Human Institute. It aims to provide junior engineers and medical doctors with a complete overview of state-of-the-art VPH research, following a complete pipeline from basic science and clinical needs, to model application.

The <u>3rd edition</u> of the School (https://www.upf.edu/web/bcnvph_school) will take place in Barcelona on 18-22 June 2018 and will focus on data integration, model verification and validation. CompBioMed will give its contribution with a talk and the organisation of a hands-on session by UPF and BSC.



6.8 CompBioMed training event at VPH2018 (Zaragoza, 4 Sep 2018)

As part of the <u>VPH2018 conference "VPH for In Silico Medicine"</u> (http://vph-conference.org/), running in Zaragoza on 5-7 September 2018, CompBioMed will organize a training session titled "<u>High Performance Computing for the VPH - A practical introduction to HPC usage</u>" (http://vph-conference.org/pre-courses/course-b/). The course will take place the day before the start of the conference, on 4 September 2018, at the conference venue, the University of Zaragoza.

The course targets early phase researchers and aims to provide a short and concise introduction to HPC programming as well as 2 application examples. All lectures will be hands-on, using BSC's MareNostrum supercomputer. A maximum of 30 participants will be admitted to the course. The event will be recorded and the recording will be made freely available on the CompBioMed Training Portal. UvA has taken the lead in organising the course.

Feedback on the training will be collected by means of a paper feedback questionnaire to be distributed to the attendees and collected at the end of the session.

6.9 Training Portal and Repository

The <u>Training Portal</u> (http://www.compbiomed.eu/training/) has been developed, populated and is continuously updated by UCL and CBK. The Portal aims to be a sustainable open access educational and training resource for Computational Biomedicine, including HPC. It displays:

- the announcement of the upcoming training events organized within CompBioMed
- the previous training events organized within CompBioMed, including the video recordings, where available, and the training material developed for each course (course slides, code examples, exercises)
- the training activities offered by the partners that are relevant for the CompBioMed user community (training repository)

The <u>Training Repository</u> (http://www.compbiomed.eu/training/training-portal/) displays all those training activities and related material that are relevant to the CompBioMed user community, as offered by the project partners. The Repository features a filter engine to allow for a quick search, with the filter options shown in Figure 7.



Topic:	User Type:	Skill Level:	Course Type:			
Advanced computing	Academia	Novice	Face2Face			
Application	Clinical	Semi	моос			
Application codes	Industry	Expert	Online self-drive			
Big Data			Webinar			
Cloud						
Data Management	Data Management					
How to get access to and	How to get access to and					
Intro Computing						
Linux command line						
Modelling + simulation						
Visualisation						

Figure 7 - Training Portal filtering options

For each filtered course the following information appears:

- Title of the course
- Organisation delivering the course
- Short description
- URL
- Training dates
- Recurrence

The repository currently displays approx. 40 entries and is being continuously updated.

6.10 Key Performance Indicators

CompBioMed is committed to addressing a list of Key Performance Indicators (KPIs). The 2 KPIs related to training are listed below:

- 1. If training participants report that the training was useful
 - Target: 12 months after the training with 75% positive responses
 - o Current progress: Not due yet
- 2. Number of trainees attending training events
 - Target: 150 in total (of which 25 in the first one)
 - o Current progress: Already achieved with 301 in total
 - Details: 25 participants attended the Joint BioExcel and CompBioMed training on 30 May 2017 in London; 76 attended Webinar#1; 21 attended Webinar#2; 24 attended Webinar#3; 30 students attended BSC winter school 2018; 40 medical students attended UCL undergraduate course; 85 biomedical science and biotechnology students attended UCL's undergraduate research project course.



7 Dissemination

The CompBioMed Centre of Excellence in Computational Biomedicine is distributed in nature, relying on collaboration within the project, and also with external stakeholders. To this end, CompBioMed is undertaking dissemination activities that enable us to engage external stakeholders in academia, healthcare and industry with the activities of the project. The success of CompBioMed relies on its messages, developments, activities, and results being disseminated into the wider biomedical community, including the general public, as well as growing and interacting with its users.

Dissemination and outreach plays an important role in the CompBioMed Centre of Excellence. We promote the project's outcomes (publications, codes, white papers) to stakeholders, be they members of the scientific community, user communities, vendors, other industries, regulatory authorities, and related international projects.

A combination of dedicated media work, participation in conferences, preparation and distribution of information material, and event organisation are used to implement our impact objectives. During the project, we maintain the CompBioMed website for the external world and internal project communication, and have developed a social media presence (LinkedIn, Twitter, etc.). We organise workshops which promote CompBioMed results and success stories. We also produce dissemination materials such as posters, newsletters, branded merchandise and so forth.

The dissemination activities encompass many different aspects on the use of HPC interpreted as 'computing beyond the desktop' within the biomedical sciences community. Where possible, we use existing material, and have developed a detailed dissemination plan that furnishes the full details and is updated as required.

There was a substantial amount of dissemination activity in the first 18 months of CompBioMed: The key highlights during this period include:

- Organisation of 3 workshops
- Participation in 21 major conferences and workshops
- Publication of 10 scientific papers

We are primarily targeting the project stakeholders through the following channels:

- CompBioMed website: www.compbiomed.eu
- CompBioMed Twitter account: @bio_comp
- Scientific Events (conferences, workshops, seminars etc.)
- Scientific Journals
- The mailing lists, websites, and social media channels of our core partners, associate partners, and related projects

We are targeting the various stakeholder groups using the following dissemination materials detailed in this section:

- Leaflets
- Posters
- Newsletters
- Scientific Papers
- Non-Peer Reviewed Publications

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Page 20

Version 1.2



- Website content
- Social Media Content

These plans were described in the CompBioMed dissemination action plan (Deliverable 3.2).

7.1 Dissemination Materials and Related Activity

The CompBioMed brand has been used in all of our dissemination materials, be it in the form of newsletters, videos, website content etc. CompBioMed Task 3.3 is concerned with the production of dissemination materials and runs throughout the project.

7.1.1 **Project Newsletters**

As of month 8 in the project, we began producing quarterly Newsletters, with four produced in the first 18 months of the project. These Newsletters allow us to capture the latest updates in the project and disseminate them widely in order to keep our stakeholders appraised of the Centre's progress. The newsletters contain the following features:

- The CompBioMed logo
- A URL to the CompBioMed website
- The funding line "This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675451."
- An image of the European flag
- A link to our twitter account
- A link to our LinkedIn group
- A link to our YouTube Channel
- Descriptive sections on Welcome, Recent Events, Upcoming Events, Publications, Associate Partners, and Research Articles.

An image of the cover of the Newsletter (third edition) is shown in Figure 8.



Figure 8 - CompBioMed Newsletter Third Edition, Front Page

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The PDF files of the Newsletters can be downloaded here: <u>http://www.compbiomed.eu/media-social/news-and-events/newsletter/</u>.

In addition to the quarterly newsletters, which are distributed externally as well as to the partners and related projects of CompBioMed, we also have a monthly e-newsletter, which is distributed via our mailing lists specifically to our core partners, associate partners, and related projects. This, more regular newsletter, updates those connected to CompBioMed on awards and fellowships, research, training and conferences, and other pieces of news. Figure 9 shows a sample of one of these e-newsletters.



Figure 9 - CompBioMed monthly e-newsletter

7.1.2 Website

At the core of our dissemination activity is the CompBioMed website, where the project is described, its partners are described, activities are reported, contact details are listed, and where there is a repository for the project's training programme and for project-related documents generally. The website can be accessed at the URL <u>www.compbiomed.eu</u>. The website is addressed in detail in the previous deliverable Website Release (D3.1).



Figure 10 - CompBioMed Website Homepage

Between months 12 and 18 of the project we redesigned the website to a more dynamic and considered design. The banner image is now a dynamically changing image which highlights recent and key activities in the Centre. Below the banner image we provide links for different types of users, each of which takes the visitor to a page on the website that is tailored to that user type. There we display services and content that is relevant to that user type. At present we provide tailored pages for Academic, Industry, Clinical, and General Public users. As shown in Figure 10, below the user-type links is a row of services links (i.e. Innovation, Training, etc.), which takes the visitor to our key hubs of information and services. These currently display the Innovation portal, the training portal, the software hub, and an associate partners hub.

At the time of writing, the key statistics for the website include:

- 17,150 views (up from 9,453 at month 12)
- 92 pages (up from 67 at month 12)
- 71 news/events posts (up from 52 at month 12)

2,000 1,500 1,000 500 Dec 2016 Feb 2017 Apr 2017 Jun 2017 Aug 2017 Oct 2017 Dec 2017 Feb 2018 Figure 11 - CompBioMed Website Views

Monthly visitor statistics are shown in Figure 11.

Page 23



In terms of content produced for and utilized on external websites, there were numerous articles and posts made between months 12 and 18 of the project. These are shown in Table 3 - CompBioMed Consortium Website Activity, in the Appendices, which also lists some items that were not captured in D3.4.

7.1.3 Social Media

CompBioMed has an active and continually growing social media presence. Currently we are active on Twitter, YouTube, and LinkedIn. The Twitter account has yielded a great amount of networking and dissemination activity. A snapshot of the CompBioMed Twitter account is shown in Figure 12.



Figure 12 - CompBioMed Twitter Account

Key statistics from month 1 to month 18 of the project for the CompBioMed Twitter account include:

- Tweets: 272 (up from 165 at month 12)
- Followers: 334 (up from 211 at month 12)
- Likes: 200 (up from 47 at month 12)
- Twitter Impressions: 105,333 (up from 45,226 at month 12)

YouTube 60	compbiomed		X	۹	± = 1	
HOME	ubscribers VIDEOS PLAYLISTS	icine CHANNELS	ABOUT	SUBSCRI	IBED 23	×
NG simulations of landing specific robots of the ISBN STATES States States States States	CompBicture Com CompCompBicture and the second of the sec	pBioMed Webinar 1: HP putational Biomedicine - ws • 1 week ago	PC simulations of	POPULAR Enils: SUBSCRI SUBSCRI SUBSCRI	CHANNELS a Brown BE LionFacts.org BE	
Created playlists	Free Energy	Workshop		SUBSCRI	BE cal King BE	

Figure 13 - CompBioMed YouTube Account

We also created a YouTube page for CompBioMed in April 2017, which acts as useful hub for our video content. A snapshot of the CompBioMed YouTube page is shown in Figure 13.

Key statistics from month 1 to month 18 of the project for the CompBioMed YouTube page include:

- 34 videos (up from 30 videos at month 12)
- 23 subscribers (up from 14 at month 12)
- 647 views (up from 392 at month 12)

The YouTube page can be viewed in the following link: <u>https://www.youtube.com/channel/UCUilfmesH_psiArXT3xcppA.</u>

Social Media activity on accounts other than the CompBioMed accounts is listed in Table 4 - CompBioMed Consortium Social Media Activity, in the Appendices, including some items that were not captured in D3.4.

7.1.4 Publications

In CompBioMed, we have to date published 23 peer reviewed publications (up from 13 at month 12), these are listed below:

- A. Heifetz, "Computational Methods for GPCR Drug Discovery", Methods in Molecular Biology, Springer, 1705 (2018), DOI: <u>10.1007/978-1-4939-7465-8</u> - 0 citations, impact factor 0.79
- A. Potterton, A. Heifetz, A. Townsend-Nicholson, "Synergistic Use of GPCR Modeling and SDM Experiments to Understand Ligand Binding", Methods Mol Biol., 1705, 335-343 (2018), DOI: <u>10.1007/978-1-4939-7465-8</u> <u>15</u> - 0 citations, impact factor 0.79
- A. Heifetz, M. Southey, I. Morao, A. Townsend-Nicholson, M. Bodkin, "Computational Methods Used in Hit-to-Lead and Lead Optimization Stages of Structure-Based Drug Discovery", Methods Mol Biol., 1705, 375-394 (2018), <u>DOI</u>: <u>10.1007/978-1-4939-7465-</u> <u>8 19</u> - 0 citations, impact factor 0.79

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- S. Li, J. Latt, B. Chopard, "The application of the screen model for stents in cerebral aneurysms", Computers & Fluids, Accepted (2018) 0 citations, impact factor 2.313
- S. Li, J. Latt, B. Chopard, "Model for pressure drop and flow deflection in the numerical simulation of stents in aneurysms. International journal for numerical methods in biomedical engineering", International Journal for Numerical Methods in Biomedical Engineering, Available Online (2017), <u>DOI</u>: <u>10.1002/cnm.2949</u>-0 citations, impact factor 2.192
- R. Dutta, B. Chopard, J. Lätt, F. Dubois, K. Boudjeltia, A. Mira, "Parameter estimation of platelets deposition: Approximate Bayesian computation with high performance computing", arXiv (2017), <u>https://arxiv.org/abs/1710.01054</u> - 1 citation, impact factor N/A
- A. Lyon, A. Michole, J.P.Martinez, P.Laguna, B. Rodriguez, "Computational techniques for ECG analysis and interpretation in light of their contribution to medical advances", Journal of the Royal Society Interface, 15 (138), 2017, <u>DOI</u>: <u>10.1098/rsif.2017.0821</u>- 0 citations, impact factor 3.917
- X. Zhou, A. Bueno-Orovio, B-Rodriguez, "In silicon evaluation of arrhythmia", Current Opinion in Physiology, 1, 95-103 (2017), DOI: <u>10.1016/j.cophys.2017.11.003</u> 0 citations, impact factor N/A
- R. Eccleston, P. V. Coveney, and N. Dalchau, "Host genotype and time dependent antigen presentation of viral peptides: predictions from theory", Scientific Reports, 7 (1), 14367 (2017), DOI: 10.1038/s41598-017-14415-8 0 citations, impact factor 4.259
- M. Paci, E. Passini, S. Severi, J. Hyttinen, B. Rodriguez, "Phenotypic variability in LQT3 human induced pluripotent stem cell-derived cardiomyocytes and their response to antiarrhythmic pharmacologic therapy: An in silico approach", Heart Rhythm, Available Online (2017), DOI: 10.1016/j.hrthm.2017.07.026 2 citations, impact factor 5.076
- J. Tomek, B. Rodriguez, G. Bub, J. Heijman, "β-adrenergic receptor stimulation inhibits proarrhythmic alternans in post-infarction border zone cardiomyocytes: a computational analysis", American Journal of Physiology Heart and Circulatory Physiology, Available Online (2017), <u>DOI</u>: <u>10.1152/ajpheart.00094.2017</u> 2 citations, impact factor 3.567
- G. Závodszky, B. van Rooij, V. Azizi and A. Hoekstra, "Cellular Level In-silico Modeling of Blood Rheology with An Improved Material Model for Red Blood Cells", Front. Physiol., Available Online (2017), <u>DOI: 10.3389/fphys.2017.00563</u> - 0 citations, impact factor 4.134
- S. Alowayyed, D. Groen, P. V. Coveney, A. G. Hoekstra, "Multiscale Computing in the Exascale Era", Journal of Computational Science, In Press (2017), DOI: 10.1016/j.jocs.2017.07.004 3 citations, impact factor 1.748
- I. Morao, D. G. Fedorov, R. Robinson, M. Southey, A. Townsend-Nicholson, M. J. Bodkin, A. Heifetz, "Rapid and accurate assessment of GPCR–ligand interactions Using the fragment molecular orbital-based density-functional tight-binding method", Journal of Computational Chemistry, Available Online (2017), <u>DOI</u>: <u>10.1002/jcc.24850</u>-3 citations, impact factor 3.229
- R. C. Eccleston, S. Wan, N. Dalchau, P. V. Coveney, "The role of multiscale protein dynamics in antigen presentation and T lymphocyte recognition", Frontiers in Immunology, Available Online (2017), DOI: 10.3389/fimmu.2017.00797 1 citations, impact factor 5.695
- P. S. Zun, T. Anikina, A. Svitenkov, A. G. Hoekstra, "A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data" Frontiers in Physiology, 8, 1-12 (2017), DOI:10.3389/fphys.2017.00284 – 1 citation, impact factor 4.134

PU

Page 26

Version 1.2



- A. Bueno-Orovio, K. Burrage, "Exact solutions to the fractional time-space Bloch–Torrey equation for magnetic resonance imaging", Commun Nonlinear Sci Numer Simulat., 52, 91-109 (2017), DOI:10.1016/j.cnsns.2017.04.013 0 citations, impact factor 2.784
- N. Altwaijry, M. Baron, D. Wright, P. V. Coveney, A. Townsend-Nicholson, "An Ensemble-Based Protocol for the Computational Prediction of Helix-Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics", Journal of Chemical Theory & Computation, 13 (5), 2254–2270 (2017), DOI: <u>10.1021/acs.jctc.6b01246</u> – 0 citations, impact factor 5.245
- S. Wan, A. Bhati, S. Skerratt, K. Omoto, V. Shanmugasundaram, S. Bagal, P. V. Coveney, "Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation", Journal of Chemical Information and Modelling, 57 (4), 897–909 (2017), DOI: <u>10.1021/acs.jcim.6b00780</u> – 6 citations, impact factor 3.760
- P. V. Coveney and R. Highfield, "Opinion: Is big data just big hype?", Longevity Bulletin: Big data in health, Institute and Faculty of Actuaries, 11-12 (2017), <u>ISSN 2397-7213</u>, N/A citations, impact factor N/A
- S. Wan, A. P. Bhati, S. J. Zasada, I. Wall, D. Green, P. Bamborough, and P. V. Coveney, "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: a Computational Study", J. Chem. Theory Comput., 13 (2), 784–795 (2017), DOI: <u>10.1021/acs.jctc.6b00794</u> – 6 citations, impact factor 5.245
- L. J. B. Briant, Q. Zhang, E. Vergari, J. A. Kellard, B. Rodriguez, F. M. Ashcroft, P. Rorsman, "Functional identification of islet cell types by electrophysiological fingerprinting", Journal of Royal Society Interface, 14 (128), 1-20 (2017), <u>DOI: 10.1098/rsif.2016.0999</u> – 5 citations, impact factor 3.917
- C. Shanchez, A. Bueno-Orovio, E. Pueyo, B. Rodriguez, "Atrial Fibrillation Dynamics and Ionic Block Effects in Six Heterogeneous Human 3D Virtual Atria with Distinct Repolarization Dynamics", Front. Bioeng. Biotechnol., 5, 1-13 (2017), <u>DOI:</u> <u>10.3389/fbioe.2017.00029</u> – 3 citations, impact factor 3.02
- A. Bhati, S. Wan, D. Wright, P. V. Coveney, "Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration", Journal of Chemical Theory and Computation, 13 (1), 210–222 (2017), DOI: <u>10.1021/acs.jctc.6b00979</u> 13 citations, impact factor 5.245

The CompBioMed consortium has also produced a number of non-peer reviewed publications as shown in Table 5 - CompBioMed Consortium Non-Peer Reviewed Publications, in the Appendices.

7.1.5 Activities with Related Projects

CompBioMed has conducted collaborative activity with related Horizon 2020 projects in our network; these include:

- BioExcel Centre of Excellence for Computational Biomolecular Research
- e-COST Action: OpenMultiMed
- ETP4HP The European Technology Platform for High Performance Computing
- EXDC The European Extreme Data & Computing Initiative
- MaX Materials design at the Exascale
- UKCOMES UK Consortium on Mesoscale Engineering Sciences
- EoCoE Energy orientated Centre of Excellence for Computing Applications

PU

Page 27

Version 1.2



- The Nomad Laboratory A European Centre of Excellence
- ESiWACE Centre of Excellence in Simulation of Weather and Climate in Europe
- Performance Optimisation and Productivity A Centre of Excellence in Computing Applications
- Centre of Excellence for Global Systems Science
- European HPC Centre of Excellence
- ComPat Computing Patterns for High Performance Multiscale Computing
- HPC-Europa3 Pan-European Research Infrastructure on High Performance Computing

Personnel from these projects have attended our internal and external meetings and events, and we have attended theirs. They are included in our mailing lists and act as dissemination channels in their own right. We have collaborated with these projects in a major way, and D3.4 describes some of the more significant collaborative efforts in the first 12 months of the project, and below we list a few specific instances in months 12 to 18:

- David Wright gave a presentation "Towards mutually beneficial industrial engagement with the EUDAT collaborative data infrastructure" at a EUDAT2020 meeting in Porto, Portugal, 24 January 2018
- Peter Coveney gave an invited talk on CompBioMed at the 2017 BioExcel AHM in Amsterdam, Netherlands, 22 November 2017
- We held a CompBioMed & Virtual Heart Joint Workshop in Amsterdam, Netherlands, 28 March 2018
- Emily Lumley attended the 8th cPPP Partnership Board Meeting in Brussels, Belgium
- Alex Patronis gave a presentation on "CompBioMed at pre-exascale" at 2nd EuroHPC in Brussels, Belgium

7.1.6 Other

In addition to the activities listed in the sections above, the CompBioMed consortium also engaged in other types of activities, these are listed in Table 6 - CompBioMed Consortium Other Activities, in the Appendices, including some items that were omitted from D3.4.

7.2 Event Activity

7.2.1 Organisation of Events

In months 12 to 18 of the project, CompBioMed has organised and executed a number of major events. These events are shown in Table 7 - CompBioMed Event Organisation Activity, in the Appendices.

We next describe in more detail the workshop with VHeart and "The Virtual Human" IMAX event at the Science Museum Lates (expanding on what was written in D3.4).

Cardiac Modelling, Fluid-solid Interactions and Biomedical Flows

A 7-hour workshop was held on 28 March 2018. This was a collaborative effort between CompBioMed and the Spanish Network of Excellence 'The Virtual Heart' (VHeart). It involved a mixture of speakers from VHeart and CompBioMed, including 6 student presentations.



VHeart is a Spanish Network of Excellence aimed at sharing tools and software with members of the network to improve the overall knowledge and capacity to develop a personalised virtual heart. It is made up of 9 universities and research centres throughout Spain. This workshop brought together the two projects and shared the combined knowledge of the participants in the fields of cardiac modelling, fluid-solid interactions and biomedical flows.

"The Virtual Human" IMAX event at the Science Museum Lates

The CompBioMed "The Virtual Human" IMAX event on 27 September 2017 was part of the Science Museum Lates series. Science Museum Lates are adults-only, after-hours theme nights that take place in the museum every month. The hour-long event described recreating a human being *in silico* and included an IMAX video composited on BSC's MareNostrum supercomputer. The video showed stunning simulations on aspects of computational biomedicine using supercomputers.

The performance took place in front of a sold out audience of 400 members of the general public, along with invited attendees from academia, industry, the clinic, the government, and the media. The Lates event itself attracted between 4,000 – 7,000 people.

In addition to the IMAX film, the Virtual Human feature contained short presentations from the following four speakers:

- Prof Blanca Rodriguez (University Oxford)
- Prof Peter Coveney (University College London)
- Prof Marco Viceconti (University of Sheffield)
- Prof Alfons Hoekstra (University of Amsterdam)

This was followed by a discussion including questions from the audience, chaired by Dr Roger Highfield (Director of External Affairs at the Science Museum Group).

We ran a strong dissemination campaign for this event and the video due to its broad appeal as well as the impactful message it delivered in a powerful format. Details of this campaign are shown in Table 8 - Dissemination related to the CompBioMed-Science Museum "The Virtual Human" Event, in the Appendices. This includes screenings at events, a promotional video, an article on the BBC website, and social media postings on the science museum twitter account (with 667k followers).

The video itself was posted on the CompBioMed Youtube channel (1,480 views), Barcelona Supercomputing Center Youtube channel (460 views), Science Museum Youtube channel (133 views) as on 9 March 2018, giving a total of 2,073 views as of 15 March 2018.

The dissemination campaign for the video itself is ongoing as we continue to screen it at additional venues and events.

7.2.2 Participation in Events

The CompBioMed consortium participated in many events during the first 18 months of the project, giving talks and presenting posters. This includes, on top of the 42 events listed in D3.4, 21 additional major events shown below (including some that were not captured in D3.4):

CompBioMed & Virtual Heart Joint Workshop in Amsterdam, Netherlands, 28 March 2018

ΡU

Page 29

Version 1.2





- 14th Congress of The World Federation of Interventional and Therapeutic Neuroradiology (WFITN) 2017 in Budapest, Hungary, 15 October 2017
- Supercomputing 2017, Colorado, USA, 12 November 2017
- 5th CDDD Meeting Computationally Driven Drug Discovery, Milan, Italy, 16 November 2017
- The Meeting of Young Researchers in Structural Computational Biology (EJIBCE), Coimbra, Portugal, 22 December 2017
- 2nd EuroHPC in Brussels, Belgium, 31 January 2018
- Middle East Molecular Biology Sources (MEMBS) Congress in Abu Dhabi, UAE, 2 November 2017
- Data Intensive Studies Center (DISC) Fall Symposium, Massachusetts, USA, 8 November 2017
- HITS Colloquium, Heidelberg, Germany, 20 November 2017
- EUDAT2020 meeting in Porto, Portugal, 24 January 2018
- BioExcel AHM, Amsterdam, Netherlands, 22 November 2017
- BloodFlow 2017, Paris, France, 9 October 2017
- European Heart Rhythm Association meeting, Vienna, Austria, 21 June 2017
- Copenhagen Meeting on Cardiac Arrhythmia, Copenhagen, Denmark 31 May 2017
- Gordon Conference on Cardiac Arrhythmia Mechanisms, California, USA, 5 February 2017
- 61st Biophysical Society Meeting, Louisiana, USA, 11 February 2017
- Clinical Magnetic Resonance Research Study Day, Oxford, UK, 26 April 2017
- Scientific Visualization: From Archaeology to Astronomy, Rotterdam, Netherlands, 20 June 2017
- Blender Conference 2017 in Amsterdam, Netherlands, 27 October 2017
- Visualizing large cell-based simulations: a bloody mess?, Amsterdam, Netherlands, 12 December 2017
- Annual High Performance Computing & Big Data 2018, London, UK, 06 February 2018

The substantial list of activity of these and other events is shown in Table 9 - CompBioMed Consortium Event Participation Activity, in the Appendices.

7.3 Dissemination Network and Target Audiences

In this section, we describe the network of partners, associate partners, and related projects that aid our dissemination efforts, while also describing how we are targeting our various types of stakeholders.

7.3.1 The CompBioMed Network

The CompBioMed Centre of Excellence leverages its network of partners, associate partners, and related projects in order to help widen its dissemination reach. Some partners/projects are set up with a key aim of disseminating effectively, such as the VPH Institute and the Science Museum, but all partners have their own unique reach to different types of audiences in different domains. They represent industry (from SMEs to large companies), academia, the clinic, the general public, and many have reach in HPC poor countries.

Our 15 core partners are:

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- Acellera
- Barcelona Supercomputing Center
- Bull (ATOS)
- CBK Sci Con Limited
- Evotec AG
- Janssen
- LifeTec Group
- SURFsara
- Universitat Pompeu Fabra
- University College London
- University of Amsterdam
- University of Edinburgh
- University of Geneva
- University of Oxford
- University of Sheffield

Our 34 Associate Partners (up from 26 at month 12) include:

- Academic Computing Centre Cyfronet AGH
- Aix-Marseille University
- Alces Software
- Avicenna Alliance
- Birmingham City University
- Brunel University
- Convergence Pharma
- Dassault Systems
- Diamond Light Source
- DiaVita, Life Science
- DNA Nexus
- Electric Ant Lab BV
- European Society of Cardiology's e-Cardiology Working Group
- GSK
- Heidelberg Institute for Theoretical Studies
- Institute of Molecular Biology,
- ITMO University, St Petersburg
- KINDI Centre for Computing Research
- Leibniz Supercomputing Centre
- Lightox
- Microsoft
- National Academy of Sciences of Armenia
- Norton Straw Consultants
- Oxford NIHR Biomedical Research Centre
- Pozlab, Poznan
- Qatar Robotic Surgery Centre, Hamad Medical Corporation
- Rutgers University
- Science Museum
- The Hartree Centre
- Universidad Católica de Murcia

PU

Page 31

Version 1.2



- University of Leeds
- University of Southampton, Immunology Group
- VPH Institute
- Zayed University

There are 14 related projects (up from 13 at month 12) in our network:

- BioExcel Centre of Excellence for Computational Biomolecular Research
- CoeGSS Centre of Excellence for Global Systems Science
- ComPat Computing Patterns for High Performance Multiscale Computing
- e-COST OpenMultiMed Open Multiscale Systems Medicine
- EoCoE Energy orientated Centre of Excellence for Computing Applications
- ESiWACE Centre of Excellence in Simulation of Weather and Climate in Europe
- ETP4HPC The European Technology Platform for High Performance Computing
- E-CAM European HPC Centre of Excellence
- EXDCI The European Extreme Data & Computing Initiative
- HPC Europa 3 Infrastructure on High Performance Computing
- MaX Materials design at the Exascale
- POP Performance Optimisation and Productivity A Centre of Excellence in Computing Applications
- The Nomad Laboratory A European Centre of Excellence
- UKCOMES UK Consortium on Mesoscale Engineering Sciences

7.3.2 Targeting Academia, Industry, and the Clinic

CompBioMed is focused on three main types of stakeholders: academic, industrial and clinical users. CompBioMed deliverable D3.2 Dissemination Action Plan outlines our approach to targeting these stakeholders. Each of the tables in this document lists the type of audience reached by each piece of material or activity, including academia, industry and clinical users.

7.3.3 Targeting the General Public

CompBioMed deliverable D3.2 Dissemination Action Plan outlines our approach to targeting the general public. The most prominent activity aimed at the general public is CompBioMed's "The Virtual Human" IMAX event at the London Science Museum, as described in Section 7.2.1. Each of the tables in this document lists the type of audience reached by each piece of material or activity, including the general public.

7.3.4 Targeting HPC Poor Countries

The CompBioMed Centre of Excellence is targeting HPC-poor countries in its activities, primarily through our network of partners and via events.

To perform outreach to and engagement with countries and regions within the EU and associated states with fewer HPC resources, CompBioMed has been collaborating with the COST (European Cooperation in Science and Technology – see www.cost.eu) platform, through trans-European networking of research. COST is based on a European intergovernmental framework for co-operation in science and technology with 36 member countries and one co-operating State. It also encourages active participation by institutions from near neighbour countries and international partner countries. Near neighbour countries include Armenia, Russia, Ukraine; Lebanon, Libya, Palestine Authority, Jordan, Syria, Tunisia, Egypt and Algeria, while Turkey is currently seeking membership. Bosnia & Herzegovina are also being considered. Several CompBioMed partners (e.g. UCL, UvA) are also participants in the OpenMultiMed COST Action CA15120 on Open Multiscale Systems Medicine.

In addition to the activities held in countries with fewer HPC resources outlined in D3.4, CompBioMed also conducted the following activities and events:

- CompBioMed held a dedicated session at the 14th Congress of the World Federation of Interventional and Therapeutic Neuroradiology, WFITN 2017, Budapest, Hungary, October 2017.
- Peter Coveney gave an invited Talk on "Rapid, Accurate and Reliable Binding Affinity Calculations for Drug Discovery & Precision Medicine" at MEMBS Congress in Abu Dhabi, UAE
- Peter Coveney gave an invited Talk on "The Virtual Human: In Silico Methods for Personalised Medicine" at MEMBS Congress in Abu Dhabi, UAE
- David Wright gave a presentation "Towards mutually beneficial industrial engagement with the EUDAT collaborative data infrastructure" at a EUDAT2020 meeting in Porto, Portugal

Our Network contains a growing list of partners from HPC-poor countries:

- Zayed University, United Arab Emirates
- KINDI, Centre for Computing Research, Qatar
- Institute of Molecular Biology, National Academy of Sciences, Armenia
- DiaVita, Bulgaria

Our CompBioMed events have attracted attendees travelling from places such as Cyprus, Portugal, Romania, and United Arab Emirates.

7.4 Key Performance Indicators and Output Measurement

CompBioMed is committed to a list of Key Performance Indicators (KPIs). The 3 KPIs related to dissemination are listed below:

- 1. Number of people attending the two workshops events organised by WP3:
 - Target: 50 attendees per workshop
 - Current progress: 2 CompBioMed Workshops organised, reaching 70 and 95 attendees.
- 2. Number of publications in peer-reviewed international journals that acknowledge the support of CompBioMed.
 - Target: by the end of the three-year deployment phase, at least 10 publications (two in impact factor ten or higher journals) from 5 different research groupings with the CoE
 - Current progress: 23 Publications
- 3. Number of companies engaged.
 - Target: by the end of the three-year deployment phase, at least 20 companies, at least 30% being SMEs, have accessed CompBioMed services
 - Current progress: 83 companies engaged (38% are SMEs)

Further to these KPIs, we have a number of other types of output measurement, indicated in D3.2. These are as follows:

PU

Page 33

Version 1.2



Number of events participated in

As shown in Section 7.2.2, we participated in 21 events in months 12-18, bringing the total to 63 events to date.

Number of attendees at our events

As shown in Section 7.2.1, there were 211 attendees at our events in months 12-18, bringing the total to 1178 people to date.

Feedback from workshops and events, e.g. via surveys

We surveyed the attendees at our two major events in the first 12 months of the project, that is:

- The Cloud & High-Performance Computing in Biomedicine at UCL, London on 27 April 2017
- CompBioMed & BioExcel Free-Energy Workshop at UCL, London on 31 May 2017

The surveys asked, among other things:

- "Did you find this event useful?", with 5 available answers ranging from "Very useful" to "Not at all useful"
- "In general, I judge this meeting to be:", with 5 available answers ranging from "Excellent" to "Very poor"

At the Cloud & High-Performance Computing meeting, 18 attendees returned feedback forms. On average, the attendees answered the questions "Did you find this event useful?" at 4.33 out of 5, with 5 being "Very useful". For the question "In general, I judge this meeting to be:", the attendees answered an average of 4.44 out of 5, with 5 being "Excellent".

At the CompBioMed & BioExcel Free-Energy Workshop, 43 attendees returned feedback forms. On average, the attendees answered the questions "Did you find this event useful?" at 4.44 out of 5, with 5 being "Very useful". For the question "In general, I judge this meeting to be:", the attendees answered an average of 4.51 out of 5, with 5 being "Excellent".

Number of publications

In months 12 to 18 of the project, the CompBioMed consortium published 10 publications, taking the total to 23 since the start of the project.

Citations from publications

The citations of CompBioMed publications as of 11 February 2018 are listed in Section 7.1.4. In total our papers have been cited 47 times so far.

Publication journal impact factor

The impact factors of the journals we have published in are shown in Section 7.1.4. There are currently 5 publications in journals with an impact factor above 5, and on average the impact factor for all of our publications is 3.41.

Website stats and social media stats

Below we list cumulative statistics from the start of the project to the time of writing this report (month 17):

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Page 34

Version 1.2



At the time of writing, the key statistics for the website include:

- 17,150 views (up from 9,453 at month 12)
- 92 pages (up from 67 at month 12)
- 71 news/events posts (up from 52 news at month 12)

Key statistics for the CompBioMed Twitter account include:

- Tweets: 272 (up from 165 at month 12)
- Followers: 334 (up from 211 at month 12)
- Likes: 200 (up from 47 at month 12)
- Twitter Impressions: 105,333 (up from 45,226 at month 12)

Key statistics for the CompBioMed YouTube page include:

- 34 videos (up from 30 videos at month 12)
- 23 subscribers (up from 14 at month 12)
- 647 views (up from 392 at month 12)

Estimated sizes of audiences reached

The tables in the Appendices include a column that shows the estimated audience size for each piece of dissemination activity. Using these estimates, we can calculate the following output measurements from the start of the project to the time of writing:

- Size of audience reached by external websites: 18,368 cumulative audience size (up from 12,968 at month 12)
- Size of audience reached by the external social media activity: 1,482,973 potential impressions (up from 10,973 at month 12)
- Size of audience reached by the participation at external events: 11,342 total cumulative audience size (up from 7,613 at month 12)

7.5 Plans for the Second Half of the Project

After an extremely active and productive first 18 months of the project, we aim to continue the momentum into the second 18 months, with many plans for event participation and organisation in the pipeline, and ongoing discussions to expand our network of partners and related projects.

CompBioMed is planning to have a major presence at VPH2018 in September 2018 in Zaragoza, including a CompBioMed booth. Also, at the 8th World Congress of Biomechanics, July 2018 Dublin Ireland, CompBioMed consortium members will give multiple talks. Moreover, at Supercomputing SC18, in November 2018 in Texas, USA, we aim to have CompBioMed members give talks and to have our dissemination materials available on the exhibition floor where possible. Furthermore, we are in ongoing discussions with other H2020 Centres of Excellence to arrange our participation in their events, and their participation in our events.

We also aim to participate in an increasing number of clinical events, we have identified the following targets:

- European Society of Cardiology
- European Heart Rhythm Association
- Safety Pharmacology Society

PU

Page 35

Version 1.2



- Gordon Conference on Cardiac Arrhythmia mechanisms
- UCL-Barts Heart Centre Translational Electrophysiology Symposium
- BHF Centre of Research Excellence Annual Symposium
- TRM Forum on Computer Simulation of Cardiac Function
- Gordon Conference on Drug Safety
- World Congress of Biomechanics
- The European Congress of Biomechanics
- The International Society of Biomechanics
- The International Conference on Computational Bioengineering
- The Orthopaedic Research Society

We will continue to screen the IMAX film at various events, including the Cheltenham Film Festival in the UK, and at Barcelona Supercomputing Center in Spain.

We will continue to grow our network of Associate Partners and related projects with interest from new Associate Partners continuing.

In terms of publishing, we are currently targeting publications in various journals, including Circulation, Frontiers in Physiology, the International Journal of Numerical Methods in Biomedical Engineering, and the International Journal of Computer Assisted Radiology and Surgery.

8 Conclusions

As reported, there was a substantial amount of training and dissemination activity in the first 18 months of CompBioMed. The actions of the CompBioMed consortium have met and are going beyond the plans laid out in the training and dissemination action plans and the project's description of work.

On the training side, strong foundations have been laid and the first important results have been achieved. A strong collaboration with the VPH Institute has been set up, which is contributing to ensuring positive and long-lasting results. The consortium is committed to achieve the ambitious goals set.

On the dissemination front, the CompBioMed consortium targeted many events and dissemination channels of various scales and with a wide variety of themes, covering numerous domains aligned with our aims.

The project's training and dissemination KPIs are being met and exceeded on both sides.

We believe that, through our dissemination and training activities, expected impacts will be accelerated and strengthened. Through the dissemination of CompBioMed research findings to academic, industrial, and clinical users, we will contribute to the strength and leadership of the EU in HPC technologies in Computational Biomedicine, also having an impact on the emerging HPC markets. Through the building of networks between our community and the encouragement of collaboration activities, together with our training agenda, we will accelerate European excellence in Computational Biomedicine.



9 Appendices

Details	Date From	Audience(s)	Number of
Acellera posted a link and logo of CompBioMed on their website: www.acellera.com	10/01/2017	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias], [Customers]	500
The UCL Chemistry website featured a news story on the CompBioMed-Science Museum "The Virtual Human" Event. http://www.ucl.ac.uk/chemistry/news/events/2 017/virtual-human	25/08/2017	[Scientific Community (higher education, Research)]	200
The UCL Chemistry website featured a news story on the CompBioMed simulations run on the supercomputer superMUC. http://www.ucl.ac.uk/chemistry/news/news/20 17/ccs-supermuc-allocation	22/08/2017	[Scientific Community (higher education, Research)]	200
UvA published an article about the CompBioMed project on its website and newsletter: http://www.uva.nl/en/shared- content/faculteiten/en/faculteit-der- natuurwetenschappen-wiskunde-en- informatica/news/2016/04/compbiomed.html	18/04/2016	[Scientific Community (higher education, Research)]	300
SURFsara posted about the CompBioMed project ahead of its kick-off. https://www.surf.nl/en/news/2016/05/surfsara- partner-in-centre-of-excellence-in- computational-biomedicine.html	18/05/2016	[Scientific Community (higher education, Research)], [Customers], [Industry]	200
The VPH-Institute posted a news story on the CompBioMed Innovation Exchange Program. http://www.vph- institute.org/news/compbiomed-innovation- exchange-programme.html	12/01/2017	[Scientific Community (higher education, Research)]	300
The VPH-Institute advertises the CompBioMed webinar series on their website: http://www.vph-institute.org/webinar.html	01/11/2017	[Scientific Community (higher education, Research)]	300
The VPH-Institute wrote an article on CompBioMed webinar #1: http://www.vph- institute.org/news/1st-webinar-in-collaboration- compbiomed.html	07/12/2017	[Scientific Community (higher education, Research)]	300

Table 3 - CompBioMed Consortium Website Activity



Chemistry World Article "Drug binding simulations promise to get personal" featuring Peter Coveney's Computational Biomedicine research. https://www.chemistryworld.com/news/drug- binding-simulations-promise-to-get- personal/2500269.article#.WH83snhl1Z8.twitter	12/01/2017	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias], [Customers]	1000
Spanish National Newspaper published an article on CompBioMed - "Crean un nuevo centro de investigación en biomedicina computacional" http://www.lavanguardia.com/vida/20170201/4 13912002260/crean-un-nuevo-centro-de- investigacion-en-biomedicina- computacional.html	02/02/2017	[General Public], [Medias]	500
The CompBioMed-Science Museum "The Virtual Human" Event featured on the BBC Tomorrow's World website, http://www.bbc.co.uk/tomorrowsworld	01/10/2017	[General Public], [Medias]	2000
PRACE website post for the CompBioMed- Science Museum "The Virtual Human" Event. http://www.prace-ri.eu/virtual-human-imax- event-science-museum-lates/	19/09/2017	[Scientific Community (higher education, Research)]	200
UCL Events Calendar website published the CompBioMed-Science Museum "The Virtual Human" Event. http://events.ucl.ac.uk/event/event:v142- j7bnpupn-w2ab4r/the-virtual-human-imax-film- at-the-science-museum	27/09/2017	[Scientific Community (higher education, Research)]	100
Insigneo - Institute for <i>in silico</i> Medicine published a post on the CompBioMed-Science Museum "The Virtual Human" Event. http://insigneo.org/2017/10/how-to-build-a- virtual-human-at-the-science-museum-imax- theatre/	01/10/2017	[Scientific Community (higher education, Research)]	100
Insigneo - Institute for <i>in silico</i> Medicine published an article "Sheffield Biomedical Research Centre Public Launch Event hosted by SITraN" which featured the CompBioMed-Science Museum "The Virtual Human" Event. https://insigneo.org/2017/12/sheffield- biomedical-research-centre-public-launch-event- hosted-by-sitran/	01/11/2017	[Scientific Community (higher education, Research)]	100



Details	Date From	Date To	Audience(s)	Number of People
Acellera posted 14 tweets related to CompBioMed, @acellera	10/01/2017	31/03/2018	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias], [Customers]	8500
EPCC Tweeted about their booth at Supercomputing 17. https://twitter.com/EPCCed/status/92822950 0026019840	12/11/2017	17/11/2017	[Scientific Community (higher education, Research)], [Industry]	1500
The UCL Mathematical & Physical Sciences Twitter account tweeted about the Chemistry World Article "Drug binding simulations promise to get personal" featuring Peter Coveney's Computational Biomedicine research. @uclmaps https://twitter.com/uclmaps/status/82165412 0448884737	18/01/2017	18/01/2017	[Scientific Community (higher education, Research)]	1600
The UCL Mathematical & Physical Sciences Facebook account posted about the Chemistry World Article "Drug binding simulations promise to get personal" featuring Peter Coveney's Computational Biomedicine research. @uclmaps https://www.facebook.com/plugins/post.php? href=https%3A%2F%2Fwww.facebook.com%2 Fuclmaps%2Fposts%2F1490828110946028&wi dth=500	18/01/2017	18/01/2017	[Scientific Community (higher education, Research)]	1600
Samira Ahmed (BBC journalist) Twitter @SamiraAhmedUK Tweeted for the CompBioMed-Science Museum "The Virtual Human" Event https://twitter.com/SamiraAhmedUK/status/9 10409063493718017	20/09/2017	20/09/2017	[General Public], [Medias]	38000
Roger Highfield (Science Museum Group) tweeted 6 times about the CompBioMed- Science Museum "The Virtual Human" Event, @RogerHighfield	01/08/2017	01/12/2017	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	101400
The Science Museum tweeted twice about the CompBioMed-Science Museum "The Virtual Human" Event, @sciencemuseum	16/09/2017	24/09/2017	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	1324000

Table 4 -	CompBioMed	Consortium	Social	Media	Activity



Emily Lumley (UCL) & Hugh Martin (CBK) tweeted 14 times about the CompBioMed- Science Museum "The Virtual Human" Event	01/08/2017	01/12/2017	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	5000
The Mauri Lab at UCL (@Mauri_group) Tweeted about the CompBioMed-Science Museum "The Virtual Human" Event https://twitter.com/Mauri_group/status/9131 17183600943105	27/09/2017	27/09/2017	[Scientific Community (higher education, Research)]	400
The VPH-Institute regularly tweets about the CompBioMed webinar series: https://twitter.com/VPH_Institute?ref_src=tw src%5Etfw&ref_url=http%3A%2F%2Fwww.vph -institute.org%2Fnews-5.html	Regularly	-	[Scientific Community (higher education, Research)]	817

Table 5 - CompBioMed Consortium Non-Peer Reviewed Publications

Details	Date From	Date To	Audience(s)	Number of People
Alfonso Santiago (UPC) produced his Ph.D. Thesis "Fluid-electro-mechanical model of the human heart" and defended in front of an audience at BSC, Barcelona. http://doctorat.upc.edu/ca/tesi/llistats-de- tesis/tesis-autoritzades-per-a-defensa	22/03/2018	22/03/2018	[Scientific Community (higher education, Research)]	20
Emily Lumley (UCL) prepared the CompBioMed Newsletter January 2018. http://www.compbiomed.eu/wp- content/uploads/2018/01/newsletter3.pdf	01/01/2018	31/01/2018	[Scientific Community (higher education, Research)], [Industry], [General Public]	200
Alex Heifetz (Evotec) edited the book "Computational Methods for GPCR Drug Discovery", published by Springer	01/01/2018	31/01/2018	[Scientific Community (higher education, Research)], [Industry], [General Public]	100

Table 6 - CompBioMed Consortium Other Activities

Details	Date From	Date To	Audience(s)	Number of People
T Sloan, G Pringle, T Peete (EPCC), and E Lumley (UCL) prepared EPCC News 82 Nov'2017 (EPCC Newsletter). https://www.epcc.ed.ac.uk/sites/default/files/ EPCCNews82.pdf	01/11/2017	01/11/2017	[Scientific Community (higher education, Research)], [Industry]	200
Emily Lumley (UCL) prepared the monthly CompBioMed e-newsletter October 2017, distributed by email	01/10/2017	31/10/2018	[Scientific Community (higher education,	150



			Research)], [Industry], [General Public]	
Emily Lumley (UCL) prepared the monthly CompBioMed e-newsletter November 2017, distributed by email	01/11/2017	30/11/2017	[Scientific Community (higher education, Research)], [Industry], [General Public]	150
Emily Lumley (UCL) prepared the monthly CompBioMed e-newsletter February 2017, distributed by email	01/02/2018	28/02/2018	[Scientific Community (higher education, Research)], [Industry], [General Public]	150
Emily Lumley (UCL) prepared the monthly CompBioMed e-newsletter March 2017, distributed by email	01/03/2018	31/03/2018	[Scientific Community (higher education, Research)], [Industry], [General Public]	150
The VPH-Institute regularly advertises the CompBioMed webinar series on their newsletter: http://www.vph- institute.org/archive_newsletter.html	01/11/2017	31/03/2018	[Scientific Community (higher education, Research)]	7200
Franck Chevalier (Acellera) organised the webinar "Running simulation in the Cloud with AceCloud" for CompBioMed core and associate partners	21/02/2018	21/02/2018	[Scientific Community (higher education, Research)], [Industry]	30
Franck Chevalier (Acellera) organised the webinar "Running simulation in the Cloud with AceCloud" as an open session	22/02/2018	22/02/2018	[Scientific Community (higher education, Research)], [Industry]	30
Franck Chevalier (Acellera) organised the webinar "HTMD for drug Discovery" for CompBioMed core and associate partners	28/02/2018	28/02/2018	[Scientific Community (higher education, Research)], [Industry]	30
Franck Chevalier (Acellera) organised the webinar "HTMD for drug Discovery" as an open session	03/01/2018	03/01/2018	[Scientific Community (higher education, Research)], [Industry]	30
Franck Chevalier (Acellera) organised the webinar "Computerized Drug Discovery with PlayMolecule"	15/03/2018	15/03/2018	[Scientific Community (higher education, Research)], [Industry]	30
The CompBioMed-Science Museum "The Virtual Human" Event was posted on the weekly e-newsletter in the UCL Chemistry Department	01/09/2017	01/09/2017	[Scientific Community (higher education, Research)]	50

Table 7 - CompBioMed Event Organisation Activity

Details	Date From	Date To	Audience(s)	Number of People
Emily Lumley & Peter Coveney (UCL) & Alfons			[Scientific Community	
Hoekstra (UvA) organised the CompBioMed	26/03/2018	27/03/2018	(higher education,	60
AHM March 2018 in Amsterdam, Netherlands			Research)], [Industry]	



Emily Lumley & Peter Coveney (UCL) & Mariano Vazquez (BSC) organised the CompBioMed & Virtual Heart Joint Workshop in Amsterdam, Netherlands	28/03/2018	28/03/2018	[Scientific Community (higher education, Research)], [Industry]	30
Gabor Zavodszky (UvA) organised a workshop on "Back to the basics: How to improve the efficacy of science? Fertilizing the field of research by clinician-scientist collaboration" during WFITN 2017 in Budapest, Hungary. http://www.wfitn2017.hu	15/10/2017	15/10/2017	[Scientific Community (higher education, Research)], [Industry]	100
Franck Chevalier (Acellera) organised the workshop "HTMD and AceCloud for Drug Discovery" in the UK	24/10/2017	24/10/2017	[Industry]	21

Table 8 - Dissemination related to the CompBioMed-Science Museum "The Virtual Human" Event

Details	Date From	Date To	Audience(s)	Number of People
Samira Ahmed Twitter @SamiraAhmedUK Tweeted for the CompBioMed-Science Museum "The Virtual Human" Event https://twitter.com/SamiraAhmedUK/status/9 10409063493718017	20/09/2017	20/09/2017	[General Public], [Medias]	38000
The Mauri Lab at UCL (@Mauri_group) Tweeted about the CompBioMed-Science Museum "The Virtual Human" Event https://twitter.com/Mauri_group/status/9131 17183600943105	27/09/2017	27/09/2017	[Scientific Community (higher education, Research)]	400
The UCL Chemistry website featured a news story on the CompBioMed-Science Museum "The Virtual Human" Event. http://www.ucl.ac.uk/chemistry/news/events/ 2017/virtual-human	25/08/2017	25/08/2017	[Scientific Community (higher education, Research)]	200
The CompBioMed-Science Museum "The Virtual Human" Event featured on the BBC Tomorrow's World website, http://www.bbc.co.uk/tomorrowsworld	01/10/2017	01/10/2017	[General Public], [Medias]	2000
UvA posted an article on the event on its website and the Informatics Department newsletter: http://ivi.uva.nl/content/news/2017/09/%E2% 80%9Cthe-virtual-human%E2%80%9D-imax- event-at-the-science-museum-lates.html	26/09/2017	26/09/2017	[Scientific Community (higher education, Research)]	350
PRACE website post for the CompBioMed- Science Museum "The Virtual Human" Event. http://www.prace-ri.eu/virtual-human-imax- event-science-museum-lates/	19/09/2017	19/09/2017	[Scientific Community (higher education, Research)]	200

Page 42



D3.5 Report on Training and Dissemination

UCL Events Calendar website published the CompBioMed-Science Museum "The Virtual Human" Event. http://events.ucl.ac.uk/event/event:v142- j7bnpupn-w2ab4r/the-virtual-human-imax- film-at-the-science-museum	27/09/2017	27/09/2017	[Scientific Community (higher education, Research)]	100
Insigneo - Institute for in silico Medicine published a post on the CompBioMed-Science Museum "The Virtual Human" Event. http://insigneo.org/2017/10/how-to-build-a- virtual-human-at-the-science-museum-imax- theatre/	01/10/2017	01/10/2017	[Scientific Community (higher education, Research)]	100
Insigneo - Institute for in silico Medicine published an article "Sheffield Biomedical Research Centre Public Launch Event hosted by SITraN" which featured the CompBioMed-Science Museum "The Virtual Human" Event. https://insigneo.org/2017/12/sheffield- biomedical-research-centre-public-launch- event-hosted-by-sitran/	01/11/2017	01/11/2017	[Scientific Community (higher education, Research)]	100
BSC, Paul Melis (SURFsara), Casper van Leeuwen (SURFsara), Peter Coveney (UCL) <i>et</i> <i>al.</i> produced an IMAX animation called "Virtual Humans", which was screened at the "London Science Museum Lates". http://www.compbiomed.eu/home/how-to- build-the-virtual-human/	27/09/2017	27/09/2017	[General Public], [Medical students], [Scientific Community (higher education, Research)], [Other]	150
Science Museum the CompBioMed-Science Museum "The Virtual Human" Event YouTube Promo: https://www.youtube.com/watch?v=QGhobM PGHSM	07/09/2017	07/09/2017	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	1688
The CompBioMed-Science Museum "The Virtual Human" Event was posted on the weekly e-newsletter in the UCL Chemistry Department	01/09/2017	01/09/2017	[Scientific Community (higher education, Research)]	50
Roger Highfield (Science Museum Group) tweeted 6 times about the CompBioMed- Science Museum "The Virtual Human" Event, @RogerHighfield	01/08/2017	01/12/2017	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	101400
The Science Museum tweeted twice about the CompBioMed-Science Museum "The Virtual Human" Event, @sciencemuseum	16/09/2017	24/09/2017	[General Public], [Medias], [Scientific Community (higher education, Besearch)], [Industry]	1324000



Peter Coveney (UCL) screened the "The Virtual Human" IMAX video at an invited talk on "The Virtual Human: In Silico Methods for Personalized Medicine" at the Data Intensive Studies Center (DISC) Fall Symposium in Massachusetts, USA.	08/11/2017	08/11/2017	[Scientific Community (higher education, Research)], [Industry]	150
Peter Coveney (UCL) screened "The Virtual Human" IMAX film at an invited talk on "Exploiting HPC to Change the Way Neurosurgeons Operate in the Future and Improve Outcomes for Patients" at the Annual High Performance Computing & Big Data 2018 conference in London, UK.	06/02/2018	06/02/2018	[Scientific Community (higher education, Research)], [Industry]	100
Emily Lumley (UCL) & Hugh Martin (CBK) tweeted 14 times about the CompBioMed- Science Museum "The Virtual Human" Event	01/08/2017	01/12/2017	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	5000
Emily Lumley (UCL) included the CompBioMed- Science Museum "The Virtual Human" Event in the November 2017 CompBioMed e- Newsletter	01/11/2017	30/11/2017	[Scientific Community (higher education, Research)], [Industry]	100
Emily Lumley (UCL) included the CompBioMed- Science Museum "The Virtual Human" Event in the May 2017 CompBioMed Newsletter	01/05/2017	31/05/2017	[Scientific Community (higher education, Research)], [Industry]	100
Emily Lumley (UCL) included the CompBioMed- Science Museum "The Virtual Human" Event in the September 2017 CompBioMed Newsletter	01/09/2017	30/09/2017	[Scientific Community (higher education, Research)], [Industry]	100
Emily Lumley (UCL) included the CompBioMed- Science Museum "The Virtual Human" Event in the January 2018 CompBioMed Newsletter	01/01/2018	31/01/2018	[Scientific Community (higher education, Research)], [Industry]	100

Table 9 - CompBioMed Consortium Event Participation Activity

Details	Date From	Date To	Audience(s)	Number of People
Toni Collis staffed an EPCC exhibition booth at Supercomputing 17 in Denver, Colorado, USA to discuss CompBioMed, distributed EPCCNews with CompBioMed article (see below) and distributed CompBioMed promotion material. https://sc17.supercomputing.org/ https://twitter.com/EPCCed/status/92822950 0026019840	12/11/2017	17/11/2017	[Scientific Community (higher education, Research)], [Industry]	500



Acellera gave a talk at CDDD, Milan, Italy on "Optimizing Proteins and Ligands for	16/11/2017	17/11/2017	[Scientific Community (higher education.	80
Computerized Drug Discovery"		,,	Research)]. [Industry]	
Acellera gave a talk at EJIBCE Coimbra			Scientific Community	
"Optimizing Proteins and Ligands for	22/12/2017	22/12/2017	(higher education.	50
Computerized Drug Discovery"	, , -	, , -	Research)]. [Industry]	
Alberto Marzo (USED) gave a Keynote seminar			///////////////////////////////////////	
on cardiovascular modelling titled "Use of 1D			[Scientific Community	
models to improve the diagnosis of cerebral	28/12/2017	28/12/2017	(higher education,	100
vasospasm" organised at the University of			Research)],	200
Cagliari, Italy, Dec 2017			[Clinicians] [Industry]	
David Wright (UCL) gave a presentation				
"Towards mutually beneficial industrial			[Scientific Community	
engagement with the FLIDAT collaborative	24/01/2018	24/01/2018	(higher education	10
data infrastructure" at a ELIDAT2020 meeting	24/01/2010	24/01/2010	(Inglier education, Research)] [Industry]	10
in Porto, Portugal			Research), [maastry]	
Alex Patronis (UCL) gave a presentation on			[Scientific Community	
"CompBioMed at pre-evascale" at 2nd	31/01/2018	31/01/2018	(higher education	70
EuroHPC in Brussels, Belgium	51/01/2010	51/01/2010	(higher education, Research)] [Industry]	70
Peter Coveney (LICL) gave an invited talk on			[Scientific Community	
CompBioMed at the Cambridge	06/09/2017	08/09/2018	(higher education	50
Ophthalmological Symposium, Cambridge, LIK	00/03/201/	00/05/2018	(higher education,	50
Deter Coveney (UCL) gave an invited Talk on			Researchyj	
"Banid Accurate and Beliable Binding Affinity			[Scientific Community	
Calculations for Drug Discovery & Presidion	02/11/2017	02/11/2017	(higher education	100
Calculations for Drug Discovery & Precision	02/11/2017	02/11/2017	(Ingher education,	100
			Research)j, [industry]	
Deter Coveney (UCL) gave an invited Talk on				
"The Virtual Human: In Silice Methods for			[Scientific Community	
Deverselized Medicine" at MEMDE Congress in	04/11/2017	04/11/2017	(higher education,	100
Abu Dhabi LLAE			Research)], [Industry]	
"The Mistual Human In Silice Matheda for			[Colontific Community	
Demonstrated Medicine," at the Data Interaction	00/11/2017	00/11/2017	(bisher education	100
Studies Canton (DISC) Fell Suma situation	08/11/2017	08/11/2017	(nigner education,	100
Studies Center (DISC) Fail Symposium in			Research)], [Industry]	
Massachusetts, USA.				
"The Virtual Luman In Silice Methods for			[Scientific Community	
Demonstrated Medicine," at the UITS Collections	20/11/2017	20/11/2017	(higher education,	30
Personalised Medicine" at the HITS Colloquium			Research)]	
In neuerony, Germany			[Colontific Community	
Complia Mod at the 2017 Discuss Autoria	22/11/2017	22/11/2017	(bigher advection	40
Compulsionied at the 2017 BIOEXCELAHIM IN	22/11/201/	22/11/201/	(nigner education,	40
Amsterdam, Netherlands			Kesearch)j	
Peter Coveney (UCL) gave an invited talk on	00/02/2010	00/02/2010	[Scientific Community	100
Exploiting HPC to Change the Way	06/02/2018	06/02/2018	(nigner education,	100
			DESEMICITY, HUQUSTRVI	



Improve Outcomes for Patients" at the Annual High Performance Computing & Big Data 2018				
Gabor Zavodszky (UvA) gave a plenary talk on "Blood flow simulations: what have we learned recently?" at WFITN 2017 in Budapest, Hungary. http://www.wfitn2017.hu	17/10/2017	17/10/2017	[Scientific Community (higher education, Research)], [Industry]	1400
Gabor Zavodszky (UvA) gave a conference talk on "Fast patient-specific flow diverter simulation" at WFITN 2017 in Budapest, Hungary. http://www.wfitn2017.hu	16/10/2017	16/10/2017	[Scientific Community (higher education, Research)]	80
Gabor Zavodszky (UvA) presented a poster on "In-silico investigation of the effect of cytoplasm viscosity on blood transport mechanics" at BloodFlow 2017 in Paris, France. http://www.fz-juelich.de/ics/ics- 2/EN/Leistungen/ConferencesAndWorkshops/ Blood-Flow-2017/_node.html	09/10/2017	11/10/2017	[Scientific Community (higher education, Research)]	90
Benjamin Czaja (UvA) presented a poster on "The effects of pulsatility in 2D cell resolved blood flow simulations of curved vessels with aneurysms" at BloodFlow 2017 in Paris, France. http://www.fz-juelich.de/ics/ics- 2/EN/Leistungen/ConferencesAndWorkshops/ Blood-Flow-2017/_node.html	09/10/2017	11/10/2017	[Scientific Community (higher education, Research)]	90
Britt van Rooij (UvA) gave a conference talk on "Cell-based platelet aggregation modelling in Hemocell" at BloodFlow 2017 in Paris, France. http://www.fz-juelich.de/ics/ics- 2/EN/Leistungen/ConferencesAndWorkshops/ Blood-Flow-2017/_node.html	09/10/2017	11/10/2017	[Scientific Community (higher education, Research)]	90
CompBioMed talk at the European Heart Rhythm Association meeting, Vienna (delivered by Blanca Rodriguez, UOXF).	21/06/2017	21/06/2017	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
CompBioMed talk at Copenhagen Meeting on Cardiac Arrhythmia, Denmark (delivered by Dr Bueno-Orovio, UOXF)	31/05/2017	31/05/2017	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
CompBioMed talk "Experimentally Calibrated Population of Models Predicts and Explains Inter-Subject Variability" at Gordon Conference on Cardiac Arrhythmia Mechanisms, CA, USA (delivered by Blanca Rodriguez, UOXF)	05/02/2017	05/02/2017	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100



CompBioMed talk on "Computational Cardiology" given at 61st Biophysical Society Meeting, New Orleans, LA, USA (delivered by Blanca Rodriguez, UOXF)	11/02/2017	11/02/2017	[Scientific Community (higher education, Research)]	200
Keynote presentation on Computational Biomedicine given by Peter Coveney (UCL) at the 1st Kennedy Institute Student Symposium in Oxford	17/11/2016	17/11/2016	[Scientific Community (higher education, Research)]	100
CompBioMed talk given at Oxford Centre for Clinical Magnetic Resonance Research Study day held at University of Oxford (delivered by Dr. Mincholé, UOXF)	26/04/2017	26/04/2017	[Scientific Community (higher education, Research)], [Medical Students]	30
CompBioMed talk given at the Cardiac Arrhythmia Centre, Washington University in St Louis, MO, USA (delivered by Blanca Rodriguez, UOXF)	01/03/2017	01/03/2017	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Acellera gave a seminar "Towards Computerized Drug Discovery" given at Complutense University, Madrid, Faculty of Chemistry	24/01/2018	24/01/2018	[Scientific Community (higher education, Research)]	14
Acellera gave training on HTMD, Boston, USA	10/02/2017	10/06/2017	[Industry]	10
Acellera gave a talk at Winter school at BSC, "High Throughput Molecular Dynamics Simulations for Drug Discovery"	14/02/2018	16/02/2018	[Scientific Community (higher education, Research)], [Industry]	20
Gabor Zavodszky (UvA) and Paul Melis (SURFsara) gave a presentation on "Visualization of large-scale cellular simulations of blood" at "Scientific Visualization: From Archaeology to Astronomy", Rotterdam, NL (including short video clip). https://www.esciencecenter.nl/event/progra m/scivis17/ https://www.youtube.com/watch?v=Y3XjiSf3 MOc	20/06/2017	20/06/2017	[Scientific Community (higher education, Research)], [Other]	80
Paul Melis (SURFsara) gave a presentation (including short video clip) on "Visualizing large-scale simulations of blood" at the Blender Conference 2017 in Amsterdam, NL. https://www.blender.org/conference/2017/pr esentations/376	27/10/2017	27/10/2017	[Scientific Community (higher education, Research)], [Other]	50
Paul Melis (SURFsara) gave a presentation (including short video clip) on "Visualizing large cell-based simulations: a bloody mess?" at Super D Event in Amsterdam NI	12/12/2017	12/12/2017	[Scientific Community (higher education, Research)], [Other]	30



https://super-d.surf.nl/programme/december- 12				
Alberto Marzo (USFD) gave a lecture on "VPH video within the context of the VPH initiative and its vision" in a module in Cardiovascular Biomechanics at the University of Sheffield	01/02/2018	01/02/2018	[Scientific Community (higher education, Research)]	15
Bastien Chopard (UNIGE) gave an invited talk on "A physical description of platelets deposition" at Tohoku University	23/03/2017	23/03/2017	[Scientific Community (higher education, Research)]	30
Bastien Chopard (UNIGE) gave an invited talk on "Computer models and numerical simulations of complex systems" at Brown University	22/06/2017	22/06/2017	[Scientific Community (higher education, Research)]	30
Bastien Chopard (UNIGE) gave an invited talk on "Bloodflow: how much do we understand it?" at Tohoku University	23/02/2018	23/02/2018	[Scientific Community (higher education, Research)]	30