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Table of Contents

1	Version Log	4
2	Contributors	4
3	Definitions and Acronyms	5
4	Executive summary	6
5	Introduction	6
6	Training.....	7
6.1	CompBioMed webinar series.....	8
6.2	Training events	13
6.2.1	CompBioMed Winter School 2018 at BSC (Barcelona, 14-16 Feb 2018)	15
	Training evaluation.....	16
6.2.2	CompBioMed training event at VPH2018 (Zaragoza, 4 Sep 2018).....	16
6.2.3	CompBioMed Winter School 2019 at BSC (Barcelona, 13-15 Feb 2019)	17
6.3	University education.....	19
6.3.1	CompBioMed in medical curriculum at UCL	19
6.3.2	CompBioMed in the Science and Engineering curriculum at UCL.....	20
6.4	Other training activities	20
6.4.1	CompBioMed presence in PATC Course at BSC (Barcelona, 14-16 Feb 2017) ..	20
6.4.2	BioExcel & CompBioMed joint workshop (London, 30 May 2017)	21
6.4.3	CompBioMed's presence in VPH Summer School 2018 (Barcelona, 18-22 June 2018) ..	21
6.5	Training Portal and Repository	21
6.6	Training Package.....	22
6.7	Key Performance Indicators	23
7	Dissemination.....	23
7.1	Dissemination Materials.....	24
7.1.1	Publications.....	24
7.1.2	Newsletters	26
7.1.3	Posters	26
7.1.4	Other materials	27
7.1.5	Film and Video	27
7.2	Online Presence.....	29
7.2.1	Social Media.....	29
7.2.2	Websites	30
7.3	Events	33
7.3.1	Event Organisation.....	33
7.3.2	Event Participation.....	36
7.4	Other Dissemination	37
7.5	Targeted Activity.....	37
7.5.1	Targeting the General Public.....	38
7.5.2	Targeting Clinicians	38
7.5.3	Targeting Other H2020 Projects and CoEs	40
7.6	Key Performance Indicators	43
8	Conclusions	43
9	Appendices	45
9.1	CompBioMed Publications	45
9.2	Popularised Publications	49
9.3	Film and Video	50



9.3.1	Film and Video not related to the Virtual Humans Film	50
9.3.2	Activity Specifically related to the Virtual Humans Film	50
9.4	Social Media	56
9.5	Website.....	56
9.6	Organisation of Events.....	58
9.7	Participation in Events	59
9.8	Other.....	69

List of Tables and Figures

Figure 1 – Overview of CompBioMed webinar series.....	8
Table 1 - CompBioMed webinar series calendar and attendance overview.....	10
Figure 2 – Country of residence of webinars’ registrants	11
Figure 3 – Gender composition (%) of webinars’ registrants	12
Figure 4 – User groups’ representation among webinars’ registrants	12
Figure 5 – Replies to webinars’ feedback questionnaire's question	13
Figure 6 – Overview of the 3 training courses organised by CompBioMed	14
Table 2 - CompBioMed training events and attendance overview	15
Figure 7 - Replies to BSC Winter School feedback questionnaire's last question	16
Figure 8 – Recording of one of the VPH2018 pre-course sessions.....	17
Figure 9 – Recording of one of the Winter School 2019 sessions	18
Figure 10 - Replies to BSC Winter School feedback questionnaire.....	19
Figure 11 - Training Portal filtering options	22
Figure 12: The CompBioMed Training Flyer	22
Figure 13: CompBioMed paper featured on the cover of the Physics of Fluids Journal	25
Figure 14: Book on Computational Methods for GPCR Drug Discovery	25
Figure 15: CompBioMed print newsletters from the second half of the project	26
Figure 16: Four of the posters produced in the second half of the project.	27
Figure 15: Screenshot from the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm"	27
Figure 18: Screenshots from the Virtual Humans film	28
Figure 19: Visitor traffic to the CompBioMed website	30
Figure 22: The general public page of the CompBioMed website.....	31
Figure 23: The CompBioMed Software Hub page.....	31
Figure 24: The CompBioMed Conference Website.....	32
Figure 25: The leading homepage banner from the CompBioMed Conference 2019 website	34



1 Version Log

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V0.1	23/08/2019	Manuela Corsini (UvA)/Hugh Martin (CBK)	First draft, sent to internal reviewers
V0.2	13/09/2019	Manuela Corsini (UvA)/Hugh Martin (CBK)	Second draft, revised based on reviewers' comments
V0.3	23/09/2019	Manuela Corsini (UvA)/Hugh Martin (CBK)	Third draft, revised based on additional reviewers' comments
V1.0	30/09/2019	Emily Lumley (UCL)	Final version, submitted

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3 Definitions and Acronyms

Acronyms	Definitions
BSC	Barcelona Supercomputing Center, partner of CompBioMed
CBK	CBK Sci Con Limited, 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
HPC	High Performance Computing
INSIGNEO	Institute for <i>in silico</i> Medicine
KPI	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
TP	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 undertook, 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, D3.4 Report on Dissemination and Training Material and D3.5 Report on Training and Dissemination).

The present WP3 deliverable, D3.6 Final Training and Dissemination Report, aims at providing an overview of the dissemination and training activities carried out and the material developed in the course of the CompBioMed project.

Through the dissemination of CompBioMed research findings to academic, industrial, and clinical users, we contributed 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 contributed to the acceleration of 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, aimed at providing a focal point for the collaboration within the project, and also with external stakeholders, by developing and coordinating the training (led by UvA) and dissemination (led by CBK) activities that enabled us to engage external stakeholders in academia, healthcare and industry with the activities of the project.

Within work package 3, six deliverables have 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 would 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.



- D3.5 Report on Training and Dissemination (UvA) – month 18 - Report on training and dissemination actions undertaken and materials produced, as well as update to the training plan and dissemination action plan.
- D3.6 Final Training and Dissemination Report (UvA) – month 36 - Report on training and dissemination actions undertaken and materials produced (present deliverable).

The present deliverable aims at providing an overview of the training and dissemination activities carried out and the material developed within the CompBioMed project (months 1 to 36).

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) aimed 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 were targeted at the user groups that lie at the heart of CompBioMed: academic, industrial and clinical users.

The training was delivered by CompBioMed scientists alongside HPC experts within the project. The material was provided by those experts. Our approach was 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 relied fully on its partners to avoid duplication and exploit the already available training courses and material.

CompBioMed training activities comprised 10 webinars (section 6.1), 3 face-to-face training events (section 6.2), university education courses (section 6.3), and other training activities (section 6.4), **for a total of approximately 600 live participants and more than 5,000 YouTube views.**

All the available training recordings and materials are made publicly available on the CompBioMed Training Portal (section 6.5): 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.



All the resources on the Training Portal are advertised and disseminated as one unique consistent Training Package (section 6.6).

CompBioMed met a list of Key Performance Indicators (KPIs). The two KPIs related to training are described in section 6.7.

The following sections provide the details of the training activities, the Training Portal, the Training Package and the KPIs.

6.1 CompBioMed webinar series

The CompBioMed D3.3 Training Plan foresaw the organisation, every 2-3 months, of webinars on a range of topics, for various audiences.



Figure 1 – Overview of CompBioMed webinar series

To meet this the CompBioMed webinar series started in November 2017 and ran until the end of the project. It comprised 10 webinars, each one focussing on a distinctive topic and delivered by a different partner, for a total of ±250 live participants, ±1.500 YouTube views (

Table 1) and 32 different countries represented¹ (Figure 2).

¹ Registrations' data



Table 1 - CompBioMed webinar series calendar and attendance overview

Number and title	Broadcast date and delivering partner	Number of live participants	Number of YouTube views
CompBioMed webinar #1 - HPC simulations of cardiac electrophysiology using patient specific models of the heart (using CHASTE and Alya)	22 Nov 2017 (UOXF)	76	332
CompBioMed webinar #2 - Introduction to Cloud Computing for the VPH	30 Jan 2018 (Surfsara+USFD)	21	73
CompBioMed webinar #3 - Lattice Boltzmann method for CompBioMed (incl. Palabos)	19 March 2018 (UNIGE)	24	655
CompBioMed webinar #4 - Introduction to Biomedical Applications on High Performance Computers	07 June 2018 (EPCC+ UvA)	19	233
CompBioMed webinar #5 - High Throughput Molecular Dynamics for Drug Discovery	25 October 2018 (UPF)	12	101
CompBioMed webinar #6 - CompBioMed: Innovations on medical student training	5 December 2018 (UCL)	14	35
CompBioMed webinar #7 - Sensitivity analysis of a strongly coupled cardiac electro-mechanical model	20 March 2019 (UOXF)	45	86
CompBioMed webinar #8 - The EOSC Digital Innovation Hub: open data services for biomedicine and business	28 May 2019 (EOSC-Hub)	9	37
CompBioMed webinar #9 - EUDAT Services for FAIR Data Management	27 June 2019 (Surfsara)	13	12
CompBioMed webinar #10 - HemeLB – Simulation of cardiovascular flow on high performance computers	9 September 2019 (UCL)	10	22
Total		243	1,586

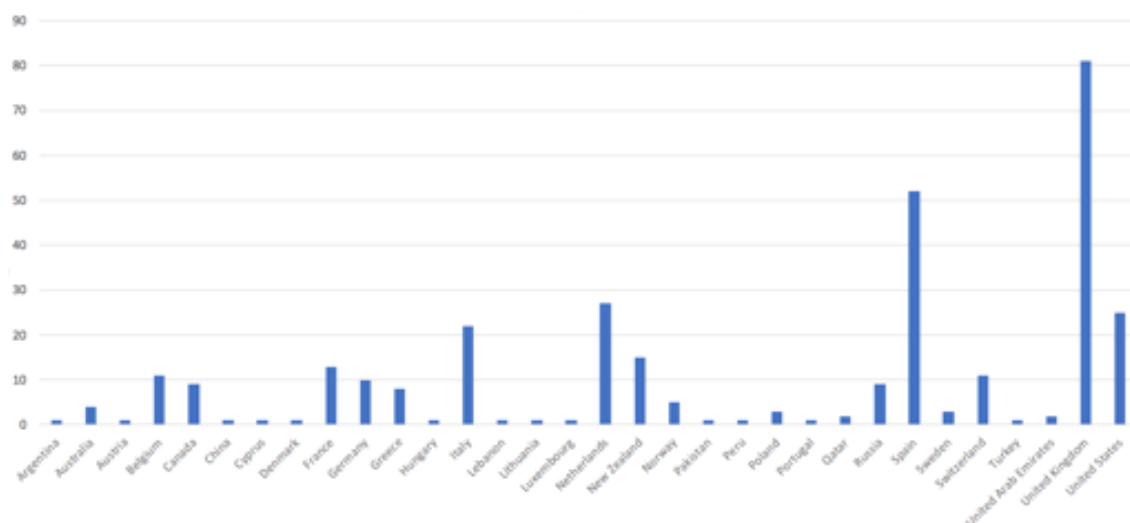


Figure 2 – Country of residence of webinars' registrants

The University of Amsterdam (UvA) was in charge of the planning, organisation, hosting and facilitation of the series.

In order to ensure that the webinar series maintained the CompBioMed flavour, the topics alternated between the 3 CompBioMed application fields (i.e. cardiovascular, molecularly-based and neuro-musculoskeletal medicine) and the HPC/Cloud perspective.

The webinar series was advertised through CompBioMed's website (www.compbioimed.eu/training), the quarterly newsletter (this reached over 200 people), the monthly e-newsletter (reached 144 people), website, social media channels, the VPH Institute's newsletter (reached approximately 7.200 people), website, and social media channels, as well as the partners' relevant formal and informal networks. For each webinar, a flyer was produced to facilitate its dissemination, also offline at meetings and conferences.

Each webinar was recorded, and these were uploaded a few hours after the event on the CompBioMed YouTube channel 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 were asked to fill in a feedback questionnaire. If needed, the questions were tailored to the specific content of the webinar.

After the responses were collected, a full report was produced for each webinar, which was saved in the project's intranet and shared with the speakers. They were particularly useful for those partners running subsequent webinars.

From an analysis of the responses to the registration questions and the feedback questionnaires of the first 9 webinars (337 responses to the registration questions and 92 respondents to the feedback questionnaire in the overall), it was possible to generate some statistics. A few highlights are reported below.

As regards the gender composition of the registrants to the webinars, the majority of them were male, although females were also well represented (66% and 34%, respectively) (Figure 3).

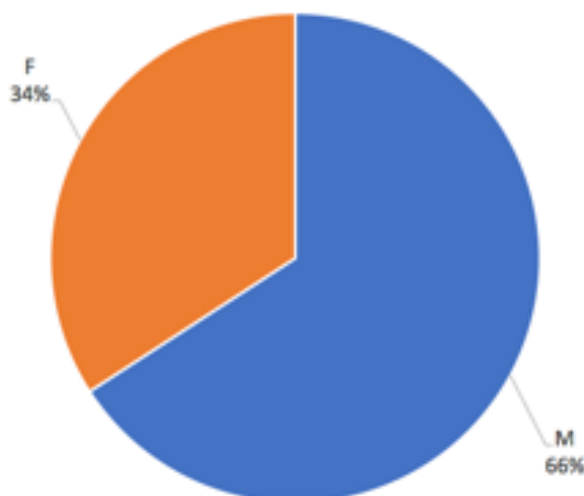


Figure 3 – Gender composition (%) of webinars’ registrants

The vast majority of respondents belonged to the Academic user group (80%), while Industry was represented by 13% of the respondents, Clinical user group by 4% and Other groups by 3% (Figure 4).

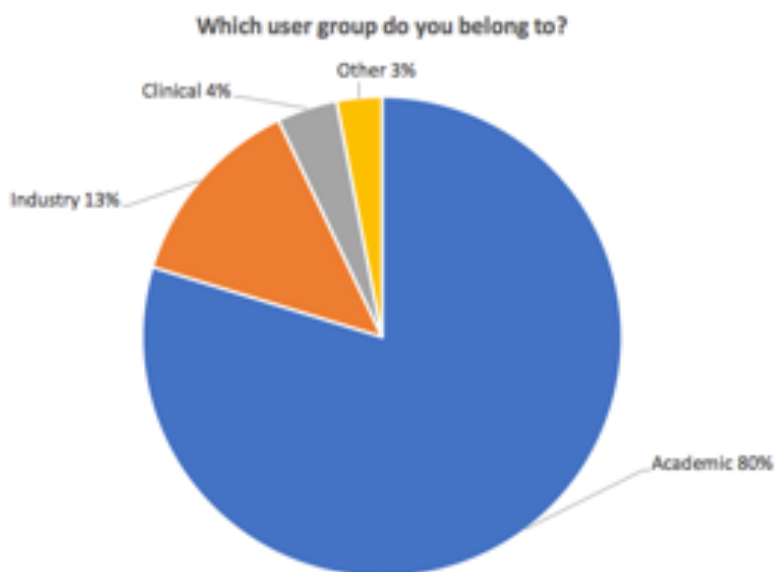


Figure 4 – User groups’ representation among webinars’ registrants

As regards the feedback questionnaire, to the question “Would you recommend the webinar?” almost all responded positively (96%) (Figure 5).

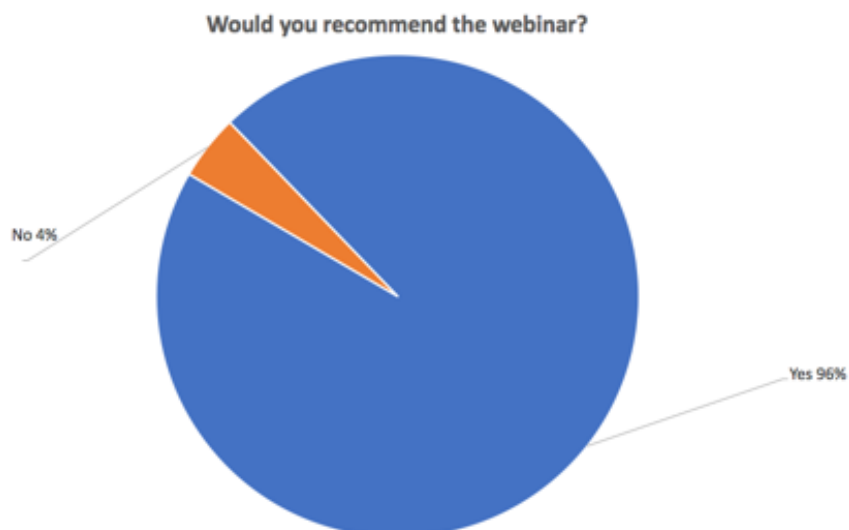


Figure 5 – Replies to webinars' feedback questionnaire's question

6.2 Training events

Three training events were organised within the CompBioMed project, as reported in Figure 6 and

Table 2, for a total of 72 live participants and 3,596 YouTube views.

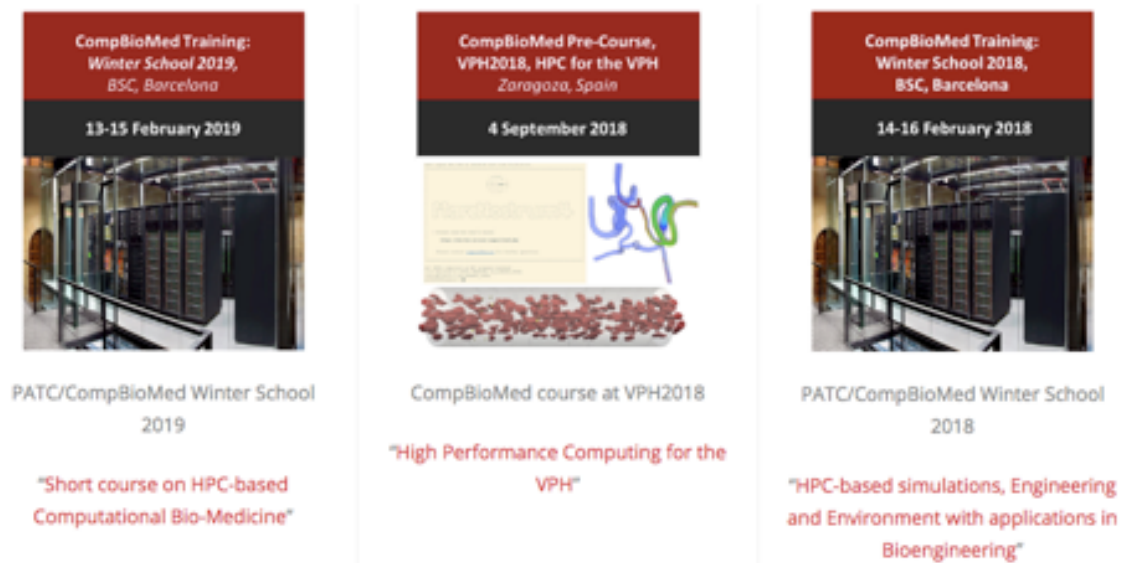


Figure 6 – Overview of the 3 training courses organised by CompBioMed

Table 2 - CompBioMed training events and attendance overview

Title	Date, place and responsible partner	N. live participants	N. YouTube views	Section
CompBioMed Winter school 2018 at BSC "HPC-based simulations, Engineering and Environment with applications in Bioengineering"	14-16 Feb 2018, Barcelona (BSC)	30	3,583	6.2.1
CompBioMed training event at VPH2018 "High Performance Computing for the VPH"	4 Sep 2018, Zaragoza (UvA)	17	291	6.2.2
CompBioMed Winter school 2019 at BSC "Short course on HPC-based Computational Bio-Medicine"	13-15 Feb 2019, Barcelona (BSC)	25	109	6.2.3
	Total	72	3,983	

The following paragraphs provide the details of such training events.

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

The Barcelona Supercomputing Center's Winter School "HPC-based simulations, Engineering and Environment with applications in Bioengineering" (<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.

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 was announced 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** 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 website², 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.

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 a highlight, Figure 7 shows that, on a sliding scale of 1 – 5, a clear majority (67%) assigned at least 4 out of 5 to the course, when asked the last question "How would you rate the overall value of this course?".

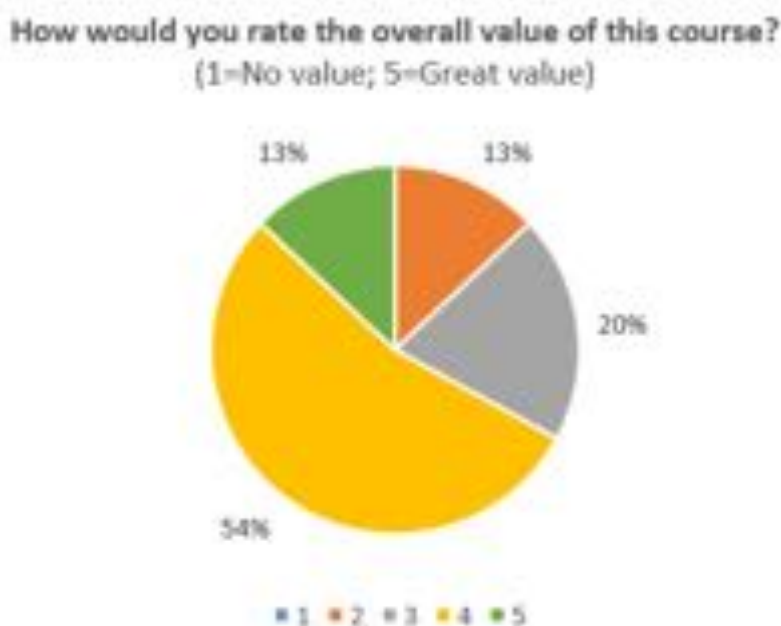


Figure 7 - Replies to BSC Winter School feedback questionnaire's last question

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

As part of the VPH2018 conference "VPH for In Silico Medicine", running in Zaragoza on 5-7 September 2018, CompBioMed organized a training session titled "High Performance Computing for the VPH - A practical introduction to HPC usage"

² <https://www.compbiomed.eu/events-2/compbiomed-training-winter-school-2018-at-bsc/>

(<https://www.compbioimed.eu/events-2/high-performance-computing-for-the-vph>). The course took place the day before the start of the conference, on 4 September 2018, at the conference venue, the University of Zaragoza.

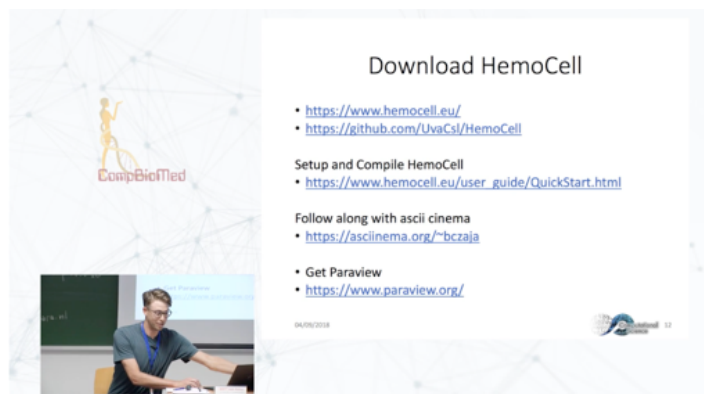


Figure 8 – Recording of one of the VPH2018 pre-course sessions

The course targeted early phase researchers and aimed to provide a short and concise introduction to HPC programming as well as 2 application examples. All lectures were hands-on, using BSC's MareNostrum supercomputer. The course was fully booked with 30 registrants. **17 students participated in the course.** The event was recorded, and the recording was made freely available on the CompBioMed Training Portal. UvA has taken the lead in organising the course.

Feedback on the training was collected by means of a paper feedback questionnaire distributed to the attendees and collected at the end of the session. All the respondents (16) to the questionnaire replied that they would recommend the course.

6.2.3 CompBioMed Winter School 2019 at BSC (Barcelona, 13-15 Feb 2019)

The CompBioMed Winter School 2019, titled “Short course on HPC-based Computational Bio-Medicine” (<https://www.compbioimed.eu/patc-compbioimed-winter-school-2019>), took place at Barcelona Supercomputing Center (BSC) on 13-15 February 2019.

The objective of the course was to give a panorama on the use of HPC-based computational mechanics in Engineering and Environment through the projects BSC is carrying out. This panorama included the basics of what is behind the main tools: computational mechanics and parallelization. The training was delivered in collaboration with PRACE.

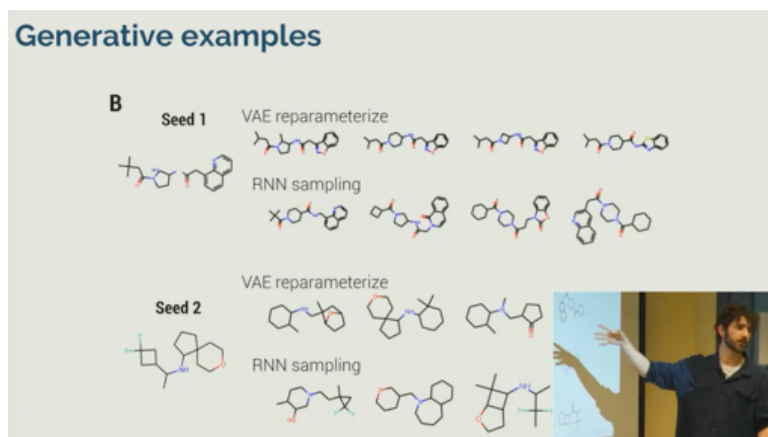


Figure 9 – Recording of one of the Winter School 2019 sessions

The course gave a wide perspective and the latest trends of how HPC helps in industrial, clinical and research applications allowing to achieve more realistic multiphysics simulations. In addition, the students had the opportunity of visiting and running jobs on the Marenostrum supercomputer. The course targeted trainees with some theoretical and practical knowledge, PhD students, master students, engineers, specialists with at least 1st cycle degree or similar background experience.

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

The course was free of charge and 5 travel grants were awarded to a selected number of participants for covering part of their travelling expenses.

The final agenda, the recordings of the sessions and the reports from the travel grantees are available on CompBioMed's website³.

Feedback on the training was collected by means of a paper feedback questionnaire distributed to the attendees and collected at the end of the session (16 responses were collected). As a highlight, Figure 10 shows that 94% of the respondents to the questionnaire replied that they would recommend the course (Figure 10).

³ <https://www.compbiomed.eu/patc-compbiomed-winter-school-2019/>

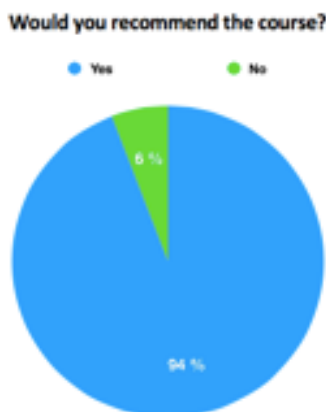


Figure 10 - Replies to BSC Winter School feedback questionnaire.

6.3 University education

CompBioMed University Education is an experimental-computational workflow in molecularly-based medicine that can be delivered to medical students, to science and engineering students, or as part of a bespoke training programme to familiarise trainees with genome-based computational biomedicine using state-of-the-art experimental and computational resources.

The course of study involves a combination of field work, wet laboratory-based experimental work, taught lectures, supervised workshops, and small group tutorial sessions and data analysis using high performance computing. Participants purify microbial genomic DNA from environmental samples and use conserved regions of the gene encoding the 16S bacterial ribosomal RNA for amplification of genomic microbial DNA. This DNA is sequenced using Illumina Next Generation Sequencing on an iSeq-100 machine and a bioinformatics pipeline is used on the raw data to understand microbial diversity by performing microbiome analysis on HPC.

All course resources are placed on GitHub and made available to students via the UCL institutional virtual learning environment, Moodle.

6.3.1 CompBioMed in medical curriculum at UCL

The Student Selected Component (SSC) of UCL's Medical School Curriculum provided an opportunity to educate medical students in Years 1, 2 and 6. This was an 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 was an entirely novel training element introduced in CompBioMed, albeit not originally planned.

The Skin Microbiome SSC was offered to Year 1 and Year 2 Medical Students. This course provided 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 were determined. Under supervision, students designed and carried out original experimental work, analysed data, compared results of their specific experiments with the group and wrote a report

on the findings. A test of the theoretical aspects of the experimental techniques was taken. SSC activities included 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) involved 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) involved 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,
 - b. “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.

60 students in total (20 each from years 1 and 2 in 2017-2018 and 20 from year 1 in 2018-2019) have successfully completed the course. The course was delivered by UCL and the HPC workshop was run by EPCC.

6.3.2 CompBioMed in the Science and Engineering curriculum at UCL

UCL's undergraduate research project course BIOC0023 – Specialist Research Project 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 samples.

Following a workshop “Rough Guide to HPC for Bioscientists”, they were given access to high-performance computing clusters to analyse their data.

185 students in total (85 in 2017-2018 and 100 students in 2018-2019) took this course as part of their degree programme studies (BSc Biochemistry, BSc Molecular Biology, BSc Biotechnology and MSci Biochemistry).

The course was delivered by UCL and the HPC workshop was run by EPCC.

6.4 Other training activities

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

Two CompBioMed sessions were held within the PATC Course: “HPC-based simulations, Engineering and Environment” organised by BSC (<https://www.bsc.es/education/training/patc-courses/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.

6.4.2 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.

6.4.3 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 3rd edition of the School (https://www.upf.edu/web/bcnvph_school) took place in Barcelona on 18-22 June 2018 and focussed on data integration, model verification and validation. CompBioMed’s contribution consisted of a talk and the organisation of a hands-on session by UPF and BSC.

6.5 Training Portal and Repository

The Training Portal (<http://www.compbiomed.eu/training/>) has been developed, populated and is continuously updated. 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 portal is included in the common catalogue for e-Infrastructure services of eInfraCentral (<http://einfracentral.eu/>) and the EOSC-hub catalogue (<https://www.eosc-portal.eu/services-resources/training>).

The Training Repository (<https://www.compbiomed.eu/training/training-repository>) 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 11.



Topic:	User Type:	Skill Level:	Course Type:
<input type="checkbox"/> Advanced computing	<input type="checkbox"/> Academia	<input type="checkbox"/> Novice	<input type="checkbox"/> Face2Face
<input type="checkbox"/> Application	<input type="checkbox"/> Clinical	<input type="checkbox"/> Semi	<input type="checkbox"/> MOOC
<input type="checkbox"/> Application codes	<input type="checkbox"/> Industry	<input type="checkbox"/> Expert	<input type="checkbox"/> Online self-drive
<input type="checkbox"/> Big Data			<input type="checkbox"/> Webinar
<input type="checkbox"/> Cloud			
<input type="checkbox"/> Data Management			
<input type="checkbox"/> How to get access to and...			
<input type="checkbox"/> Intro Computing			
<input type="checkbox"/> Linux command line			
<input type="checkbox"/> Modelling + simulation			
<input type="checkbox"/> Visualisation			

Figure 11 - 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 63 entries and is being continuously updated.

6.6 Training Package

All the resources on the Training Portal will be advertised and disseminated as one unique consistent package.

A flyer has been prepared to allow its promotion and dissemination, see Figure 12.



Figure 12: The CompBioMed Training Flyer

This is then advertised through:

- B2find of EUDAT

- eInfra Central
- EOSC-hub catalogue
- CompBioMed conference and other conferences
- VPH institute
- Avicenna Alliance
- PRACE
- Partners' networks

6.7 Key Performance Indicators

CompBioMed was committed to addressing a list of Key Performance Indicators (KPIs). The two KPIs related to training have both been achieved and are listed below:

- 1) **KPI:** If training participants report that the training was useful
Target: 12 months after the training with 75% positive responses
Result: Achieved with 78% positive responses
Details: Survey sent out to the attendants of the Free-Energy Training Workshop (22 responses collected) and the Winter School 2018 (7 responses collected)
- 2) **KPI:** Number of trainees attending training events
Target: 150 in total (of which 25 in the first one)
Result: Achieved with 585 (5056 YouTube views) in total
Details: 25 participants attended the Joint BioExcel and CompBioMed training; 76 attended Webinar#1; 21 attended Webinar#2; 24 attended Webinar#3; 19 attended Webinar#4; 30 students attended BSC Winter School 2018; 60 medical students attended UCL undergraduate course; 185 biomedical science and biotechnology students attended UCL's undergraduate research project course; 17 students attended the VPH2018 pre-course; 12 attended Webinar #5; 14 attended Webinar #6; 25 students attended Winter School 2019; 45 attended Webinar #7; 9 attended Webinar #8; 13 attended Webinar #9; 10 attended Webinar #10.

7 Dissemination

In order to be an active, effective and visible Centre of Excellence, CompBioMed sought to reach a wide audience with a high quantity of high impact content, via a targeted dissemination campaign that informs those already in the field of Computational Biomedicine, as well as those outside of the field that need convincing of its merits and potential.

Across the full 36 months of the project, the CompBioMed consortium produced a massive 502 separate dissemination activities, with 204 of these done in the first 18 months, and 298 done in the second 18 months. These activities include:

- 83 Publications
- 82 YouTube Videos
- 804 Tweets
- 2 Conferences
- 8 Workshops
- 4 Sessions within external events
- 6 booths



and much more besides. In this section, we describe our dissemination campaign in the second half of the project.

7.1 Dissemination Materials

In this section, we describe the dissemination materials that were produced and/or harnessed in the second half of the project. The strategy shows a wide-reaching approach to peer reviewed publications that targets Academia, Industry and the Clinic, while popularised publications target the general public in addition to those same groups. Our video content gains attention thanks to a high number of recorded talks, as well as our major dissemination campaign surrounding the Virtual Humans film. Meanwhile, our newsletters, posters, and other materials have kept a steady flow of dissemination into the world throughout the second half of the project.

7.1.1 Publications

In this section we look at our peer reviewed publications and popularised publications.

Peer Reviewed Publications

The CompBioMed CoE has published 83 peer reviewed publications that acknowledge the project's grant number (675451). These are listed in Appendix 9.1, and are also listed on the CompBioMed website along with summaries of each paper⁴. The summaries help visitors from all backgrounds to understand the work being done in CompBioMed.

At month 18 there were 24 publications, in the second half of the project, there has been a dramatic rise in the number of publications, with an additional 59 being published. The target was originally as follows:

“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”

Each research grouping within the project has published papers, and two of those were in journals with an impact factor more than 10:

- Unlocking data sets by calibrating populations of model to data density: A study in atrial electrophysiology, B. A. J. Lawson, C. C. Drovandi, N. Cusimano, P. Burrage, B. Rodriguez, K. Burrage, Science Advances, 4 (1), 2018, 10.1126/sciadv.1701676
Impact Factor: 12.804
- Machine Learning of Coarse-Grained Molecular Dynamics Force Fields, J. Wang, S. Olsson, C. Wehmeyer, A. Pérez, N. E. Charron, G. de Fabritiis, F. Noé, and C. Clementi, ACS Central Science, 755-767 (2019), 10.1021/acscentsci.8b00913
Impact Factor: 12.837

Other highlights among the publications in the last 18 months of the project include a cutting-edge and unique book on *Computational Methods for GPCR Drug Discovery* published by Alexander Heifetz of Evotec. The book acts as a resource for structural and molecular biologists,

⁴ <https://www.compbiomed.eu/media-social/publications-2/>



computational and medicinal chemists, pharmacologists, and drug designers. The front cover of the book is shown in Figure 14.

Additionally, a paper written by the team at University of Amsterdam (UvA) was selected for the front cover of the Physics of Fluids journal:

- Red blood cell and platelet diffusivity and margination in the presence of cross-stream gradients in blood flows, G. Závodszy, B. van Rooij, B. Czaja, V. Azizi, D. de Kanter, A. G. Hoekstra, Physics of Fluids, 31, 031903 (2019), 10.1063/1.5085881

The cover image is shown in Figure 13 below.



Figure 14: Book on Computational Methods for GPCR Drug Discovery

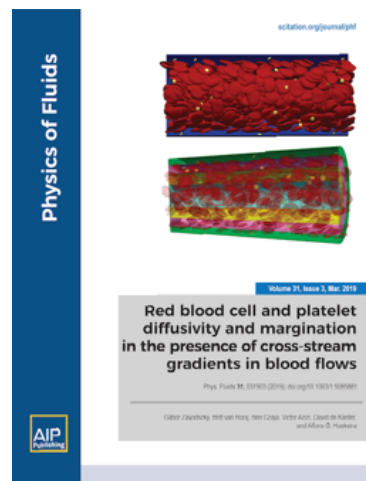


Figure 13: CompBioMed paper featured on the cover of the Physics of Fluids Journal

Popularised Publications

In the second half of the project, the consortium published 10 substantial popularised publications that featured CompBioMed and its research. Each publication is listed in Appendix 9.2. Across these 10 publications, conservative audience size estimates show the collective audience reached was 1,124,537 people. Three particularly notable publications are listed below.

- Roger Highfield (Science Museum – CompBioMed Associate Partner) published an online and printed WIRED article on “How weather forecasts could help develop ‘designer’ drugs personalised to your illness”. This featured CompBioMed’s JCTC paper on "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study", WIRED.com receives 19,087,927 unique visitors per month and the printed edition has 870,101 subscribers.
- Andrea Townsend-Nicholson (UCL) published an article on “The Body Double that could improve your health” in the September 2019 online and printed version of "The Healthy Food Guide" featuring CompBioMed. The issue focuses on the benefits to health from computational biomedicine and the Virtual Human. The Healthy Food Guide receives 25,000 visitors per month, and the printed version has 45,000 subscribers.

- Elisa Passini, Blanca Rodriguez, Patricia Benito (Oxford) published an article on "Why computer simulations should replace animal testing for heart drugs" in "The Conversation". The article was tweeted 50 times and shared on facebook 539 times.

7.1.2 Newsletters

As of month 8 in the project, we began producing quarterly Newsletters, with four produced in the second 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 apprised of the Centre's progress. The PDF files of the newsletters can be downloaded from the project website⁵. The newsletters were distributed electronically on our website, social media, and mailing lists, and were also printed and distributed at various events along with our other materials.

In addition to the quarterly newsletters, which are distributed externally as well as to the partners and related projects of CompBioMed, we also had a monthly e-newsletter, which was 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, fellowships, research, training and conferences, and other pieces of news. 8 e-newsletters were produced in the second half of the project.



Figure 15: CompBioMed print newsletters from the second half of the project

7.1.3 Posters

In addition to the 30 instances of presenting posters listed in D3.4 and D3.5, 18 further instances of poster presentations have now been given, taking the total instances during the project to 48. These are listed in among the items in Appendix 9.7. A selection of the latest posters is shown in Figure 16 below.

⁵ <http://www.compbiomed.eu/media-social/news-and-events/newsletter/>



Figure 16: Four of the posters produced in the second half of the project.

7.1.4 Other materials

The popular CompBioMed branded stress toys and project leaflets (described in D3.4) continued to be re-stocked and distributed at the various events discussed in Section 7.3.

7.1.5 Film and Video

The CompBioMed project continued to heavily leverage its video output in the second half of the project. At month 18, the CompBioMed YouTube channel housed 34 videos, at the end of the project the channel hosted 81 videos. These included the Virtual Humans film, while the remainder were recordings of CompBioMed talks and webinars. The videos on the CompBioMed YouTube channel gained a cumulative view count of 13,687.

BSC, Sheffield, and Medtronic created and posted a video on "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" on The Barcelona Supercomputing Center YouTube⁶. This video shows the effect of the Pipeline Embolization Device by Medtronic, over the blood flow inside an artery. The first part shows visualizations of a CFD simulation inside an intracranial artery with an aneurysm, without the stent. The second part is an accurate recreation of the stent delivery process. The final part shows visualizations of a CFD simulation of the blood, after diverter stent implantation. The stunning graphics in this video are shown in Figure 18. The voiceover for this video is soon to be implemented.



Figure 17: Screenshot from the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm"

Blanca Rodriguez (Oxford) appeared in an interview video titled "Professor Blanca Rodriguez on how computer models can replace animal research" on the YouTube channel "National Centre for the 3Rs". During the interview she discussed developing computer models of the human heart with the potential to replace animal experiments.

⁶ https://www.youtube.com/watch?v=Pn1_bD4r1cg

7.1.5.1 The Virtual Humans Video

CompBioMed continued to dedicate a considerable amount of effort towards a major dissemination campaign for the “Virtual Humans” film. The film was initially released on 27 September 2017 at an event at the London Science Museum in a ‘Lates’ event before a crowd of 400 members of the general public. More details on that event are available in D3.4.

The film itself was produced using structural data taken directly from simulations, and enhanced using advanced graphics techniques, then rendered in 4k resolution on the MareNostrum supercomputer at Barcelona Supercomputing Center. Six screenshots from the film are shown in Figure 18.

The Virtual Humans film is intended to describe the core concept of Computational Biomedicine, looking towards a future where digital avatars are used to inform medical decisions. The concept is described in a simple manner than can be understood by the general public. In describing computational biomedicine, the film also introduces viewers to the main areas of research in CompBioMed. By delivering the message alongside striking high fidelity graphics, the resulting video is a high impact, broadly appealing, and extremely versatile piece of content.

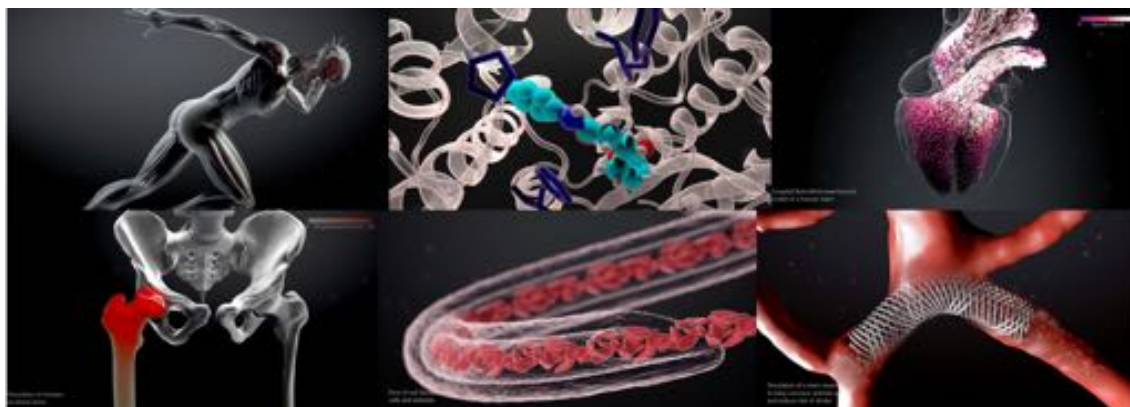


Figure 18: Screenshots from the Virtual Humans film

Appendix 9.3.2 shows the activity undertaken to disseminate the Virtual Humans film, along with the types of audiences targeted, and the estimated numbers of people reached.

Highlights of the campaign include:

- A screening of the video during the Dutch TV programme “De Wereld Van Morgen”, with reported viewer estimates of 1,000,000.
- A link to the video in an article in “The Healthy Food Guide” print magazine to a subscriber base of 45,000.
- Postings of the film on YouTube channels, amassing 11,438 views.
- The film was a finalist in the 5th Raw Science Film Festival in Los Angeles. It won the 2nd place of the Professional Documentary of less than 10 minutes.
- The film was shortlisted for the Short Film Competition at the AFO (Academic Film Olomouc) Festival of Science in the Czech Republic.
- The film won an award for Technical Merit at the 2018 SCINEMA International Science Film Festival.
- The film was presented in a segment on “Building A Virtual Human” at the Cheltenham Science Festival 2018, UK.

- The film was shown to various groups of medical students in the courses described in Section 6.
- The Science Museum Lates event featured on the BBC Tomorrow's World website.
- Prominent people tweeted about the Science Museum Lates event include Samira Ahmed (SamiraAhmedUK) with 44,600 followers, the Science Museum (@sciencemuseum) with 662,000 followers, and Roger Highfield (@RogerHighfield) with 17,200 followers.
- The film was shown to school children in six schools across the Netherlands and Italy.
- Versions of the film have been made available with subtitles in English, Dutch, and French.

All in all, 106 dissemination actions were taken, reaching an estimated audience of 2,555,552. This audience figure is heavily weighted by activity on the extremely popular Science Museum Twitter account (2 x 662,000), and the appearance of the video on the Dutch TV programme “De Wereld Van Morgen” (reported viewer estimates of 1,000,000). But even taking those aside, the dissemination campaign reached an estimated 231,552 people.

The campaign's dissemination activities were targeted as follows:

- 16 items targeted at clinicians or medical students
- 43 items targeted at the general public
- 50 items targeted at industry
- 78 items targeted at the scientific community
- 5 items targeted at policy makers
- 28 items targeted at medias

For full details, see Appendix 9.3.2.

The dissemination campaign is an ongoing one, with the following plans in the pipeline:

- French voiceover version of the film is imminently due for release.
- German voiceover version of the film is scripted and is due for recording and then release.
- We are in discussions with the London BodyWorlds Exhibit to construct a temporary exhibit dedicated to Computational Biomedicine, which will screen the film. The exhibit is planned to run for 6 weeks in 2020, and then be used across Europe.

There are additional plans for the film which are in the preliminary stages of development.

7.2 Online Presence

In this section, we describe CompBioMed's online presence in the second half of the project, covering the social media and website presence that has been employed. The strategy shows a social media campaign designed to focus on the effective platforms of Twitter and YouTube in an impactful way and ensuring that the CompBioMed website acts as a highly functional and feature-rich home for the Centre of Excellence.

7.2.1 Social Media

CompBioMed's social media activity in the second half of the project is listed in Appendix 9.4. As discussed in previous dissemination deliverables, we have chosen to focus our social media efforts only on effective platforms, namely YouTube and Twitter.



On YouTube, the CompBioMed channel posted 82 videos (up from 34 videos at month 18), yielding 14,429 views across all content (up from 647 views at month 18). The channel has 215 subscribers (up from 23 at month 18). The numbers have risen enormously since month 18, with the views and video count being the highest of the HPC CoEs. In terms of subscribers, we are second among the HPC CoEs only to BioExcel, which started a year earlier than CompBioMed. The 11,438 views for 'Virtual Humans' shows that the film is, by a considerable distance, the most popular single piece of YouTube content among the HPC CoEs, with the next nearest being 1.4k views.

On twitter, the CompBioMed account (@bio_comp) tweeted 804 times (up from 272 at month 18), gaining 327,120 impressions (up from 105,333 at month 18). The account has 787 followers (up from 334 at month 18). The tweets collected a total of 884 likes (up from 200 at month 18). These numbers, which were already strong at month 18, have risen substantially. These numbers rank comfortably as the second strongest among the HPC CoEs, behind only BioExcel2 which started a year earlier than CompBioMed.

Various prominent twitter accounts have tweeted about our activities in the second half of the project, a selection of these are listed in Appendix 9.4. A notable piece of activity amongst those listed is the 539 facebook accounts that shared Oxford's article on "Why computer simulations should replace animal testing for heart drugs" in 'The Conversation'⁷. Other instances of significant social media sharing of CompBioMed content are also listed in the appendix.

7.2.2 Websites

In this section, we describe changes and improvements to the CompBioMed website, the new CompBioMed Conference website, and other website activity.

The CompBioMed Website

In this section we describe what's new on the CompBioMed website in the second half of the project. In terms of visitor traffic, the number of visitors and visits coming to the CompBioMed website since the start of the project is shown in Figure 19.

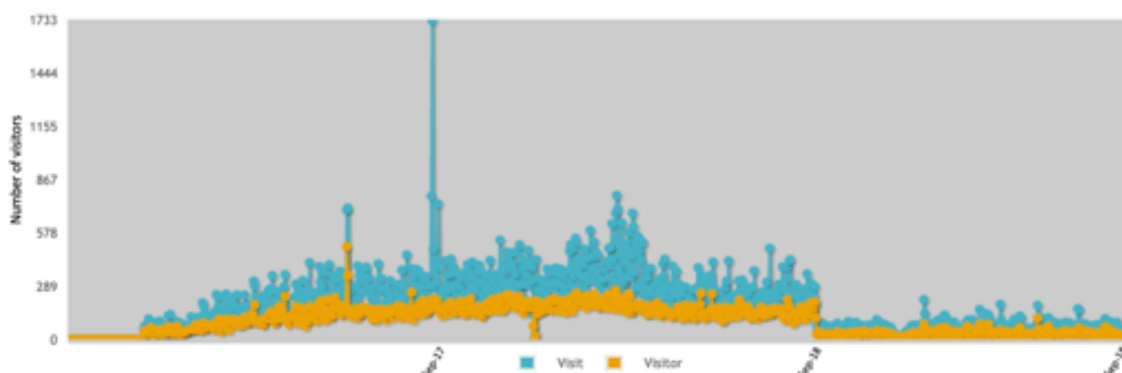


Figure 19: Visitor traffic to the CompBioMed website

In total there were 109,908 visitors and 199,669 visits to the website's 129 pages. It should be noted that the large peak in visits during September 2017 does not correlate to a rise in the number of visitors. It is therefore likely due to the action of automated bots and should therefore be ignored. Additionally, there is a notable drop in both visitors and visits around September

⁷ <https://theconversation.com/why-computer-simulations-should-replace-animal-testing-for-heart-drugs-93409>

2018 and the numbers are lower thereafter. Such a shift is often regarded as the result of a change in the algorithm that was being used to calculate the numbers.

The CompBioMed website⁸ has undergone continual development since month 18 of the project.

As described in D3.5, the front page gives prime screen space to buttons that take visitors to content that is tailored to the type of user that they are: Academic, Industry, Clinical, and General Public visitors. The images on the buttons have been upgraded to attractive animations from the Virtual Humans film, which, combined with the scrolling banner image that shows key highlights, gives a dynamic feel to the website's front page.

The General Public page is now designed to take visitors through the core ideas behind CompBioMed and Computational Biomedicine, harnessing the Virtual Humans film to achieve this. Also, on this page are other videos, a news feed, and a twitter feed. The general public page is shown in Figure 20.

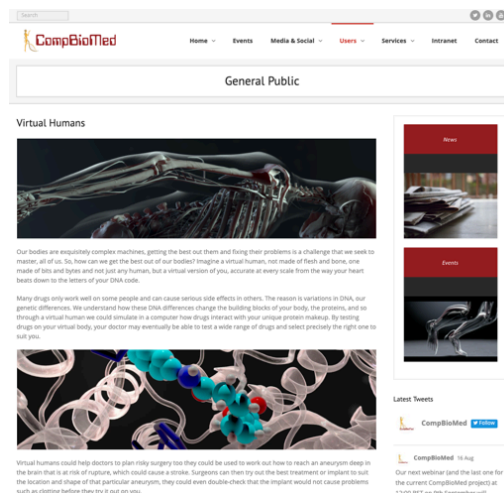


Figure 20: The general public page of the CompBioMed website

To further help the general public and other visitors, the publications page of the website is now formatted into a presentable table that shows short summaries of the research in each paper.

The Clinicians page has also been revamped, now showing short summaries of each of CompBioMed's software applications, along with two descriptive examples of CompBioMed software being used in a way that will interest clinicians.

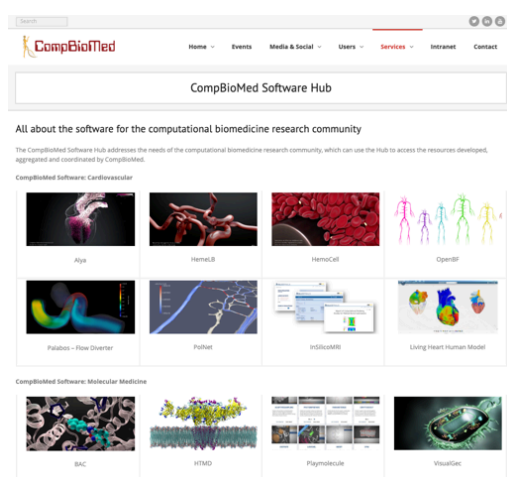


Figure 21: The CompBioMed Software Hub page

We have also set up a forum on the website that will be used as a support forum for each piece

We've added a High Performance Computer Allocations page so that partners, associate partners and even external parties can apply to take advantage of computational resources under the control of CompBioMed. The new page provides details of available allocations and a contact email address in order that visitors can make official requests for resources.

The CompBioMed Software Hub page, which lists each CompBioMed software application, has been revamped to now show a relevant image for each piece of software. When the image or link is clicked, the user is taken to a page dedicated to that application, which shows a description, use scenario, relevant links and related publications.

⁸ <https://www.compbiomed.eu>

of software, which will be monitored by a moderator for that application. The link to the relevant part of the forum will be added to the Software Hub page in due course. The Software Hub page is shown in Figure 21.

The Visitor Programme page has also been revamped. The programme promotes and monitors internships between academia, healthcare, and industry in the field of biomedical computing. In this programme, experts from the research community spend time embedded within industrial organisations looking for assistance, applying the latest research techniques in their software. The Visitor Programme page provides details about the scheme as well as a contact form to make official requests for visitor internships.

The Associate Partner and Related Projects Pages have been given a new slick look. The lists of partners and projects have continued to be updated, with now 40 Partners enjoying the benefits of being a CompBioMed Associate Partner, as well as 17 related projects.

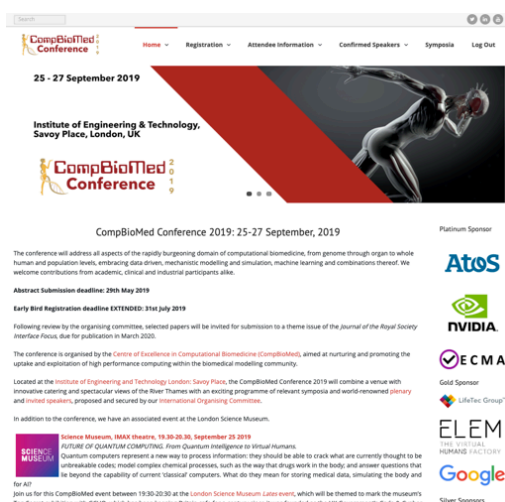


Figure 22: The CompBioMed Conference Website

The CompBioMed Conference Website

As discussed later in Section 7.3.1, CompBioMed organised a major conference in September 2019. In order to aid in the management and operation of the event, we created a standalone website for the CompBioMed Conference⁹.

The website featured pages covering: the homepage summarising the event, the organising committee, registration, call for papers, the programme, hotels & accommodation, plenary speakers, invited speakers, and the symposia. The homepage is shown in Figure 22, and the programme page is shown in **Error! Reference source not found.** Each page also lists the many sponsors of the event along the right-hand side.

Other Website Activity

In addition to the CompBioMed-owned websites, there was also plenty of dissemination activity occurring on external websites. Appendix 9.5 lists the activity in the second half of the project on external websites other than the popularised publication activity already listed in Appendix 9.2.

A couple of notable items among this list include Roger Highfield's (Science Museum) blog article on "Using Virtual Hearts to Reduce Animal Testing in Medicine", and his blog article on "How to build a Virtual Human", both of which were posted on the Science Museum Blog website.

⁹ <https://www.compbioimed-conference.org/>

7.3 Events

In this section, we describe the various events that CompBioMed organised and those in which they participated. We strongly leveraged our active consortium in the second half of the project, giving talks and presenting posters at a vast number of events that targeted all of our stakeholders (discussed further in Section 7.5). We also organised a number of events or aspects within events, including the major CompBioMed Conference in September 2019.

7.3.1 Event Organisation

In Appendix 9.6, the events organised by the CompBioMed consortium in the M18 - M36 are listed. These include:

- A 3-day CompBioMed Conference in London in September 2018
- A 2-day CompBioMed Workshop on "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications" in Amsterdam Netherlands on in March 2019
- A 2-day meeting on "HemeLB: cardiovascular modelling and simulation in UKCOMES" in London UK in May 2019
- CompBioMed Booths at VPH2018, Teratec Forum 2018, Supercomputing 2018, Supercomputing 2019, and ISC 2018
- A Birds of a Feather session on "Personalized Medicine and HPC" at Supercomputing 2018 in Dallas in November 2018
- A joint CompBioMed and ETP4HPC BoF entitled "The Computational Biomedicine Community and the HPC Industry: Working together to advance Personalised Medicine" at ISC19 in Frankfurt Germany in June 2019.
- A session on "Computational challenges in multi scale modelling in biomechanics" at the World Congress in Biomechanics in Dublin Ireland in July 2018

Across the full project, the CompBioMed consortium has co-organised or fully organised:

- 2 Conferences
- 8 Workshops
- 4 Sessions within external events
- 6 booths

Some of the major events organised by CompBioMed in months 18-36 of the project are described below.

Container Technologies in Cloud and High Performance Computing Research and Commercial Applications

In March 2019, we organised the 2-day event "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications", which took place at the Amsterdam Science Park Conference centre in Amsterdam, Netherlands.

The use of container technologies for scientific applications is growing every day, thanks to the evolution of the cloud computing landscape and the rapid development of tools for efficient deployment and scaling of services. Containerisation is now beginning to impact the world of high performance computing (HPC) in a major way. These technologies also support the portability and reproducibility of the results, which are essential for addressing many scientific problems and industrial applications, including the burgeoning field of biomedicine.



In this meeting we congregated computational services developers and users from academia, industry, and the healthcare sectors to discuss the most recent advances in container technology, cybersecurity and related services. The focus was on the use of these technologies in computational modelling and their integration within HPC and cloud computing infrastructures. The event featured presentations of diverse applications and services arising in academic, industrial and clinical contexts. 35 attendees participated in the event, with 19 speakers and two panel discussions among the agenda. These presentations were made available on the CompBioMed YouTube channel.

HemeLB: cardiovascular modelling and simulation in UKCOMES

CompBioMed, along with the EPSRC UKCOMES project and the FETHPC VECMA project, organised a 2-day meeting on “HemeLB: cardiovascular modelling and simulation in UKCOMES” centred around lattice Boltzmann simulations for blood flow. As part of the day’s proceedings, researchers at UCL introduced and demonstrated the use of the HemeLB application and the progress made towards simulating the whole arterial tree. There were talks from other users of HemeLB in addition to alternative LB applications, including Palabos and DL_MESO.

There were 15 speakers, including a roundtable discussion, and 30 attendees participated. The meeting took place in May 2019 at UCL in London.

The CompBioMed Conference

In September 2019, the CompBioMed Centre of Excellence ended its 3-year run with bang: a major 3-day conference dedicated to computational biomedicine. Many of the CompBioMed consortium contributed to the organisation of the event and of its symposia, with many giving talks as part of the event’s agenda. Appendix 9.6 and Appendix 9.7 list these various contributions.

As discussed in Section 7.2.2, the conference received its own dedicated website in order to aid in the organisation and operation of the event. The leading homepage banner on the website is shown in Figure 23.

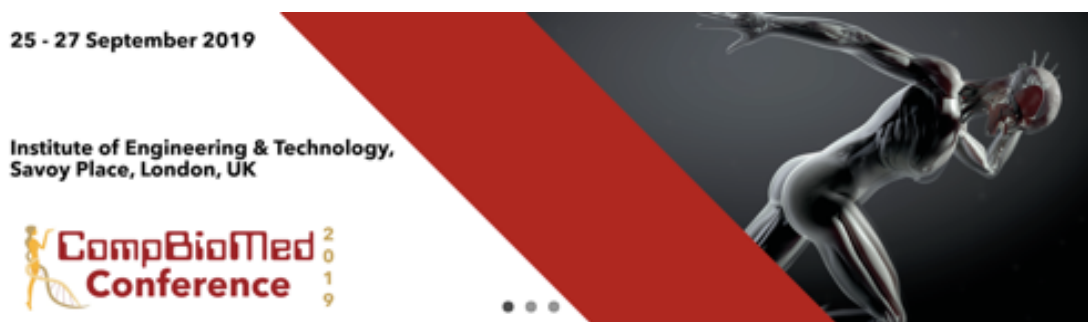


Figure 23: The leading homepage banner from the CompBioMed Conference 2019 website

The conference addressed all aspects of the rapidly burgeoning domain of computational biomedicine, from genome through organ to whole human and population levels, embracing data driven, mechanistic modelling and simulation, machine learning and combinations thereof. It had the aim of nurturing and promoting the uptake and exploitation of high performance computing within the biomedical modelling community. The conference targeted participation

from academic, clinical, and industrial participants alike, and was held at the Institute of Engineering and Technology London on Savoy Place, London, UK.

There were 15 symposia during the event, separated into 3 themes, multiple talks were delivered within each symposium, which were organised by dedicated chairs.

Biomedical Applications

- Genomics
- Molecular Medicine
- Organ Modelling and Simulation
- Oncology

Methodology

- Multiscale Modelling
- Role of Theory, Modelling and Simulation in Biomedicine
- Machine Learning, Big Data & AI
- Uncertainty Quantification
- From Quantum AI to the Virtual Human

Technology and Outreach

- Imaging & Visualisation
- Regulatory Science and in silico Trials
- Cloud & High Performance Computing
- Innovation in Modern Biotechnology
- Education, Training & Public Awareness

Sponsors of the conference were given access to meetings rooms, booths, and distribution of dissemination materials. Some major companies participated as sponsors: ATOS, NVIDIA, VECMA, LifeTec Group, ELEM, Google, Medtronic, Pie Medical Imaging, LIGHTOX, Janssen, Microsoft, CBK Sci Con, Journal of Chemical Theory and Computation and The Royal Society Publishing.

Furthermore, selected papers were invited for submission to a theme issue of the *Journal of the Royal Society Interface Focus*, due for publication in March 2020.

In addition to the conference itself, CompBioMed, along with the London Science Museum, also organised a satellite event at the London Science Museum on the evening of 25 September 2019. The event was called “Future of Quantum Computing, From Quantum Intelligence to Virtual Humans”. This satellite event explored how quantum computers represent a new way to process information: cracking unbreakable codes; model complex chemical processes, such as the way that drugs work in the body; and what this means for storing medical data, simulating the body, and for AI. The Satellite event was held at the London Science Museum as part of their ‘Lates’ series, similarly to that of the launch of the Virtual Humans film in 2017 and was again sold out.

All in all, 200 attendees participated at the CompBioMed Conference, which acted as a strong statement of the importance of computational biomedicine now and into the future. The intention is to consider running the conference as a regular feature in the scientific event calendar, possibly with future versions taking place every 2 or 3 years.



7.3.2 Event Participation

The CompBioMed consortium was extremely active in the second half of the project in terms of event participation. Appendix 9.7 shows the full listing of event participation, which includes keynote presentations, invited talks, talks, posters, meetings, and panel discussions. In total, a massive 176 event participations are recorded here for the second half of the project alone. The events ranged from conferences, workshops, seminars, themed weeks, bird-of-a-feathers, webinars, launches, meetings, and sessions. They targeted all of CompBioMed's stakeholders: academia, industry, clinicians, the general public, policy makers, medias, and investors. For more on the targeting of specific types of stakeholders, see Section 7.5. Some highlights among these event participations are presented below.

Sense About Science: Evidence Week

Andrea Townsend-Nicholson (UCL) and Clint Davies-Taylor (Dassault Systèmes), with the help of UCL, UvA, and the Biophysical Society, gave a briefing at an evidence pod during Evidence Week in London UK in June 2019. At this event, more than 100 British MPs and peers got involved in the proceedings at UK Parliament, run by Sense about Science (an independent charity that promotes the public interest in sound science and evidence). The MPs received 3-minute briefings at 'evidence pods' in Upper Waiting Hall in the UK House of Commons, on how to handle the evidence on 20 pressing policy issues.

Evidence Week in Parliament aimed to equip MPs with the tools they need to interrogate evidence across a range of policy issues. Between elections, parliament is fundamental to scrutinising the evidential reasoning of policy. Increasingly, this means asking searching questions of new sources of data, as well as complex interactions between variables and trade-offs to consider.

The MPs and Lords were shown a beating virtual heart via a special tablet provided by Dassault Systèmes to show a 3D version of the virtual heart in action. The pod also displayed a Macarena-dancing skeleton looping in the background, showing the work of the University of Sheffield to simulate the muscles and skeleton of a virtual human. The pod then ran a raffle to build a dancing skeleton for one parliamentarian.

Prof Andrea Townsend-Nicholson presented how the virtual human uses digital evidence – from the 'letters' in genetic code to medical imaging of the heart – to seek real improvements to healthcare by delivering truly personalised medicine, via exascale computing hardware.

Visitors to the pod included: Lord Cameron of Dillington, Countess Mar, Thangam Debbonaire MP, Lilian Greenwood MP, Jim Sturdy MP, Chris Leslie MP, Neil Parish MP, and Tony Lloyd MP.

Newton Dinner at the Science Museum

The Newton Dinner is a series of exclusive dinners for the London Science Museum's top-level donors who enjoy premium access to top scientists in an elegant setting. Peter Coveney (UCL) presented CompBioMed's work exploring computational methods in creating biological models which could be used to aid clinical decision making.

SCALE18 Prize at CCGrid

UCL's work executing and managing large and complex campaigns of ligand binding simulations (using domain specific middleware, HTBAC) won the 11th IEEE International Scalable Computing Challenge (SCALE 2018) at the IEEE/ACM International Symposium on Cluster, Cloud, and Grid



Computing (CCGrid) 2018 held in Washington DC. The prize rewards real-world problem-solving using computing that scales.

7.4 Other Dissemination

This section covers instances of dissemination that did not easily fit into the categories in the previous sections. These instances are listed in Appendix 9.8, with a couple of highlights described below.

Matthew Wright Show on Talk Radio

Elisa Passini (Oxford) gave an interview appearance on the Matthew Wright show on TalkRadio. The segment was a feature on women in science. Elisa spoke about her and University of Oxford's research in mathematical modelling of cardiac electrophysiology, by combining clinical and experimental data with modelling and simulation, in order to gain new insights into the ionic mechanisms underlying cardiac arrhythmias in humans.

International 3Rs prize

University of Oxford and Janssen won the major 'International 3Rs prize', as a result of their research providing evidence that drug testing could one day be conducted in a computer rather than on animals.

Awarded by the National Centre for the Replacement, Refinement and Reduction of Animals in Research (NC3Rs), and sponsored by GSK, the prizewinning research was conducted by Dr Elisa Passini at the University of Oxford's Department of Computer Science, with Janssen Pharmaceutica.

The winning paper describes a 'drug trial', where 62 drugs and reference compounds were tested at various concentrations in more than a thousand simulations of human heart cells. Their computer model predicted the risk that drugs would cause abnormal heart rhythms in patients with 89% accuracy. They compared these computer predictions with data obtained from previously conducted comparable animal studies and found the animal research was less accurate (75%) than the computer predictions of how the drugs would behave in the body.

This prestigious award consisted of a £28k prize grant and a £2k personal award.

7.5 Targeted Activity

The dissemination activity in CompBioMed was targeted towards all of its stakeholders, be it academics, industry personnel, clinicians, or the general public. The academic and industry backgrounds of the CompBioMed consortium naturally mean that these groups of stakeholders are often targeted. In total, 263 items of dissemination activity (shown across Appendix 9) included the scientific community as targets, while 191 items targeted industry. With these stakeholders clearly well catered for, it is the targeting of clinicians and the general public that this section will address. In addition to that, we take a look at CompBioMed's work with other H2020 funded projects and CoEs.



7.5.1 Targeting the General Public

Communicating complicated science to the general public is a challenging, yet rewarding and important endeavour. In CompBioMed, many of our activities were targeted at the general public, 46 dissemination activities were targeted at the general public in the second half of the project, each of these are listed amongst the items in Appendix 9. 44 such activities were undertaken in the first half, bringing the total to 90. In the latter half of the project, much of the general public dissemination activity was centred around the Virtual Humans film, which was specifically designed for communicating the key concepts of computational biomedicine, and of CompBioMed, to the layman. In fact, 43 items of dissemination activity in the second half of the project involved showing or linking to the Virtual Humans video.

Some highlights amongst the general public targeted dissemination in months 18-36 of the project include:

- Alfons Hoekstra (UvA) and Peter Coveney (UCL) gave a lecture and debate on "Your digital twin: closer than you think" at a UvA University Day to the public.
- Elisa Passini (Oxford) gave an interview appearance on a feature on women in science on the Matthew Wright show on TalkRadio.
- A screening of the Virtual Humans video during the Dutch TV programme "De Wereld Van Morgen", with reported viewer estimates of 1,000,000
- A link to the Virtual Humans video in an article in "The Healthy Food Guide" print magazine to a subscriber base of 45,000
- Postings of the Virtual Humans film on YouTube channels, amassing 11,438 views
- The Virtual Humans film was screened at the 5th Raw Science Film Festival in Los Angeles.
- The Virtual Humans film was screened at the AFO (Academic Film Olomouc) Festival of Science in the Czech Republic.
- The Virtual Humans film was screened at the 2018 SCINEMA International Science Film Festival.
- The Virtual Humans film was screened at the "Building A Virtual Human" at the Cheltenham Science Festival 2018, UK.
- The Virtual Humans film was shown to school children in six schools across the Netherlands and Italy.
- As discussed in Section 0, we created and updated a page dedicated to general public visitors to the CompBioMed website.

For further examples and some exciting future plans, see Section 7.1.5, for the full list of items see throughout Appendix 9. This wide-ranging set of targeted activities reached a vast number of the general public with high impact content throughout the project.

7.5.2 Targeting Clinicians

One of the goals of the CompBioMed Centre of Excellence is to enhance the awareness and acceptance of Computational Biomedicine in the clinical domain. The activities described in Section 6.3.1 and D3.4 "Report on Dissemination and Training Material" cover our activities working directly with medical students and clinicians; delivering 'HPC for medics' training courses to medical students, and collaborating directly with clinicians on software such as CT2S and AngioSupport. Beyond that, it was important that CompBioMed raises awareness of



Computational Biomedicine more broadly to clinicians across Europe and the world, through targeted dissemination activity.

Across the various dissemination activities listed in Appendix 9, 79 activities were targeted at the clinical domain in the second half of the project. 25 such activities were undertaken in the first half, bringing the total to 104. This shows a substantial ramping up of such activity in the latter half of the project as recommended by our Innovation Advisory Board and the European Commission during our periodic review meeting.

Some highlights from these activities include:

- BSC, Sheffield and Medtronic showed the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" at LINCC 2019 in Paris France and at ESMINT Congress 2019 in Nice France.
- Bettine van Willigen and Tim van den Boom (LifeTec Group) demoed AngioSupport for the Amsterdam Medical Center and the Catharina Hospital Eindhoven the Netherlands
- As discussed in Section 7.2.2, we created a dedicated page for clinicians on the CompBioMed website.
- Marco Viceconti (USFD) gave a talk on "Do virtual patients see electric Doctors?" to patients and carers at the launch of the Sheffield NIHR Biomedical Research Centre in neurodegenerative Disease.
- Marco Viceconti (USFD) showed the Virtual Humans film in a talk during the Insigneo Showcase in 2018, which specifically targets clinical attendees, among others.
- Jazmín Aguado-Sierra (BSC) gave a talk on "The role of High Performance Computing in Pharmacology Safety" at the Safety Pharmacology Society Annual Meeting in Barcelona Spain.
- A CompBioMed talk was given by Blanca Rodriguez (Oxford) at the Cardiac Arrhythmia Centre, Washington University in St Louis USA.
- Jenny Wang (Oxford) and Hector Martinez (Oxford) gave talks on "Electrophysiological response of HCM myocardium to disopyramide" and "Human in-silico investigations into therapeutic strategies in acute myocardial ischemia", and presented posters at the Gordon seminar on cardiac arrhythmias in Barga Italy.
- Alfonso Bueno-Orovio (Oxford) will give an invited talk on "Data, AI and the android electrophysiologist: Machine learning for you, your patients and your job" at the 2019 Heart Rhythm Congress in Birmingham UK in October 2019.
- Alfonso Bueno-Orovio (Oxford) presented a posters on "Computational methods for safety pharmacology and anti-arrhythmic drug discovery: Towards in silico clinical trials in human" and "Prediction of all form drug-induced cardiotoxicity by combining transcriptome analysis, structural data and machine learning" at the "World congress of basic and clinical pharmacology" in Kyoto Japan.
- For the CompBioMed conference, we included clinicians on the organising committee to ensure that the content was appealing to clinicians generally (for instance, with the inclusion of an Oncology and Immunology Symposium).

There are many more such activities listed in Appendix 9.

Additionally, as shown in Appendix 9.1, many of CompBioMed's publications were in journals targeting clinicians. There were publications in clinically relevant journals such as:

- International Journal of Computer Assisted Radiology and Surgery



- Heart Rhythm
- Clinical Biomechanics
- Current Osteoporosis Reports
- American Journal of Physiology – Heart and Circulatory Physiology
- Cardiovascular Engineering and Technology

As well as in journals that bridge the clinical-academic gap such as:

- Computers in biology and medicine
- Frontiers in Immunology
- Current Opinion in Physiology
- The Journal of Physiology
- Frontiers in Physiology

Overall, a great deal of dissemination activities and CompBioMed publications were aimed at reaching clinicians.

7.5.3 Targeting Other H2020 Projects and CoEs

We share the view of the European Commission that its H2020 funded projects should align and collaborate where possible in order to maximise their collective output and impact. This is particularly true for the HPC CoEs, who share a great deal of common interest and aims. In this section, we describe some of the collaborative activity with the other CoEs and H2020 projects that CompBioMed has undertaken.

POP CoE

UCL-CCS has collaborated with the POP Centre of Excellence on two fundamentally different codes: HemeLB and DeaLAMMPS. HemeLB is a highly optimized lattice-Boltzmann solver for sparse geometries, designed for very large monolithic runs on supercomputers. Through collaboration with the Julich Supercomputing Centre, HemeLB was profiled on ~100k cores on EPCC ARCHER, ~250k cores on BlueWaters and later ~150k cores on the new LRZ SuperMUC NG supercomputer. The profiling revealed excellent scaling, even for modest problem sizes, while also highlighting the importance of the load decomposition on the performance, especially for the efficient use on exascale computing. DeaLAMMPS, on the other hand, is a cyclically coupled Finite Element/Molecular dynamics code which spawns an a priori unknown number of MD simulations per step with varying run times. Through collaboration with the Barcelona Supercomputing Centre, this code has also been profiled, and an avenue for improvement has been identified. This will involve the use of BSC's modified LAMMPS code and OpenMP-based library that dynamically reallocates cores to different LAMMPS processes during runtime according to need.

POP CoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

E-CAM CoE

CompBioMed has had a fruitful collaboration with the E-CAM project, which has been improving HemeLB's load balance decomposition with a view to the exscale, both in terms of the time taken and the resulting balance, through integration of ALL - A Load-balancing Library. This



collaboration has taken the form of a co-design relationship, with new load balancing algorithms being designed according to feedback from the HemeLB developers.

ECAM joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

BioExcel CoE

CompBioMed and BioExcel co-organised an event on “Free Energy Calculations from Molecular Simulation: Applications in Life and Medical Sciences” in London in 2017. The event was themed on the calculation of free energies of various binding processes between compounds and proteins with high levels of accuracy and precision, as well as speed and reliability. The meeting assessed the state of the art, through the participation of leading practitioners from academia and industry, and discussed methods, applications, and experimental validation. This event was livestreamed via YouTube, and recordings of the talks were uploaded to the CompBioMed YouTube channel.

Herman van Vlijmen (Janssen) gave a talk on “Prediction of Activity Cliffs Using FEP+ and Gromacs FEP” at the BioExcel Alchemical Free Energy Workshop in Göttingen Germany in May 2019. Peter Coveney (UCL) gave an invited talk on CompBioMed at the 2017 BioExcel AHM in Amsterdam Netherlands in November 2017. Peter Coveney (UCL) sat on the Scientific Advisory Board for the BioExcel CoE, including for the BioExcel AHM in 2018

BioExcel CoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

HiDALGO CoE

CompBioMed shares a strong interest in Uncertainty Quantification with the new CoE, HiDALGO. Peter Coveney (UCL), who leads the VECMA FETHPC project (looking at multiscale VVUQ on peta- and exascale machines), is in the early stages of collaboration with HiDALGO CoE, via VECMA and CompBioMed.

Excellerat CoE

Gavin Pringle (EPCC) provided guidance to Excellerat CoE regarding Innovation concepts and processes, as well planning for sustainability. We are in discussions with the new CoE, Excellerat, for them to join as Associate Partner.

Max CoE

Max CoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

EoCoE

EoCoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.



NOMAD CoE

NOMAD CoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

ESIWACE CoE

ESIWACE CoE joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

CoeGSS

CoeGSS joined CompBioMed as an Associate Partner, meaning that they were signed up to CompBioMed's mailing list, have access to CompBioMed's available resources, and are listed on CompBioMed's website.

FocusCoE

FocusCoE contributes to the success of the EU HPC Ecosystem and the EuroHPC Initiative by supporting the EU HPC CoEs to more effectively fulfil their role within the ecosystem and initiative: ensuring that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges.

Several CompBioMed consortium members are also part of the FocusCoE consortium, and we have been working with FocusCoE in a number of ways. Firstly, CompBioMed will be sharing its training repository and resources to feed into the training portal being constructed by FocusCoE WP4. Similarly, CompBioMed will be providing details on its services to be included in the CoE services portal being constructed by FocusCoE WP5. CompBioMed has been and will continue to make use of FocusCoE's dissemination channels.

Hugh Martin (CBK) pitched the CompBioMed Containerisation meeting to each of the H2020 HPC CoEs as a meeting with common interest during the FocusCoE Kick-Off Meeting in Frankfurt Germany in February 2019. He also discussed CompBioMed with each of the H2020 HPC CoEs during that meeting. He also provided information on CompBioMed's dissemination, innovation, resources, and contacts directly to FocusCoE in order to help them coordinate their activities.

Other CoE targeted activity

Emily Lumley (UCL) and Gavin Pringle (EPCC) participated in the PRACE CoE FET-HPC EXDCI Workshop in Brühl Germany in October 2018, the event involved each of the H2020 HPC CoEs. The event was a great opportunity to network with various other EU projects working on highly related projects. CompBioMed was able to share best practices with Training, Dissemination and Links with Industry, also discussions were held on the road to the Exascale and Services within the projects. Gavin Pringle presented CompBioMed's work within the Operational Services session and took part in the sessions related to New Technologies and Application Enabling at Exascale. Emily Lumley gave presentations in the Dissemination, Training and Links with Industry Sessions, discussing the Virtual Humans video among other items.

Other H2020 related activity

- CompBioMed members participated in the COST OpenMultiMed Survey on Multiscale Computing in Biomedicine in December 2017



- Gabor Zavodszky (UvA) gave an invited talk on "Zoom in on blood - Using supercomputers in hemodynamics" at the (PRACE Advanced Training Centre) PATC 2019 HPC training event in Barcelona Spain in February 2019
- Alfonso Santiago (BSC) gave a talk on "A verification and validation process for a fluid-electro-mechanical model of the human heart" at the VECMA AHM in Amsterdam Netherlands in May 2019
- Alberto Marzo and Ahmed Mustafa (USFD) gave a talk on "1D modelling of thrombectomy" at the All Hands Meeting of INSIST (In Silico Clinical Trials for treatment of Acute ischemic stroke) project in Milan Italy in April 2019

CompBioMed has communicated and collaborated with the other HPC CoEs and related H2020 projects and has yielded fruitful returns for those efforts.

7.6 Key Performance Indicators

We have comfortably exceeded each of the KPIs that relate to dissemination:

- 1) **KPI:** Number of publications in peer-reviewed international journals that acknowledge the support of CompBioMed
Target: 10 publications (2 in impact factor ≥ 10 journals) from 5 different research groupings with the CoE
Result: Achieved, with 83 publications (2 in impact factor ≥ 10 journals) from each of CompBioMed's different research groupings
- 2) **KPI:** Number of people attending the 2 workshops events organised by WP3
Target: 50 attendees per workshop
Result: Achieved, with 70 participants in the HPC/Cloud Workshop and 95 in the Free-Energy Workshop
- 3) **KPI:** Number of companies engaged
Target: ≥ 20 companies, at least 30% being SMEs, have accessed CompBioMed services
Result: Achieved, with 94 companies engaged, 38% of those are SMEs

8 Conclusions

As reported, there was a substantial amount of training and dissemination activity in the course of CompBioMed. The actions of the CompBioMed consortium have met and gone 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 were laid down and important results have been achieved. A strong collaboration with the VPH Institute was set up, which contributed to ensuring positive and long-lasting results. The consortium achieved 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. Each of our key stakeholders was targeted with impactful content, reaching a vast number of people.

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



We believe that, through our dissemination and training activities, expected impacts were accelerated and strengthened. Through the dissemination of CompBioMed research findings to academic, industrial, and clinical users, we contributed 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 contributed to the acceleration of European excellence in Computational Biomedicine.



9 Appendices

9.1 CompBioMed Publications

1. Ensemble-based replica exchange alchemical free energy methods: the effect of protein mutations on inhibitor binding, A. P. Bhati, S. Wan, and P. V. Coveney, J. Chem. Theory Comput., 2018, 10.1021/acs.jctc.8b01118
2. Fully coupled Fluid-electro-mechanical model of the human heart for supercomputers, Santiago A, Zavala-Aké M, Aguado-Sierra J, Doste R, Gómez S, Arís R, Cajas J C, Casoni E, Vázquez M, Int. J. Numer. Meth. Biomed. Engng., 2018, 10.1002/cnm.3140
3. Implications of bipolar voltage mapping and magnetic resonance imaging resolution in biventricular scar characterisation after myocardial infarction, M. López-Yunta, D. G. León, J. M. Alfonso-Almazán, M. Marina-Breyse, J. G. Quintanilla, J. Sánchez-González, C. Galán-Arriola, V. Cañadas-Godoy, D. Enríquez-Vázquez, C. Torres, B. Ibáñez, J. Pérez-Villacastín, N. Pérez-Castellano, J. Julie, M. Vázquez, J. Aguado-Sierra, D. Filgueiras-Rama, Europace, 2018, 10.1093/europace/euy192
4. Influence of fiber connectivity in simulations of cardiac biomechanics, D. Gil, R. Aris, A. Borrás, E. Ramírez, R. Sebastian, M. Vazquez, International Journal of Computer Assisted Radiology and Surgery, 2018, 10.1007/s11548-018-1849-9
5. PlayMolecule BindScope: large scale CNN-based virtual screening on the web, M. Skalic, G. Martínez-Rosell, J. Jiménez, G. De Fabritiis, Bioinformatics, 35, 1237–1238, 2018, 10.1093/bioinformatics/bty758
6. Numerical Investigation of the Effects of Red Blood Cell Cytoplasmic Viscosity Contrasts on Single Cell and Bulk Transport Behaviour, M. de Haan, G. Závodszky, V. Azizi, A. G. Hoekstra, Applied Sciences, 8(9), 1616, 2018, 10.3390/app8091616
7. Cell-resolved blood flow simulations of saccular aneurysms: effect of pulsatility and aspect ratio, B. Czaja, G. Závodszky, V. Azizi Tarksalooyeh, A. G. Hoekstra, Journal of the Royal Society Interface, 2018, 10.1098/rsif.2018.0485
8. Inflow and outflow boundary conditions for 2D suspension simulations with the immersed boundary lattice Boltzmann method, V. Azizi Tarksalooyeh, G. Závodszky, B. J. M. van Rooij, A. G. Hoekstra, Computers & Fluids, 2018, 10.1016/j.compfluid.2018.04.025
9. Patterns for High Performance Multiscale Computing, S. Alowayyed, T. Piontek, J. L. Suter, O. Hoenen, D. Groen, O. Luk, B. Bosak, P. Kopta, K. Kurowski, O. Perks, K. Brabazon, V. Jancauskas, D. Coster, P.V. Coveney, A.G. Hoekstra, Future Generation Computer Systems, 91, 335-346 2018, 10.1016/j.future.2018.08.045
10. Uncertainty Quantification of a Multiscale Model for In-Stent Restenosis, A. Nikishova, L. Veen, P. Zun, A. G. Hoekstra, Cardiovascular Engineering and Technology, 1-4, 2018, 10.1007/s13239-018-00372-4
11. Parameter Estimation of Platelets Deposition: Approximate Bayesian Computation with High Performance Computing, R. Dutta, B. Chopard, J. Latt, F. Dubois, K.Z. Boudjeltia, A. Mira, Front Physiol, 2018, 10.3389/fphys.2018.01128
12. LigVoxel: Inpainting binding pockets using 3D-convolutional neural networks, M. Skalic, A. Varela-Rial, J. Jimenez, G. Martinez-Rosell, G. De Fabritiis, Bioinformatics , 2018, 10.1093/bioinformatics/bty583
13. Simulations meet machine learning in structural biology, A. Perez, G. Martinez-Rosell, G. De Fabritiis, Current Opinion in Structural Biology, 2018, 10.1016/j.sbi.2018.02.004
14. Left Ventricular Trabeculations Decrease the Wall Shear Stress and Increase the Intra-Ventricular Pressure Drop in CFD Simulations, F. Sacco, B. Pain, O. Lehmkuhl, T.L. Iles, P.A. laizzo, G. Houzeaux, M. Vazquez, C. Butakoff, J. Aguado-Sierra, Frontiers in Physiology, 2018, 10.3389/fphys.2018.00458
15. Evaluating the roles of detailed endocardial structures on right ventricular haemodynamics by means of CFD simulations, F. Sacco, B. Pain, O. Lehmkuhl, T.L. Iles, P.A. laizzo, G. Houzeaux, M. Vazquez, C. Butakoff, J. Aguado-Sierra, International Journal for Numerical Methods in Biomedical Engineering, 2018, 10.1002/cnm.3115
16. A mechanistic model for predicting cell surface presentation of competing peptides by MHC class I molecules, D. S. M. Boulanger, R. C. Eccleston, A. Phillips, P. V. Coveney, T. Elliott, N. Dalchau, Frontiers Immunology, 2018, 10.3389/fimmu.2018.01538
17. Validation of patient-specific cerebral blood flow simulation using transcranial Doppler measurements, D. Groen, R. A. Richardson, R. Coy, U. D. Schiller, H. Chandrashekar, F. Robertson, P. V. Coveney, Frontiers Physiology, 2018, 10.3389/fphys.2018.00721
18. PolNet: A Tool to Quantify Network-Level Cell Polarity and Blood Flow in Vascular Remodeling, M. O. Bernabeu, M. L. Jones, R. W. Nash, A. Pezzarossa, P. V. Coveney, H. Gerhardt, and C. A. Franco, Biophysical Journal, 114 (9), 2052-2058 2018, 10.1016/j.bpj.2018.03.032
19. Uncertainty Quantification in Alchemical Free Energy Methods, A. Bhati, S. Wan, Y. Hu, B. Sherborne, P. V. Coveney, Journal of Chemical Theory and Computation, 14 (6), 2867-2880 2018, 10.1021/acs.jctc.7b01143



20. Investigating the mechanical response of paediatric bone under bending and torsion using finite element analysis, Z. Altai, M. Viceconti, A. C. Offiah, X. Li, Biomechanics and Modeling in Mechanobiology, 2018, 10.1007/s10237-018-1008-9
21. Modeling Patient-Specific Magnetic Drug Targeting Within the Intracranial Vasculature, A. Patronis, R. A. Richardson, S. Schmieschek, B. J. N. Wylie, R. W. Nash, P. V. Coveney, Frontiers in Physiology, 2018, 10.3389/fphys.2018.00331
22. Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation, L. Pérez-Benito, H. Keränen, H. van Vlijmen & G. Tresadern, Scientific Reports, 8, 4833, 2018, 10.1038/s41598-018-23039-5
23. KDEEP: Protein-Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks, J. Jimenez, M. Skalic, G. Martinez-Rosell, G. De Fabritiis, J. Chem. Inf. Model., 52 (8), 287-296, 2018, 10.1021/acs.jcim.7b00650
24. Computational Methods for GPCR Drug Discovery, A. Heifetz, Springer, 1705, 2018, 10.1007/978-1-4939-7465-8
25. Synergistic Use of GPCR Modeling and SDM Experiments to Understand Ligand Binding, A. Potterton, A. Heifetz, A. Townsend-Nicholson, Methods Mol Biol., 1705, 335-343, 2018, 10.1007/978-1-4939-7465-8_15
26. Unlocking data sets by calibrating populations of model to data density: A study in atrial electrophysiology, B. A. J. Lawson, C. C. Drovandi, N. Cusimano, P. Burrage, B. Rodriguez, K. Burrage, Science Advances, 4 (1), 2018, 10.1126/sciadv.1701676
27. Computational Methods Used in Hit-to-Lead and Lead Optimization Stages of Structure-Based Drug Discovery, A. Heifetz, M. Southey, I. Morao, A. Townsend-Nicholson, M. Bodkin, Methods Mol Biol., 1705, 375-394 2018, 10.1007/978-1-4939-7465-8_19
28. The application of the screen model for stents in cerebral aneurysms, S. Li, J. Latt, B. Chopard, Computer Fluids., 172, 651-660 2018, 10.1016/j.compfluid.2018.02.007
29. Dynamic and Kinetic Elements of μ -Opioid Receptor Functional Selectivity, A. Kapoor, G. Martinez-Rosell, D. Provasi, G. Fabritiis, M. Filizola, Scientific Reports, 7, 11255 2017, 10.1038/s41598-017-11483-8
30. Model for pressure drop and flow deflection in the numerical simulation of stents in aneurysms. International journal for numerical methods in biomedical engineering, S. Li, J. Latt, B. Chopard, International Journal for Numerical Methods in Biomedical Engineering, 2017, 10.1002/cnm.2949
31. Parameter estimation of platelets deposition: Approximate Bayesian computation with high performance computing, R. Dutta, B. Chopard, J. Lätt, F. Dubois, K. Boudjeltia, A. Mira, arXiv, 2017, arxiv.org/abs/1710.01054
32. Computational techniques for ECG analysis and interpretation in light of their contribution to medical advances, A. Lyon, A. Michole, J.P.Martinez, P.Laguna, B. Rodriguez, Journal of the Royal Society Interface, 15 (138)2017, 10.1098/rsif.2017.0821
33. In silico evaluation of arrhythmia, X. Zhou, A. Bueno-Orovio, B-Rodriguez, Current Opinion in Physiology, 1, 95-103, 2017, 10.1016/j.cophys.2017.11.003
34. Host genotype and time dependent antigen presentation of viral peptides: predictions from theory, R. Eccleston, P. V. Coveney, and N. Dalchau, Scientific Reports, 7 (1), 14367, 2017, 10.1038/s41598-017-14415-8
35. Phenotypic variability in LQT3 human induced pluripotent stem cell-derived cardiomyocytes and their response to antiarrhythmic pharmacologic therapy: An in silico approach, M. Paci, E. Passini, S. Severi, J. Hyttinen, B. Rodriguez, Heart Rhythm, 2017, 10.1016/j.hrthm.2017.07.026
36. β -adrenergic receptor stimulation inhibits proarrhythmic alternans in post-infarction border zone cardiomyocytes: a computational analysis, M. J. Tomek, B. Rodriguez, G. Bub, J. Heijman, American Journal of Physiology – Heart and Circulatory Physiology, 2017, 10.1152/ajpheart.00094.2017
37. Cellular Level In-silico Modeling of Blood Rheology with An Improved Material Model for Red Blood Cells, G. Závodszy, B. van Rooij, V. Azizi and A. Hoekstra, Front. Physiol., 2017, 10.3389/fphys.2017.00563
38. Multiscale Computing in the Exascale Era, S. Alowayyed, D. Groen, P. V. Coveney, A. G. Hoekstra, Journal of Computational Science, 2017, 10.1016/j.jocs.2017.07.004
39. Rapid and accurate assessment of GPCR–ligand interactions Using the fragment molecular orbital-based density-functional tight-binding method, I. Morao, D. G. Fedorov, R. Robinson, M. Southey, A. Townsend-Nicholson, M. J. Bodkin, A. Heifetz, Journal of Computational Science, 2017, 10.1002/jcc.24850
40. The role of multiscale protein dynamics in antigen presentation and T lymphocyte recognition, R. C. Eccleston, S. Wan, N. Dalchau, P. V. Coveney, Frontiers in Immunology, 2017, 10.3389/fimmu.2017.00797
41. A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data, P. S. Zun, T. Anikina, A. Svitenkov, A. G. Hoekstra, Frontiers in Physiology, 8, 1-12, 2017, 10.3389/fphys.2017.00284
42. Exact solutions to the fractional time-space Bloch–Torrey equation for magnetic resonance imaging, A. Bueno-Orovio, K. Burrage, Commun Nonlinear Sci Numer Simulat., 52, 91-109, 2017, 10.1016/j.cnsns.2017.04.013
43. An Ensemble-Based Protocol for the Computational Prediction of Helix-Helix Interactions in G Protein-Coupled Receptors using Coarse-Grained Molecular Dynamics, N. Altwaijry, M. Baron, D. Wright, P. V. Coveney, A. Townsend-Nicholson, Journal of Chemical Theory & Computation, 13 (5), 2254-2270, 2017, 10.1021/acs.jctc.6b01246
44. Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation, S. Wan, A. Bhati, S. Skerratt, K. Omoto, V. Shanmugasundaram, S.



- Bagal, P. V. Coveney, Journal of Chemical Information and Modelling, 57 (4), 897-909, 2017, 10.1021/acs.jcim.6b00780
45. Opinion: Is big data just big hype?, P. V. Coveney and R. Highfield, Longevity Bulletin: Big data in health, Institute and Faculty of Actuaries, 11-12, 2017, ISSN 2397-7213
46. Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: a Computational Study, S. Wan, A. P. Bhati, S. J. Zasada, I. Wall, D. Green, P. Bamborough, and P. V. Coveney, J. Chem. Theory Comput., 13 (2), 784-795, 2017, 10.1021/acs.jctc.6b00794
47. Functional identification of islet cell types by electrophysiological fingerprinting, L. J. B. Briant, Q. Zhang, E. Vergari, J. A. Kellard, B. Rodriguez, F. M. Ashcroft, P. Rorsman, Journal of Royal Society Interface, 14 (128), 1-20, 2017, DOI: 10.1098/rsif.2016.0999
48. Atrial Fibrillation Dynamics and Ionic Block Effects in Six Heterogeneous Human 3D Virtual Atria with Distinct Repolarization Dynamics, C. Sanchez, A. Bueno-Orovio, E. Pueyo, B. Rodriguez, Front. Bioeng. Biotechnol., 5, 1-13, 2017, DOI: 10.3389/fbioe.2017.00029
49. Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration, A. Bhati, S. Wan, D. Wright, P. V. Coveney, Journal of Chemical Theory and Computation, 13 (1), 210-222, 2017, 10.1021/acs.jctc.6b00979
50. PathwayMap: Molecular pathway association with self-normalizing neural networks, J. Jiménez, D. Sabbadin, A. Cuzzolin, G. Martínez-Rosell, Journal of Chemical Information and Modeling, 59, 1172-1181 (2018), 10.1021/acs.jcim.8b00711
51. Shape-Based Generative Modeling for de Novo Drug Design, M. Skalic, J. Jiménez, D. Sabbadin and G. De Fabritiis, Journal of Chemical Information and Modeling, 59, 1215-1214 (2019), 10.1021/acs.jcim.8b00706
52. Machine Learning of Coarse-Grained Molecular Dynamics Force Fields, J. Wang, S. Olsson, C. Wehmeyer, A. Pérez, N. E. Charron, G. de Fabritiis, F. Noé, and C. Clementi, ACS Central Science, 755-767 (2019), 10.1021/acscentsci.8b00913
53. Characterising GPCR-ligand interactions using a fragment molecular orbital-based approach, A. Heifetz, T. James, M. Southey, I. Morao, M. Aldeghi, L. Sarrat, D. G. Fedorov, M. J. Bodkin, A. Townsend-Nicholson, Current Opinion in Structural Biology, 55, 85-92 (2019), 10.1016/j.sbi.2019.03.021
54. Computational prediction of GPCR oligomerisation, A. Townsend-Nicholson, N. Altwaijry, A. Potterton, I. Morao, A. Heifetz, Current Opinion in Structural Biology, 55, 178-184 (2019), 10.1016/j.sbi.2019.04.005
55. Identifying inter-helical interactions involved in GPCR structure-function and the forces that determine ligand residence time, A. Heifetz, A. Potterton, I. Morao, T. James, M. Southey, D. Fedorov, M. Bodkin, A. Townsend-Nicholson, Abstracts of Papers of the American Chemical Society, 256 (2018)
56. Systematic electrophysiology analysis of four biventricular, anatomically normal human heart models, F. Sacco, R. Doste, C. Bederián, T. L. Iles, P. A. Iaizzo, G. Houzeaux, M. Vázquez, O. Cámara, C. Butakoff, J. Aguado-Sierra, Journal of the Royal Society: Interface Focus, Accepted (2019)
57. Toward full GPU implementation of fluid-structure interaction, J. Beny, C. Kotsalos and J. Latt, ISPDC-2019 Conference Proceedings, IEEE Xplore, 16-22 (2019)
58. Application of the ESMACS Binding Free Energy Protocol to a Highly Varied Ligand Dataset: Lactate Dehydrogenase A, D. Wright, F. Hussein, S. Wan, C. Meyer, H. van Vlijmen, G. Tresadern, P. V. Coveney, ChemRxiv (2019)
59. Computational drug design applied to the study of metabotropic glutamate receptors, C. Llinas del Torrent, L. Pérez-Benito, G. Tresadern, G. Molecules, 24, 1098 (2019), 10.3390/molecules24061098
60. Mechanisms Underlying Allosteric Molecular Switches of Metabotropic Glutamate Receptor 5, C. Llinas del Torrent, N. Casajuana-Martin, L. Pardo, G. Tresadern, L. Pérez-Benito, J. Chem. Inf. Model. 59, 2456-2466 (2019), 10.1021/acs.jcim.8b00924
61. Predicting Activity Cliffs with Free Energy Perturbation, L. Pérez-Benito, N. Casajuana-Martin, M. Roses-Jimenez, H. van Vlijmen, G. Tresadern, J. Chem. Theory. Comput., 15, 1884-1895 (2019), 10.1021/acs.jctc.8b01290
62. Systematic electrophysiological analysis of four biventricular, anatomically normal human heart models, F. Sacco, R. Doste, C. Bederián, T.L. Iles, P.A. Iaizzo, G. Houzeaux, M. Vazquez, O. Camara, C. Butakoff, J. Aguado-Sierra, Journal of the Royal Society: Interface Focus (2019)
63. Suppression of alternans in the border zone of healed infarcts via β -adrenergic stimulation, J. Tomek, G. Hao, M. Tomková, C. Carr, A. Lewis, D. J. Paterson, B. Rodriguez, N. Herring, G. Bub, Frontiers in Physiology, 10, 350 (2019) 10.3389/fphys.2019.00350
64. Investigating the complex arrhythmic phenotype caused by the gain-of-function mutation KCNQ1-G229D, X. Zhou, A. Bueno-Orovio, R. J. Schilling, C. Kirkby, C. Denning, D. Rajamohan, K. Burrage, A. Tinker, B. Rodriguez, S. Harmer, Frontiers in Physiology, 10, 259 (2019) 10.3389/fphys.2019.00259
65. The effect of boundary and loading conditions on patient classification using finite element predicted risk of fracture, Z. Altai, M. Qasim, X. Li, M. Viceconti, Clinical Biomechanics, 68, 137-143 (2019) 10.1016/j.clinbiomech.2019.06.004



66. Improved biomechanical metrics of cerebral vasospasm identified via sensitivity analysis of a 1D cerebral circulation model, A.Melis, F.Moura, I.Larrabide, K.Janot, R.H.Clayton, A.P.Narata, A.Marzo, Journal of Biomechanics, 90, 24-32 (2019), 10.1016/j.jbiomech.2019.04.019
67. Multiple Aneurysms AnaTomy CHallenge 2018 (MATCH)—phase II: rupture risk assessment, P. Berg, S. Voß, G. Janiga, S. Saalfeld, A. W. Bergersen, K. Valen-Sendstad, J. Bruening, L. Goubergrits, A. Spuler, T. Lok Chiu, A. Chun On Tsang, G. Copelli, B. Csippa, G. Paál, G. Závodszy, F. J. Detmer, B. J Chung, J. R Cebra, S. Fujimura, H. Takao, C. Karmonik, S. Elias, N. M. Cancelliere, M. Najafi, D. A. Steinman, V. M. Pereira, S. Piskin, E. A. Finol, M. Pravditsseva, P. Velvaluri, H. Rajabzadeh-Oghaz, N. Paliwal, H. Meng, S. Seshadhri, S. Venguru, M. Shojima, S. Sindeev, S. Frolov, Y. Qian, Y. Wu, K. D. Carlson, D. F. Kallmes, D. Dragomir-Daescu, O. Beuing, International journal of computer assisted radiology and surgery, 1-10 (2019), 10.1007/s11548-019-01986-2
68. A new hypothesis on the role of vessel topology in cerebral aneurysm initiation, B. Csippa, G. Závodszy, G. Paál, I. Szikora, Computers in biology and medicine, 103, 244-251 (2019), 10.1016/j.combiomed.2018.10.018
69. Red blood cell and platelet diffusivity and margination in the presence of cross-stream gradients in blood flows, G. Závodszy, B. van Rooij, B. Czaja, V. Azizi, D. de Kanter, A. G. Hoekstra, Physics of Fluids, 31, 031903 (2019), 10.1063/1.5085881
70. Understanding Malaria induced red blood cell deformation using data-driven Lattice Boltzmann Simulations, J. Sing Yee Tan, G. Závodszy, P. M. A. Slood, International Conference on Computational Science, 393-402 (2018), 10.1007/978-3-319-93698-7_30
71. Optimizing parallel performance of the cell based blood flow simulation software hemocell, V. A. Tarksalooyeh, G. Závodszy, A. G. Hoekstra, International Conference on Computational Science, 11538, 537-547 (2019), 10.1007/978-3-030-22744-9_42
72. Bridging the computational gap between mesoscopic and continuum modeling of red blood cells for fully resolved blood flow, C. Kotsalos, J. Latt, B. Chopard, arXiv:1903.06479 (2019)
73. Strategies of data layout and cache writing for input-output optimization in high performance scientific computing: Applications to the forward electrocardiographic problem, L. Cardone-Noott, B. Rodriguez, A. Bueno-Orovio, PLOS ONE, 13, e0202410 (2018), 10.1371/journal.pone.0202410
74. Load balancing of parallel cell-based blood flow simulations, S. Alowayyed, G. Závodszy, V. Azizi, A.G. Hoekstra, Journal of Computational Science, 24, 18777503 (2018), 10.1016/j.jocs.2017.11.008
75. Modelling variability in cardiac electrophysiology: a moment-matching approach, E. Tixier, D. Lombardi, B. Rodriguez, J. Gerbeau, Journal of The Royal Society Interface, 14, 20170238 (2017), 10.1098/rsif.2017.0238
76. Are CT-Based Finite Element Model Predictions of Femoral Bone Strengthening Clinically Useful?, M. Viceconti, M. Qasim, P. Bhattacharya, X. Li, Current Osteoporosis Reports, 16, 216-223 (2018), 10.1007/s11914-018-0438-8
77. Variational Inference over Non-differentiable Cardiac Simulators using Bayesian Optimization, A. McCarthy, B. Rodriguez, A. Minchile, arXiv:1712.03353 (2017)
78. Big data: the end of the scientific method?, S. Succi, P. V. Coveney, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 377, 20180145 (2019), 10.1098/rsta.2018.0145
79. Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations, J. Dakka, K. Farkas-Pall, M. Turilli, D. Wright, P. V. Coveney, S. Jha, arXiv:1801.01174 (2018)
80. High-throughput Binding Affinity Calculations at Extreme Scales, J. Dakka, M. Turilli, D. Wright, S. Zasada, V. Balasubramanian, S. Wan, P. V. Coveney, S. Jha, arXiv:1712.09168 (2017)
81. Human In Silico Drug Trials Demonstrate Higher Accuracy than Animal Models in Predicting Clinical Pro-Arrhythmic Cardiotoxicity, E. Passini, O. Britton, H. R. Lu, J. Rohrbacher, A. N. Hermans, D. J. Gallacher, R. J. H. Greig, A. Bueno-Orovio, B. Rodriguez, Frontiers in Physiology, 8, 668 (2017), 10.3389/fphys.2017.00668
82. δ -cells and β -cells are electrically coupled and regulate α -cell activity via somatostatin, L. J. B. Briant, T. M. Reinbothe, I. Spiliotis, C. Miranda, B. Rodriguez, P. Rorsman, The Journal of Physiology, 596, 197-215 (2018), 10.1113/JP274581
83. Quantification of the influence of detailed endocardial structures on human cardiac haemodynamics and electrophysiology using HPC, F. Sacco, PhD Thesis at UPF/BSC (2019)



9.2 Popularised Publications

Description of Activity	Audience(s) (see above table)	No. of People
Roger Highfield published an online WIRED article on "How weather forecasts could help develop 'designer' drugs personalised to your illness", featuring Peter Coveney (UCL) and CompBioMed's JCTC paper on "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study", on 29 April 2017. WIRED received 19,087,927 unique visitors per month. https://www.wired.co.uk/article/personalised-drugs-simulations	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	190,000
Roger Highfield published an article in the May 2017 printed edition WIRED on "How weather forecasts could help develop 'designer' drugs personalised to your illness", featuring Peter Coveney (UCL) and CompBioMed's JCTC paper on "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study", on 29 April 2017. The printed version of WIRED is distributed to 870,101 people per month. https://www.wired.co.uk/article/personalised-drugs-simulations	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	870,101
Andrea Townsend-Nicholson (UCL) published an online article in "The Healthy Food Guide" featuring CompBioMed, on 1 September 2019. The Healthy Food Guide receives 25,000 visitors per month.	[General Public], [Medias], [Industry]	1,000
Andrea Townsend-Nicholson (UCL) published an printed article in "The Healthy Food Guide" featuring CompBioMed, on 1 September 2019. The printed version of The Healthy Food Guide has 45,000 subscribers.	[General Public], [Medias], [Industry]	45,000
Bettine van Willigen and Tim van den Boom (LifeTec Group) published an article on AndioSupport in the career magazine of the four universities of technologie in the Netherlands, on 21 June 2019. https://www.4tu.nl/nl/publicaties/4tu.career-special-2019.pdf	[Scientific Community (higher education, Research)], [Medias], [Civil Society]	400
Gabor Zavodszky (UvA) published an ERCIM Article on "How will Your Digital Twin be born?" on 23 October 2018. https://ercim-news.ercim.eu/en115/special/2098-how-will-your-digital-twin-be-born	[General Public], [Medias], [Industry]	796
Elisa Passini, Blanca Rodriguez, Patricia Benito (Oxford) published an article on "Should Computer Simulations Replace Animal Testing for Heart Drugs?" in the Scientific American on 27 March 2018. https://www.scientificamerican.com/article/should-computer-simulations-replace-animal-testing-for-heart-drugs/	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	1,000
Elisa Passini, Blanca Rodriguez, Patricia Benito (Oxford) published an article on "Why computer simulations should replace animal testing for heart drugs" in the Conversation on 26 March 2018. This was tweeted 50 times and shared on facebook 539 times. https://theconversation.com/why-computer-simulations-should-replace-animal-testing-for-heart-drugs-93409	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	10,780
BSC published a newspaper and online article on "Barcelona alberga un proyecto para crear corazones virtuales" in El Periodico on 10 June 2019. https://www.elperiodico.com/es/ciencia/20190610/proyecto-corazon-virtual-superordenador-barcelona-7497712	[General Public], [Medias], [Industry]	1,000
Bastien Chopard (UNIGE) and CompBioMed featured in the article "Artificial intelligence is invited to CHU Charleroi!" on Le Specialiste on 4 September 2018. https://www.lespecialiste.be/fr/actualites/e-health/l-rsquo-intelligence-artificielle-s-rsquo-invite-au-chu-de-charleroi.html	[Clinicians], [Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	500
Ana Mincholé and Blanca Rodriguez (Oxford) published the article "Artificial intelligence for the electrocardiogram" in Nature Medicine on 7 Jan 2019. Nature Medicine has an Impact Factor 32.621.	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	3,960

9.3 Film and Video

9.3.1 Film and Video not related to the Virtual Humans Film

Description of Activity	Audience(s) (see above table)	No. of People
Blanca Rodriguez (Oxford) appeared in an interview video titled "Professor Blanca Rodriguez on how computer models can replace animal research" on the YouTube channel "National Centre for the 3Rs" on 14 April 2019	[General Public], [Scientific Community (higher education, Research)]	486
BSC, Sheffield, and Medtronic created and posted a video on "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" on YouTube on 24 July 2019. https://www.youtube.com/watch?v=Pn1_bD4r1cg	[General Public], [Scientific Community (higher education, Research)]	303
UCL and CBK created and posted 80 videos on the CompBioMed YouTube channel (that weren't the Virtual Humans film)	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	6,323

9.3.2 Activity Specifically related to the Virtual Humans Film

Description of Activity	Audience(s) (see above table)	No. of People
Andrea Townsend-Nicholson (UCL) published an online article in "The Healthy Food Guide" featuring CompBioMed, on 1 September 2019. The Healthy Food Guide receives 25,000 visitors per month.	[General Public], [Medias], [Industry]	1,000
Andrea Townsend-Nicholson (UCL) published a printed article in "The Healthy Food Guide" featuring CompBioMed, on 1 September 2019. The printed version of The Healthy Food Guide has 45,000 subscribers.	[General Public], [Medias], [Industry]	45,000
BSC published a newspaper and online article on "Barcelona alberga un proyecto para crear corazones virtuales" in El Periodico on 10 June 2019. https://www.elperiodico.com/es/ciencia/20190610/proyecto-corazon-virtual-superordenador-barcelona-7497712	[General Public], [Medias], [Industry]	1,000
Gavin Pringle (EPCC) made the Virtual Humans video available throughout UEDIN via centralised "Media Hopper" on 11 October 2018. https://media.ed.ac.uk/media/Virtual+Humans/0_cd6algk	[Scientific Community (higher education, Research)]	11
Alfons Hoekstra (UvA) discussed Computational Biomedicine on the Dutch TV show "de wereld van morgen" (tomorrow's world), including a showing of the Virtual Humans film, on 13 June 2018. The episode had estimated viewing figures of 1,000,000.	[General Public], [Medias]	1,000,000
ELEM Biotech created a short cut of the Virtual Humans film and posted it on their Youtube channel. https://www.youtube.com/watch?v=G59PLdz8okw	[General Public], [Scientific Community (higher education, Research)]	837
Segments from the Virtual Humans Film along with Dieter Kranzlemuller (LRZ) featured in a video on 3sat on 25 September 2018. https://www.3sat.de/wissen/nano/geballte-rechenpower-100.html?mode=play&obj=76016	[General Public], [Scientific Community (higher education, Research)]	200
The Virtual Humans film was posted on the CompBioMed YouTube channel. https://youtu.be/1FvRSJ9W734	[General Public], [Scientific Community (higher education, Research)]	7,345
The Virtual Humans film was posted on the Science Museum YouTube channel. https://youtu.be/1ZrAaDsF8YY	[General Public], [Scientific Community (higher education, Research)]	2,169
The Virtual Humans film was posted on the Barcelona Supercomputing Centre YouTube channel. https://youtu.be/_rMaN1zAGxY	[General Public], [Scientific Community (higher education, Research)]	1,087
The Virtual Humans film was a finalist in the 5th Raw Science Film Festival in Los Angeles on 8 February 2019. It won the 2nd place of the Professional Documentary of less than 10 minutes.	[General Public], [Medias]	500

The Virtual Humans film was shortlisted for the Short Film Competition at the AFO (Academic Film Olomouc) Festival of Science in the Czech Republic.	[General Public], [Medias]	415
The Virtual Humans film won an award for Technical Merit at the 2018 SCINEMA International Science Film Festival on 8 June 2018. https://www.bsc.es/news/bsc-news/virtual-humans-receives-the-award-technical-merit-the-2018-scinema-international-science-film	[General Public], [Medias]	400
EPCC (@epcc_ed) retweeted the CompBioMed Twitter Account about the Virtual Humans Film	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	2,030
The Virtual Humans video was posted on Reddit on 9 March 2018 https://www.reddit.com/r/videos/comments/836xab/virtual_human/	[General Public]	200
The CompBioMed Twitter account's (@bio_comp) tweet about the Virtual Humans film was retweeted 24 times and liked 20 times	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	771
The Oxford Comp Sci Twitter account's (@CompSciOxford) tweet about the Virtual Humans film was retweeted 16 times and liked 23 times	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	4,055
Fernando Cucchiatti (BSC) tweeted (@thefercook) about the Virtual Humans video. https://twitter.com/thefercook/status/1083686230691405824	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	953
The Raw Science TV (@RawScienceTV) Twitter account tweeted about the Virtual Humans video on 11 Jan 2019. https://twitter.com/RawScienceTV/status/1083687502056120320	[Scientific Community (higher education, Research)], [General Public], [Medias], [Industry]	3,417
Roger Highfield (Science Museum) posted a blog on the CompBioMed website on CompBioMed's involvement at Evidence Week at Parliament on 26 June 2019. https://www.compbiomed.eu/the-virtual-human-enters-parliament/	[General Public], [Medias], [Industry]	47
Alberto Marzò (Sheffield), Claudia Mazza (Sheffield), Roger Highfield (Science Museum) posted a blog on Insigneo's website for CompBioMed's involvement at Evidence Week at Parliament on 26 June 2019. https://insigneo.org/2019/07/the-virtual-human-enters-parliament/	[General Public], [Medias], [Industry]	100
Oxford published a website dedicated for their research on drug safety using computational models. http://www.cs.ox.ac.uk/insilicocardiotox/home	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians], [General Public]	200
Alberto Marzò (USFD) posted a news item about CompBioMed's involvement at Evidence Week at Parliament on the University of Sheffield website on 4 July 2019. https://www.sheffield.ac.uk/faculty/engineering/news	[Scientific Community (higher education, Research)]	50
BSC posted an article on "Virtual Humans receives the award for Technical Merit at the 2018 SCINEMA International Science Film Festival" on their website on 13 April 2018. https://www.bsc.es/news/bsc-news/virtual-humans-receives-the-award-technical-merit-the-2018-scinema-international-science-film	[Scientific Community (higher education, Research)], [Industry]	50
An article on "Your digital twin: closer than you think" was posted on the UvA website on 19 April 2018. https://www.uva.nl/en/shared-content/subsites/informatics-institute/en/news/2018/04/your-digital-twin.html?origin=kUP%2BByx6UTZquvJiCJknnEQ	[Scientific Community (higher education, Research)]	50
Roger Highfield (Science Museum) wrote an article on "USING 'VIRTUAL HEARTS' TO REDUCE ANIMAL TESTING IN MEDICINE" on the Science Museum Blog on 12 March 2018. https://blog.sciencemuseum.org.uk/using-virtual-humans-to-reduce-medical-animal-testing/	[General Public], [Medias]	500
Roger Highfield (Science Museum) wrote an article on "HOW TO BUILD A VIRTUAL HUMAN" on the Science Museum Blog on 11 August 2017. https://blog.sciencemuseum.org.uk/build-virtual-human/	[General Public], [Medias]	1,000
CBK and UCL created 2 pages on the CompBioMed.eu website that focus on the Virtual Humans film.	[Clinicians], [Scientific Community (higher education, Research)], [Industry], [General Public]	724
The Virtual Humans video was posted on the UCL Biosciences website as an innovation case study on 9 November 2018. https://www.ucl.ac.uk/biosciences/partnerships-and-innovation/innovation/virtual-human-project and https://www.ucl.ac.uk/biosciences/home/study/partnerships-and-innovation/innovation	[Scientific Community (higher education, Research)]	50

Peter Coveney (UCL) was the conference chair for the CompBioMed Conference in London on 25-27 September 2019. Andrea Townsend-Nicholson (UCL), David Wright (UCL), and Francesco Gervasio (UCL) were on the local organising committee. Emily Lumley (UCL) was the head of conference administration. Hugh Martin (CBK), Apostolos Evangelopoulos (UCL), Xuanye Gu (UCL) were on the administrative committee.	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
ATOS held a booth at the Teratec Forum in Palaiseau France on 19 and 20 June 2018. CompBioMed flyers and stress toys were distributed, CompBioMed posters were displayed, and the Virtual Humans video was presented.	[Scientific Community (higher education, Research)], [Industry]	200
UCL and CBK organised a CompBioMed booth at VPH2018, showing the Virtual Humans video, displaying CompBioMed posters, and distributing flyers and stress toys, in Zargoza Spain on 5-7 September 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) gave 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 on 6 February 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, gave a talk on "Practical challenges for biomedical modeling using HPC" at the Second HPC Applications in Precision Medicine Workshop at ISC18 in Frankfurt Germany on 28 June 2018	[Scientific Community (higher education, Research)], [Industry]	25
Peter Coveney (UCL), Ana Mincholé (Oxford), and Andrea Townsend-Nicholson (UCL), along with Roger Highfield (Science Museum), presented the Virtual Humans film in a segment on "Building A Virtual Human" at the Cheltenham Science Festival 2018, UK, on 9 June 2018	[General Public], [Medias]	200
Natalia Jimenez (ATOS) gave a Keynote Presentation on Precision Medicine which promoted CompBioMed at the International Supercomputing Conference (ISUM) in Mexico on 26-29 March 2019	[Industry], [Scientific Community (higher education, Research)], [General Public]	50
Erwan Raffin (ATOS) presented a poster on "CompBioMed Biomedical Applications on High Performance Computers" at the Teratec Forum - European Research Café on 19-20 June 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Policy makers]	1,300
Jazmín Aguado-Sierra (BSC) gave a talk on "The role of High Performance Computing in Pharmacology Safety" at the Safety Pharmacology Society Annual Meeting in Barcelona Spain on 23-26 September 2019	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
Christos Kotsalos (UNIGE) gave a talk on "Optimizing performance of the blood flow simulation software hemocell" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community], [Industry], [General Public], [Medias], [Clinicians], [Policy makers], [Customers], [Investors]	200
Marco Verdicchio (SURFsara) gave a talk promoting CompBioMed at the EOSC Hub week 2019 in Prague Czech Republic on 10-12 April 2019	[Scientific Community (higher education, Research)], [Industry]	50
Marco Verdicchio (SURFsara) gave a talk on "New trends in High Performance Computing: from commodity clusters to exascale machines" at Numerical Combustion 2019 in Aachen Germany on 6-8 May 2019	[Scientific Community (higher education, Research)], [Industry]	50
Gábor Zavodszky (UvA) gave a talk on "Coupling scheme for a high-performance multiscale blood flow simulation workflow" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	300
Gabor Zavodszky (UvA) gave an invited talk on "How do Red Blood Cells and Platelets move in our Arteries? The circulatory system of the Virtual Human" at Super Day 2018 in Amsterdam Netherlands on 18 December 2018	[Scientific Community (higher education, Research)], [Industry]	150
Peter Coveney (UCL) gave a talk on "The Virtual Human: In Silico Methods for Personalised Medicine" at the Digital Transformation Conference 2018 in Lebanon on 12-13 March 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) presented the Virtual Humans video at the event Think Science, held at the World Trade Center in Dubai on 16 April 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Medias]	400
Peter Coveney (UCL) presented the Virtual Humans video at the event Think Science, held at the World Trade Center in Dubai on 17 April 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Medias]	400
ATOS promoted CompBioMed and showed the Virtual Humans video during a talk at ISUM (International Supercomputing Conference in Mexico) in Mexico on 26-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	50

Gavin Pringle (EPCC) showed the Virtual Humans film at the Latin American Introductory School on Parallel Programming and Parallel Architecture for High Performance Computing in Mexico on 12-23 Feb 2018	Scientific Community (research)	60
Robin Richardson (UCL) gave a talk on "Development of HemeLB and adaptation to the clinic" at the UKCOMES HemeLB Meeting in London UK on 29 May 2019	[Scientific Community (higher education, Research)]	30
Gabor Zavodszky (UvA) gave an invited talk on "How do Red Blood Cells and Platelets move in our Arteries? The circulatory system of the Virtual Human" at JMBC 2019 in Delft Netherlands on 17 May 2019	[Scientific Community (higher education, Research)], [Industry]	50
Gabor Zavodszky (UvA) gave an invited talk on "The virtual artery - A multiscale model for vascular pathophysiology" at the MultiScale Workshop in the Lorentz Center in Leiden Netherlands on 16-20 April 2018	[Scientific Community (higher education, Research)], [Industry]	50
Peter Coveney (UCL) showed the CompBioMed "Virtual Humans" film at the LRZ event "Next-Gen HPC - The Path to Exascale: Artificial Intelligence & Personalized Medicine" in Garching on 29-30 June 2018	[Scientific Community (higher education, Research)]	30
Natalia Jimenez (ATOS) gave a talk on "Challenges and opportunities in Life Sciences" at the ELIXIR Bioinformatics Suppliers Forum in London on 7 May 2019	[Scientific Community (higher education, Research)], [Industry]	30
Emily Lumley (UCL) gave a talk on CompBioMed Dissemination, Training and Links with Industry, discussing the Virtual Humans Video at the PRACE CoE FET-HPC EXDCI Workshop in Brühl Germany on 30 October 2018	[Scientific Community (higher education, Research)]	30
Peter Coveney (UCL) met with representatives at the Istituto Italiano di Tecnologia (including the Computational modelling of Nanoscale and bioPhysical systems lab) in Genova Italy to discuss CompBioMed on 18 July 2018	[Scientific Community (higher education, Research)]	10
Andrea Townsend-Nicholson (UCL) and Clint Davies-Taylor (Dassault Systèmes) gave presentations at "Sense About Science's Evidence Week at Parliament 2019" at the UK House of Parliament, Upper Waiting Hall on 26 June 2019	[Policy makers], [Medias], [General Public]	50
Andrea Townsend-Nicholson (UCL) gave a talk at "UCL Biochemistry Open Day Research Talks" in London UK on 28-29 June 2019	[General Public]	700
Cyril Mazauric (ATOS) and Natalia Jimenez (ATOS) gave a technical talk at the Atos Scientific Community Meeting in Paris France on 19-20 February 2019	[Industry]	120
Natalia Jimenez (ATOS) gave an Industry Talk on "Challenges and opportunities in Life Sciences" at the Elixir Bioinformatics Supplier Forum in London UK on 7 May 2019	[Industry]	50
Jazmin Aguado-Sierra (BSC) gave a seminar on "Computers Simulating the heart: How close are we to recreating physiology?" at the Cardiovascular Seminar Series, Division of Cardiovascular Sciences, University of Manchester in Manchester UK on 2 May 2019	[Scientific Community (higher education, Research)]	25
The Virtual Humans film was presented by Alfons Hoekstra (UvA) during the event "Bessensap" in the Netherlands on 15 June 2018	[Medias], [Scientific Community (higher education, Research)]	400
Marco Viceconti (USFD) gave a talk on "Do virtual patients see electric Doctors?" to patients and carers at the public launch of the Sheffield NIHR Biomedical Research Centre in neurodegenerative Disease on 14 Dec 2017. http://sheffieldbrc.nihr.ac.uk/public-launch-event/	[Clinicians], [General Public]	100
Marco Viceconti (USFD) showed the Virtual Humans film in a talk during the Insigneo Showcase on 3 May 2018. https://insigneo.org/event/insigneo-showcase-2018/	[Clinicians], [Policy makers], [Investors], [Scientific Community (higher education, Research)]	300
EPCC showed the Virtual Humans film at the Bayes Centre VIP launch at the University of Edinburgh in Edinburgh UK on 10 October 2018	[Policy makers], [Investors], [Scientific Community (higher education, Research)]	50
Jazmin Aguado (BSC) presented the Virtual Humans video and distributed CompBioMed flyers at the Cardiovascular Seminar Series at the Division of Cardiovascular Sciences, University of Manchester in Manchester UK on 2nd May 2019	[Scientific Community (higher education, Research)]	30
Alfons Hoekstra (UvA) and Peter Coveney (UCL) gave a lecture and debate on "Your digital twin: closer than you think" at the UvA University Day. https://alumni.uva.nl/en/services/university-day/en-your-digital-twin.html	[General Public]	100
Sauro Succi showed the Virtual Humans film at the event "Master in HPC" at the International Centre for Theoretical Physics in Trieste Italy on 14 Feb 2019	[Scientific Community (higher education, Research)]	30

Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to the Director - Institute for Computational Biomedicine, Weill Cornell Medical College, and Englander Institute for Precision Medicine in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	2
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Chief Business Officer - New York Genome Center in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Managing Director - Biolabs in New York USA in September 2018	[Industry]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Executive Director - Institute of Computational Medicine, NYU Langone Health in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Academic Partnerships - Broad Institute of Harvard and MIT in Boston USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Chief Operating Officer - CIMIT Boston in Boston USA in September 2018	[Industry]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Manager - Cambridge Innovation Center in Boston USA in September 2018	[Industry]	2
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Associate Director (Research) - Massachusetts General Hospital Center for Computational and Integrative Biology, Harvard University in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Director R&D - Mitra Biotech in Boston USA in September 2018	[Industry]	3
Gavin Pringle (EPCC) showed the Virtual Humans video during the two 'HPC for Medics' course in London on 7th Dec 2017	[Medical Students], [Clinicians]	20
Gavin Pringle (EPCC) showed the Virtual Humans video during the two 'HPC for Medics' course in London on 8th Dec 2017	[Medical Students], [Clinicians]	20
Gavin Pringle (EPCC) showed the Virtual Humans video during the 'HPC for Bioscientist' in London on 7th March 2018	[Scientific Community (higher education, Research)]	20
Alfons Hoekstra (UvA) presented the Virtual Humans film to pupils aged 16/17 in 3 schools in Amsterdam on 3 November 2018	[General Public]	90
Sauro Succi showed the Virtual Humans film at various school around Italy in 2018 and 2019	[General Public]	60
Alberto Marzo (USFD) presented the Virtual Humans film to 15 Year 4 undergraduate students in Mechanical Engineering at the University of Sheffield on 1 February 2018	[Scientific Community (higher education, Research)]	15
Alberto Marzo (USFD) presented the Virtual Humans film to 100 Year 1 undergraduate students in Bioengineering at the University of Sheffield on 1 November 2018	[Scientific Community (higher education, Research)]	100
Alberto Marzo (USFD) presented the Virtual Humans film to 15 Year 4 undergraduate students in Mechanical Engineering at the University of Sheffield on 1 February 2019	[Scientific Community (higher education, Research)]	15
Gabor Zavodszky (UvA) gave an invited talk on "Zoom in on blood - Using supercomputers in hemodynamics" at the PATC 2019 HPC training event in Barcelona Spain on 13-14 February 2019	[Scientific Community (higher education, Research)]	30
Samira Ahmed Twitter @SamiraAhmedUK Tweeted for the CompBioMed-Science Museum "The Virtual Human" Event. https://twitter.com/SamiraAhmedUK/status/910409063493718017	[General Public], [Medias]	38,000
The Mauri Lab at UCL (@Mauri_group) Tweeted about the CompBioMed-Science Museum "The Virtual Human" Event. https://twitter.com/Mauri_group/status/913117183600943105	[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	[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	[General Public], [Medias]	2,000
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	[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/	[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-j7bnpu-pn-w2ab4r/the-virtual-human-imax-film-at-the-science-museum	[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/	[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/	[Scientific Community (higher education, Research)]	100
BSC, Paul Melis (SURFsara), Casper van Leeuwen (SURFsara), Peter Coveney (UCL) <i>et al.</i> produced an IMAX animation called "Virtual Humans", which was screened at the "London Science Museum Lates". http://www.compbioed.eu/home/how-to-build-the-virtual-human/	[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=QGhobMPGHSM	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	1,688
The CompBioMed-Science Museum "The Virtual Human" Event was posted on the weekly e-newsletter in the UCL Chemistry Department	[Scientific Community (higher education, Research)]	50
Roger Highfield (Science Museum Group) tweeted 6 times about the CompBioMed-Science Museum "The Virtual Human" Event, @RogerHighfield	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	101,400
The Science Museum tweeted twice about the CompBioMed-Science Museum "The Virtual Human" Event, @sciencemuseum	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	1,324,000
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.	[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.	[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	[General Public], [Medias], [Scientific Community (higher education, Research)], [Industry]	5,000
Emily Lumley (UCL) included the CompBioMed-Science Museum "The Virtual Human" Event in the November 2017 CompBioMed e-Newsletter	[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	[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	[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	[Scientific Community (higher education, Research)], [Industry]	100

9.4 Social Media

Description of Activity	Audience(s) (see above table)	No. of People
Acellera (@acellera) retweeted the CompBioMed Twitter Account 12 times	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	8,292
Acellera (@acellera) Tweeted 4 times about CompBioMed	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	2,764
EPCC (@epcc_ed) retweeted the CompBioMed Twitter Account 9 times	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	18,270
EPCC (@epcc_ed) tweeted the CompBioMed's Webinars on 7 June 2019	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	2,030
The UCL PR team tweeted about the CompBioMed article on "Drug binding simulations promise to get personal" on 18 Jan 2017. https://twitter.com/uclmaps/status/821654120448884737	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	2,381
The Virtual Humans video was posted on Reddit on 9 March 2018 https://www.reddit.com/r/videos/comments/836xab/virtual_human/	[General Public]	200
UCL and CBK posted 771 tweets on the CompBioMed Twitter Account (@bio_comp)	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	302,411
UCL and CBK created and posted 81 videos on the CompBioMed YouTube channel	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	13,668
Fernando Cucchiatti (BSC) tweeted (@thefercook) about the Virtual Humans video. https://twitter.com/thefercook/status/1083686230691405824	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	953
The Raw Science TV (@RawScienceTV) Twitter account tweeted about the Virtual Humans video on 11 Jan 2019. https://twitter.com/RawScienceTV/status/1083687502056120320	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	3,417
Oxford Comp Sci tweeted about Elisa Passini appearing on the Matthew Wright Show on TalkRadio on 14 June 2019 https://twitter.com/CompSciOxford/status/1139445092085903360	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	4,049
The AnimalFreeResearchUK (@AFR_UK) Twitter account tweeted about Oxford's article on "Why computer simulations should replace animal testing for heart drugs" in The Conversation on 18 April 2018	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	5,735
Dr Jenny Morber's (@JRMorber) Twitter account tweeted about Oxford's article on "Should Computer Simulations Replace Animal Testing for Heart Drugs?" in the Scientific American on 27 March 2018	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	2,884
45 Twitter Accounts tweeted about Oxford's Nature Medicine article on "Artificial intelligence for the electrocardiogram" on 18 August 2019	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	9,000
539 Facebook Accounts shared Oxford's article on "Why computer simulations should replace animal testing for heart drugs" in the Conversation on 26 March 2018. https://theconversation.com/why-computer-simulations-should-replace-animal-testing-for-heart-drugs-93409	[General Public]	5,390
50 Twitter Accounts tweeted about Oxford's article on "Why computer simulations should replace animal testing for heart drugs" in the Conversation on 26 March 2018	[Scientific Community (higher education, Research), [General Public], [Medias], [Industry]	10,000
Joan Rangel Tarrés's (@rangeltarres) Twitter account tweeted about BSC's newspaper and online article on "Barcelona alberga un proyecto para crear corazones virtuales" in El Periodico on 10 June 2019	[General Public]	5,030

9.5 Website

Description of Activity	Audience(s) (see above table)	No. of People
On Acellera.com, the logo of CompBioMed was posted. https://www.acellera.com/science/	[Scientific Community (higher education, Research), [Industry]	200

Joao Damas posted a blog on the Acellera website on the participation of Acellera at the CompBioMed Containerisation meeting. https://www.acellera.com/index.php/2019/04/29/acellera-at-the-first-compbiomed-containerisation-meeting/	[Scientific Community (higher education, Research)], [Industry]	200
Roger Highfield (Science Museum) posted a blog on the CompBioMed website on CompBioMed's involvement at Evidence Week at Parliament on 26 June 2019. https://www.compbiomed.eu/the-virtual-human-enters-parliament/	[General Public], [Medias], [Industry]	47
Alberto Marzo (Sheffield), Claudia Mazza (Sheffield), Roger Highfield (Science Museum) posted a blog on Insigneo's website for CompBioMed's involvement at Evidence Week at Parliament on 26 June 2019. https://insigneo.org/2019/07/the-virtual-human-enters-parliament/	[General Public], [Medias], [Industry]	100
Andrea Townsend-Nicholson (UCL) posted an article on "The Virtual Human: A case study in collaborative data" on the Biochemical Society website on 25 June 2019. https://biochemistry.org/home/science-policy/evidence-pod-virtual-human/	[General Public], [Medias], [Industry]	300
Andrea Townsend-Nicholson (UCL) posted a blog for CompBioMed's involvement at Evidence Week at Parliament on the UCL Faculty of Life Sciences website on 31 July 2019	[General Public], [Medias], [Industry]	50
Bettine van Willigen and Tim van den Boom (LifeTec Group) published a news item on AngioSupport on LifeTec Group website. https://www.lifetecgroup.com/cases-papers-products-services/case-angiosupport	[Industry], [General Public]	50
Oxford published a website dedicated for their research on drug safety using computational models. http://www.cs.ox.ac.uk/insilicocardiotox/home	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians], [General Public]	200
Alberto Marzo (USFD) posted a news item about CompBioMed's involvement at Evidence Week at Parliament on the University of Sheffield website on 4 July 2019. https://www.sheffield.ac.uk/faculty/engineering/news	[Scientific Community (higher education, Research)]	50
An Article was posted on the VPH Institute website which introduced the CompBioMed Innovation Exchange Programme, on 12 January 2017. https://www.vph-institute.org/news/compbiomed-the-european-center-of-excellence-in-computational-medicine.html	[Scientific Community (higher education, Research)], [Industry]	200
An article was posted on "'Virtual Artery' takes us closer to improved prediction of treatment side-effects" on the Europa Cordis website on 17 August 2017. https://cordis.europa.eu/news/rcn/128702/en	[Scientific Community (higher education, Research)], [Industry], [Policy Makers]	50
BSC posted an article on "Virtual Humans receives the award for Technical Merit at the 2018 SCINEMA International Science Film Festival" on their website on 13 April 2018. https://www.bsc.es/news/bsc-news/virtual-humans-receives-the-award-technical-merit-the-2018-scinema-international-science-film	[Scientific Community (higher education, Research)], [Industry]	50
An article on "Your digital twin: closer than you think" was posted on the UvA website on 19 April 2018. https://www.uva.nl/en/shared-content/subsites/informatics-institute/en/news/2018/04/your-digital-twin.html?origin=kUP%2Byx6UTZquvJiCJknnEQ	[Scientific Community (higher education, Research)]	50
An article was posted on "Novel cardiovascular device will help reduce re-blocking of arteries" on the Europa Cordis website on 2 August 2017. https://cordis.europa.eu/news/rcn/131362/en	[Scientific Community (higher education, Research)], [Industry], [Policy Makers]	50
Roger Highfield (Science Museum) wrote an article on "USING 'VIRTUAL HEARTS' TO REDUCE ANIMAL TESTING IN MEDICINE" on the Science Museum Blog on 12 March 2018. https://blog.sciencemuseum.org.uk/using-virtual-humans-to-reduce-medical-animal-testing/	[General Public], [Medias]	500
Roger Highfield (Science Museum) wrote an article on "HOW TO BUILD A VIRTUAL HUMAN" on the Science Museum Blog on 11 August 2017. https://blog.sciencemuseum.org.uk/build-virtual-human/	[General Public], [Medias]	1,000
CompBioMed's Training Portal was listed on einfraCentral on 11 September 2018. https://www.einfracentral.eu/service/compbiomed.compbiomed_training_portal	[Scientific Community (higher education, Research)], [Industry]	43
CBK and UCL created 129 pages on the CompBioMed.eu website	[Clinicians], [Scientific Community (higher education, Research)], [Industry], [General Public]	199,577
CBK and UCL created 35 pages on the compbiomed-conference.eu website	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	1,000

The Virtual Humans video was posted on the UCL Biosciences website as an innovation case study on 9 November 2018. https://www.ucl.ac.uk/biosciences/partnerships-and-innovation/innovation/virtual-human-project and https://www.ucl.ac.uk/biosciences/home/study/partnerships-and-innovation/innovation	[Scientific Community (higher education, Research)]	50
Oxford published an article titled "International 3Rs Prize awarded for computer modelling that predicts human cardiac safety better than animal studies" on the NC3RS website on 12 March 2018. https://www.nc3rs.org.uk/news/international-3rs-prize-awarded-computer-modelling-predicts-human-cardiac-safety-better-animal	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
CompBioMed featured in the eInfracentral website in an article called "Seven new Service Providers join eInfracentral service catalogue" on 19 November 2018. http://project.einfracentral.eu/news/seven-new-service-providers-join-einfracentral-service-catalogue	[Scientific Community (higher education, Research)], [Industry]	50

9.6 Organisation of Events

Description of Activity	Audience(s) (see above table)	No. of People
Peter Coveney (UCL) and Emily Lumley (UCL) were on the organising committee for workshop "HemeLB: cardiovascular modelling and simulation in UKCOMES" in London on 29 May 2019	[Scientific Community (higher education, Research)], [Industry]	30
Peter Coveney (UCL) was the conference chair for the CompBioMed Conference in London on 25-27 September 2019. Andrea Townsend-Nicholson (UCL), David Wright (UCL), and Francesco Gervasio (UCL) were on the local organising committee. Emily Lumley (UCL) was the head of conference administration. Hugh Martin (CBK), Apostolos Evangelopoulos (UCL), XuanYe Gu (UCL) were on the administrative committee.	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Nikolas Maniatis (UCL) and Andrea Townsend-Nicholson (UCL) co-chaired the Genomics symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney (UCL) and Herman Van Vijmen (Janssen) co-chaired the Molecular Medicine symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Blanca Rodriguez (Oxford) and Claudia Mazza (Sheffield) co-chaired the Organ Modelling and Simulation symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Andrea Townsend-Nicholson (UCL) co-chaired the "Role of Theory, Modelling and Simulation in Biomedicine" symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney (UCL) and Alfons Hoekstra (UvA) co-chaired the Uncertainty Quantification symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Marco Viceconti (UNIBO) and Alfons Hoekstra (UvA) co-chaired the "Regulatory Science and in silico Trials" symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Marco Verdicchio (SURFsara) chaired the "Cloud & High Performance Computing" symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Herman Van Vijmen (Janssen) chaired the "Innovation in Modern Biotechnology" symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Andrea Townsend-Nicholson (UCL) chaired the "Education, Training & Public Awareness" symposium at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200

Marcin Ostasz (BSC), Mariano Vazquez (BSC) and Peter Coveney (UCL) organised and ran a Birds of a Feather session on "Personalized Medicine and HPC" at Supercomputing 2018 in Dallas on 14 November 2018	[Scientific Community (higher education, Research)], [Industry]	45
CompBioMed and ETP4HPC had a joint BoF entitled "The Computational Biomedicine Community and the HPC Industry: Working together to advance Personalised Medicine" at ISC19 in Frankfurt Germany on June 19th, 2019.	[Scientific Community (higher education, Research)], [Industry]	30
Alfons Hoekstra (UvA) organised a session called "Computational challenges in multi scale modelling in biomechanics" at the World Congress in Biomechanics in Dublin Ireland on 8-12 July 2018	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	100
Marco Verdicchio (SURFsara), Peter Coveney (UCL), Mariano Vazquez (BSC) and Emily Lumley (UCL) were on the organising committee for the CompBioMed Workshop on "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications" in Amsterdam Netherlands on 28-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	35
EPCC held a booth at Supercomputing 2018 which featured a rolling presentation contains CompBioMed information, and included CompBioMed flyers and stress toys, on 11-16 November 2018	[Scientific Community (higher education, Research)], [Industry]	400
EPCC held a booth at Supercomputing 2019 which featured a rolling presentation contains CompBioMed information, and included CompBioMed flyers and stress toys, on 17-22 November 2019	[Scientific Community (higher education, Research)], [Industry]	400
EPCC held a booth at ISC 2018 which featured a rolling presentation contains CompBioMed information, and included CompBioMed flyers and stress toys, on 24-28 June 2018	[Scientific Community (higher education, Research)], [Industry]	200
ATOS held a booth at the Teratec Forum in Palaiseau France on 19 and 20 June 2018. CompBioMed flyers and stress toys were distributed, CompBioMed posters were displayed, and the Virtual Humans video was presented.	[Scientific Community (higher education, Research)], [Industry]	200
UCL and CBK organised a CompBioMed booth at VPH2018, showing the Virtual Humans video, displaying CompBioMed posters, and distributing flyers and stress toys, in Zargoza Spain on 5-7 September 2018	[Scientific Community (higher education, Research)], [Industry]	100

9.7 Participation in Events

Description of Activity	Audience(s) (see above table)	No. of People
Peter Coveney (UCL) gave 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 on 6 February 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, had a paper and talk on "Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations" at IEEE eScience 2018 conference in Amsterdam Netherlands on 29 September 2018	[Scientific Community (higher education, Research)], [Industry]	500
Peter Coveney, UCL, had a poster on "Enabling Trade-offs Between Accuracy and Computational Cost: Executing Adaptive Algorithms to Reduce Time to Clinical Insight" at IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid) 2018 held in Washington DC USA on 1-4 May 2018	[Scientific Community (higher education, Research)], [Industry]	50
Peter Coveney, UCL, gave a talk on "Practical challenges for biomedical modeling using HPC" at the Second HPC Applications in Precision Medicine Workshop at ISC18 in Frankfurt Germany on 28 June 2018	[Scientific Community (higher education, Research)], [Industry]	25
Peter Coveney, UCL, gave a talk on "Accurate and Precise Binding Affinity Calculations for Drug Development and Precision Medicine" at the Second HPC Applications in Precision Medicine Workshop at ISC18 in Frankfurt Germany on 28 June 2018	[Scientific Community (higher education, Research)], [Industry]	25
Peter Coveney (UCL), Ana Mincholé (Oxford), and Andrea Townsend-Nicholson (UCL), along with Roger Highfield (Science Museum), presented the Virtual Humans film in a segment on "Building A Virtual Human" at the Cheltenham Science Festival 2018, UK, on 9 June 2018	[General Public], [Medias]	200

Peter Coveney (UCL) gave a Keynote lecture on "Accurate, precise and reliable predictions from modelling and simulation using high performance computers" at the KAUST Research Conference: Artificial Intelligence in Medicine in Saudi Arabia on 18 February 2019	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney (UCL) gave a talk on "Ensemble-based molecular dynamics: Uncertainty quantification and enhanced sampling techniques in free-energy calculations" at the ACS Spring 2019 National Meeting & Exposition in Florida on 31 March to 4 April 2019	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) gave a talk on "Personalised Medicine and the HPC Industry" at ISC 2019 in Frankfurt on 17-19 June 2019	[Scientific Community (higher education, Research)], [Industry]	30
Peter Coveney (UCL) gave a talk on "The Role of High Performance Computing in Biomedicine" at ISC 2019 in Frankfurt on 17-19 June 2019	[Scientific Community (higher education, Research)], [Industry]	50
Peter Coveney (UCL) gave a talk on "Application of ensemble based simulations and machine learning for the prediction of binding free energies and personalized drug selection" at the ACS Summer 2019 National Meeting & Exposition in San Diego on 26 August 2019	[Scientific Community (higher education, Research)], [Industry]	100
Stefan Doerr (UPF) presented a poster on "ACEMD ab-initio: Machine learning small molecule quantum energies and forces" at the IAQMS 16-ICQC Satellite Meeting on "Computational Chemistry meets Artificial Intelligence" in Lausanne Switzerland on 13-15 June 2018	[Scientific Community (higher education, Research)]	50
José Jimenez (UPF) presented a poster on "Deep Learning based protein-ligand relative affinity prediction" at RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry in London UK on 15 June 2018	[Scientific Community (higher education, Research)]	50
Raimondas Galvelis (Acellera) gave a talk on "The rise of PlayMolecule" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Natalia Jimenez (ATOS) promoted CompBioMed at STFC seminar series in Daresbury UK on 13 February 2019	[Industry], [Scientific Community (higher education, Research)]	10
Natalia Jimenez (ATOS) gave a Keynote Presentation on Precision Medicine which promoted CompBioMed at the International Supercomputing Conference (ISUM) in Mexico on 26-29 March 2019	[Industry], [Scientific Community (higher education, Research)], [General Public]	50
Natalia Jimenez (ATOS) gave a Keynote Presentation on Biotechnology which promoted CompBioMed at the International Supercomputing Conference (ISUM) in Mexico on 26-29 March 2019	[Industry], [Scientific Community (higher education, Research)], [General Public]	30
Natalia Jimenez (ATOS) participated in a roundtable discussion on Biotechnology which promoted CompBioMed at the International Supercomputing Conference (ISUM) in Mexico on 26-29 March 2019	[Industry], [Scientific Community (higher education, Research)], [General Public]	30
Erwan Raffin (ATOS) presented a poster on "CompBioMed Biomedical Applications on High Performance Computers" at the Teratec Forum - European Research Café on 19-20 June 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Policy makers]	1,300
Federica Sacco (BSC) gave a talk on "Systematic electrophysiology analysis of four biventricular, anatomically normal human heart models" at the CompBioMed Conference in London UK on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Jazmín Aguado-Sierra (BSC) gave a talk on "The role of High Performance Computing in Pharmacology Safety" at the Safety Pharmacology Society Annual Meeting in Barcelona Spain on 23-26 September 2019	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
Jazmín Aguado-Sierra (BSC) gave a talk on "Anatomically accurate electrophysiology simulations of the human heart, with application to scarred tissue, LBBB and CRT" at the ASME V&V Symposium in Las Vegas USA on 13-17 May 2019	[Scientific Community (higher education, Research)], [Industry]	50
David Wright (UCL) gave a talk on "Practical challenges for biomedical modeling using HPC" at the Second HPC Applications in Precision Medicine Workshop at ISC2018 in Frankfurt Germany on 28 June 2018	[Scientific Community (higher education, Research)], [Industry]	30
Gavin Pringle (EPCC) was a speaker in a BoF on "Personalised Medicine & HPC" at ISC18 in Frankfurt Germany on 19 June 2018	[Scientific Community (higher education, Research)]	30

Christos Kotsalos (UNIGE) gave a talk on "Modeling the Transport of Red Blood Cells and Platelets on Multiple GPUs" at PASC19 in Zurich Switzerland on 12-14 June 2019	[Scientific Community] , [Industry], [General Public], [Medias], [Clinicians], [Policy makers] , [Customers], [Investors]	500
Christos Kotsalos (UNIGE) gave a talk on "Optimizing performance of the blood flow simulation software hemocell" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community] , [Industry], [General Public], [Medias], [Clinicians], [Policy makers], [Customers], [Investors]	200
Bettine van Willigen and Tim van den Boom (LifeTec Group) presented a poster on "Clinical decision tool: AngioSupport" at the BME research day in Eindhoven Netherlands on 2 April 2019.	[Scientific Community (higher education, Research)]	100
Bettine van Willigen and Tim van den Boom (LifeTec Group) gave a talk on AngioSupport at the CompBioMed AHM in Oxford UK on 29 April 2019	[Scientific Community (higher education, Research)]	100
Marco Verdicchio (SURFsara) gave a talk promoting CompBioMed at the EOSC Hub week 2019 in Prague Czech Republic on 10-12 April 2019	[Scientific Community (higher education, Research)], [Industry]	50
Marco Verdicchio (SURFsara) gave a talk on "New trends in High Performance Computing: from commodity clusters to exascale machines" at Numerical Combustion 2019 in Aachen Germany on 6-8 May 2019	[Scientific Community (higher education, Research)], [Industry]	50
Federica Sacco (BSC) presented a poster on "Porous endocardial layer in cardiac left ventricular CFD models reproduces the effect of trabeculations on intra-ventricular pressure drop, WSS and vortex formation" at ICCFD10 in Barcelona Spain on 9-13 July 2018	[Scientific Community (higher education, Research)]	50
Federica Sacco (BSC) presented a poster on "Electrophysiology simulations of female and male human ventricles: influence of gender phenotype and endocardial anatomy on signal propagation" at the Biophysical Society meeting on "The Heart by Numbers: Integrating Theory, Computation and Experiment to Advance Cardiology" in Berlin Germany on 4-7 September 2018	[Scientific Community (higher education, Research)]	50
Federica Sacco (BSC) gave a talk on "The effect of gender and endocardial detail on anatomically normal human heart electrophysiology" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)]	200
Robin Richardson (UCL) presented a training course on "Application Simple magnetic drug targeting simulations with HemeLB" at the High Performance Computing for the Virtual Physiological Human (VPH) CompBioMed VPH2018 pre-course in Zaragoza Spain on 4 September 2018	[Scientific community (Research)]	20
Jenny Wang (Oxford) gave a talk on "Electrophysiological response of HCM myocardium to disopyramide " at the Gordon seminar on cardiac arrhythmias in Barga Italy on 30 March 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Hector Martinez (Oxford) gave a talk on "Human in-silico investigations into therapeutic strategies in acute myocardial ischemia" at the Gordon seminar on cardiac arrhythmias in Barga Italy on 5 April 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Jenny Wang, Hector Martinez, Alfonso Bueno-Orovio, Francesca Margara, Peter Marinov (Oxford) presented various CompBioMed posters at the Gordon conference on cardiac arrhythmias in Barga Italy on 30 March to 5 April 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	1,000
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Annual Public Lecture at the Department of Computer Science in Sheffield UK in June 2019	[Scientific Community (higher education, Research)]	30
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Machine Learning Meets Statistics Symposium in Cambridge UK in March 2019	[Scientific Community (higher education, Research)]	50
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the American Heart Association Scientific Sessions, Frontiers in Science Arrhythmia Research Summit in Chicago USA on 10 November 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Safety Pharmacology Society meeting in Barcelona Spain in September 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50

Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Meeting of the Italian Chapter of the European Society of Biomechanics in Bologna Italy in September 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Blanca Rodriguez (Oxford) gave an invited talk at the event "Computer Models and 3Rs of animals in research" in Germany on October, 2018.	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Blanca Rodriguez (Oxford) gave an invited talk at The 16th OXION Day on "Ion Channels and Diseases of Electrically Excitable Cells" in Oxford on 21 September 2018.	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Blanca Rodriguez (Oxford) gave an invited talk at "Frontiers of Simulation and Experimentation for Personalised Cardiovascular Management and Treatment conference" in London on 31 July 2018.	[Scientific Community (higher education, Research)]	100
Blanca Rodriguez (Oxford) gave an invited talk on "Computational Modeling of Cardiac Adverse Events" at the 2018 Gordon Research Conference on Drug Safety in Massachusetts USA on 10-15 June, 2018.	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Blanca Rodriguez (Oxford) gave a talk showcasing CompBioMed at the event "Accelerating Impact: how your research can make a difference?" at Oxford on 25 May 2018	[Scientific Community (higher education, Research)]	50
Blanca Rodriguez (Oxford) gave a talk on the role of Machine Learning and AI in biological research at "Can Computers Replace Humans in Biological Research?" in Oxford on 23 May 2018	[Scientific Community (higher education, Research)]	50
Elisa Passini (Oxford) gave a talk on "In silico human-based methodologies for evaluation of drug cardiac safety and efficacy" at the NC3R Cardiovascular Showcase in London on 23 March 2018.	[Scientific Community (higher education, Research)]	50
Hector Martinez-Navarro (Oxford) gave a talk on "HPC simulations for in-silico drug testing in humans: therapeutic strategies in acute myocardial ischemia" at the Biomedeng Conference in London UK on September 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Hector Martinez-Navarro (Oxford) gave a talk on "HPC simulations for in-silico drug testing in humans: therapeutic strategies in acute myocardial ischemia" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	200
Hector Martinez-Navarro (Oxford) gave an invited talk on "HPC simulations of cardiac electrophysiology as basis for human in-silico drug trials" at the EuroHPC Summit in Poznan Poland in May 2019	[Scientific Community (higher education, Research)],	100
Alfonso Bueno-Orovio (Oxford) gave an invited talk on "Cardiac imaging and the pharma industry" at the Biomedical Imaging Festival in Oxford UK in September 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Alfonso Bueno-Orovio (Oxford) gave an invited talk on "Computer modelling in thrombosis and heart disease" at Eurothrombosis in Barcelona Spain in October 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Alfonso Bueno-Orovio (Oxford) gave an invited talk on "Variability and cardiac arrhythmias: From drug action to acute coronary syndromes" at "Spiral waves and cardiac arrhythmias – connecting the clinic and mathematics" in Exeter UK in December 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Alfonso Bueno-Orovio (Oxford) gave an invited talk on "Realising the 3Rs in Safety Pharmacology by computational models of heart function: Always 5 years from now?" at 3Rs Research Day in Oxford UK in April 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Alfonso Bueno-Orovio (Oxford) will give an invited talk on "Data, AI and the android electrophysiologist: Machine learning for you, your patients and your job" at the 2019 Heart Rhythm Congress in Birmingham UK in October 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	100
Alfonso Bueno-Orovio (Oxford) presented a poster on "Computational methods for safety pharmacology and anti-arrhythmic drug discovery: Towards in silico clinical trials in human" at the "World congress of basic and clinical pharmacology" in Kyoto Japan in July 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	200
Alfonso Bueno-Orovio (Oxford) presented a poster on "Prediction of all form drug-induced cardiotoxicity by combining transcriptome analysis, structural data and machine learning" at the "World congress of basic and clinical pharmacology" in Kyoto Japan in July 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	200

Elisa Passini (Oxford) gave an invited talk on "Human in silico trials for evaluation of drug cardiac safety and efficacy" at the British Heart Foundation CRE Symposium in Oxford UK in September 2018	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
Elisa Passini (Oxford) gave an invited talk on "Can Human in Silico Drug Trials Replace the Need for Animal Studies?" at the British Toxicology Society Annual Meeting in Cambridge UK in April 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Xinshan Li (USFD) gave a talk on "A finite element investigation of the positioning of Arabin cerclage pessary in the prevention of spontaneous preterm birth" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Alberto Marzò (Sheffield) gave a talk on "Use of a Gaussian process emulator and 1D circulation model to characterize cardiovascular pathologies and guide clinical treatment" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Andrew Narracott (USFD) gave an invited talk on "Delivering the CT25 computational workflow directly to the clinic" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Phil Tooley (USFD) gave an invited talk on "Parallelising Image Registration and the HPC Porting Journey" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Vani Malyala (USFD) presented a poster on "Modelling of electrophysiology of the heart and treatment of Ventricular fibrillation" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Marco Viceconti (UNIBO) gave a talk on "Modelling bone at the tissue scale: the missing link between drug design and clinical outcome" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Gábor Zavodszky (UvA) gave a talk on "Multi-Scale Investigation of Cellular Flow Conditions at the Initial Stage of Thrombus Formation" at CMBE2019 in New York USA on 14-16 August 2019	[Scientific Community (higher education, Research)], [Industry]	300
Gábor Zavodszky (UvA) gave a talk on "Coupling scheme for a high-performance multiscale blood flow simulation workflow" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	200
Victor Azizi (UvA) gave a talk on "Optimizing performance of the blood flow simulation software hemocell" at ICCS2019 in Faro Portugal on 12-14 June 2019	scientific community	350
Gabor Zavodszky (UvA) presented a poster on "Transport properties of vWF proteins in blood with aneurysms" at WCB2018 in Dublin Ireland on 8 July 2018	[Scientific Community (higher education, Research)], [Industry]	400
Gabor Zavodszky (UvA) gave an invited talk on "How do Red Blood Cells and Platelets move in our Arteries? The circulatory system of the Virtual Human" at Super Day 2018 in Amsterdam Netherlands on 18 December 2018	[Scientific Community (higher education, Research)], [Industry]	150
Britt van Rooij (UvA) gave a talk on "High shear thrombosis: study the effect of shear rate on platelet aggregation and validation of a cell-based platelet aggregation model" at ISTH 2019 in Melbourne Australia on 11-15 July 2019	[Scientific Community (higher education, Research)], [Industry]	300
Britt van Rooij (UvA) gave a talk on "Platelet adhesion and aggregation: Cell-resolved simulations and In vitro experiments" at the CompBioMed Conference in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	300
Benjamin Czaja (UvA) gave a talk on "Simulation and experimental evidence for the decrease of platelet margination with an increase in volume fraction of stiffened red blood cells in flow" at the CompBioMed Conference 2019 in London UK on 25-27 September 2019	[Scientific Community (higher education, Research)], [Industry]	300
Benjamin Czaja (UvA) gave a talk on "The effect of mixing deformable and stiffened red blood cells in flow on hematocrit profiles and platelet margination" at CMBE2019 in Sendai Japan on 10 June 2019	[Scientific Community (higher education, Research)], [Industry]	300
Benjamin Czaja (UvA) gave a talk on "Pulsatile flow in 2D cell resolved blood flow simulations of curved vessels with aneurysms" at WCB2018 in Dublin Ireland on 8 July 2018	[Scientific Community (higher education, Research)], [Industry]	400

Benjamin Czaja (UvA) gave a talk on "Cell resolved simulations of saccular aneurysms: effects of pulsatility and aspect ratio" at VPH2018 in Zaragoza Spain on 5 September 2018	[Scientific Community (higher education, Research)], [Industry]	300
Dieter Kranzlmüller (LRZ) gave a talk on "Pushing personalized medicine with SuperMUC" at the 6th Munich Biomarker Conference in Munich on 30 November 2016. https://www.biom.org/fileadmin/user_upload/Veranstaltungen/2016/Biomarker_Conference/Dieter_KranzlmueLLer_LRZ.pdf	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller (LRZ) gave a talk on "Academic Supercomputing - More than just Theory" at Supercomputing 2016 in Utah on 15 November 2016	[Scientific Community (higher education, Research)], [Industry]	200
Enrico Gianluca Caiani (e-Cardiology Working Group at European Society of Cardiology) gave a talk mentioning CompBioMed at the ESC Congress in Barcelona on 26-30 August 2017 https://www.slideshare.net/EnricoGianlucaCaiani/esc-wg-on-ecardiology-2017-general-assembly	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) gave a talk on "The Virtual Human: In Silico Methods for Personalised Medicine" at the Digital Transformation Conference 2018 in Lebanon on 12-13 March 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) presented the Virtual Humans video at the event Think Science, held at the World Trade Center in Dubai on 16 April 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Medias]	400
Peter Coveney (UCL) presented the Virtual Humans video at the event Think Science, held at the World Trade Center in Dubai on 17 April 2018	[Industry], [Scientific Community (higher education, Research)], [General Public], [Medias]	400
Gianni De Fabritiis (UPF) gave a talk on "Simulations Meet Machine Learning in Computational Structural Biology and Drug Discovery" at the GPU Technology Conference in Munich Germany on 9-11 October 2018	[Scientific Community (higher education, Research)], [Industry]	100
Alfonso Santiago (BSC) presented CompBioMed at the Validation and Verification Conference 2019 in Las Vegas USA on 15-17 May 2019	[Scientific Community (higher education, Research)], [Industry]	100
ATOS promoted CompBioMed and showed the Virtual Humans video during a talk at ISUM (International Supercomputing Conference in Mexico) in Mexico on 26-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	50
ATOS promoted CompBioMed during a talk at ISUM (International Supercomputing Conference in Mexico) in Mexico on 26-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	30
Alfons Hoekstra (UvA) promoted CompBioMed during a talk at the 16th International Symposium on Computer Methods in Biomechanics and Biomedical Engineering in New York USA on 14-16 August 2019	[Scientific Community (higher education, Research)], [Industry]	50
BSC, Sheffield and Medtronic showed the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" at LINCC 2019 in Paris France on 3-5 June 2019	[Clinicians], [Industry]	400
Medtronic showed the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" at ESMINT Congress 2019 in Nice France on 4 September 2019	[Clinicians], [Industry], [Scientific Community (higher education, Research)]	200
Robin Richardson (UCL) gave a talk on "An automated pipeline for real time visualisation of blood flow during treatment of intracranial aneurysms" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
David Wright (UCL) gave a talk on "Combining molecular simulation and machine learning to INSPIRE improved cancer therapy" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Jon McCullough (UCL) gave a talk on "Developments for the Efficient Self-coupling of HemeLB" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney (UCL) gave a talk on "Quantum AI to the Virtual Human; where's the virtual human?" at the CompBioMed Conference on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200

David Wright (UCL) gave a talk on "Entropy estimation methods in ensemble end-point binding free energy simulations" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Katya Ahmad (UCL) gave a talk on "Accurate and Precise Predictions of the Influence of Salt Concentration on the Conformational Stability and Membrane-Binding Modes of Multifunctional DNA Nanopores using Ensemble-Based Coarse-Grained Molecular Dynamics" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Andrew Potterton (UCL) gave a talk on "An Ensemble-Based SMD Workflow that Predicts the Residence Time of A2A Receptor Ligands" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Mariano Vazquez (BSC) gave a talk on "ELEM Biotech – The Virtual Humans Factory" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Andrea Townsend-Nicholson (UCL) gave a talk on "Reflections on educating and engaging new communities of practice with high performance computing through the integration of teaching and research" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Alexander Gheorghiu (UCL) gave a talk on "The influence of base pair tautomerism on single point mutations in aqueous DNA" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Terry Sloan (EPCC) gave a talk on "The HemeLB Offloader" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Jazmin Aguado-Sierra (BSC) gave a talk on "The effect of gender and endocardial detail on anatomically normal human heart electrophysiology" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Fouad Hussein (UCL) gave a talk on "Simulation and experimental evidence for the decrease of platelet margination with an increase of stiffened red blood cells in flow" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Guillermo Marin (BSC) gave a talk on "Animating the Virtual Human: Applying movie-industry tools and techniques to data visualization" at the CompBioMed Conference 2019 in London on 25-27 September 2019	[Clinicians], [Scientific Community (higher education, Research)], [Industry]	200
Alessandro Melis (USFD) gave a talk on "Improved diagnosis of cerebral vasospasm through a sensitivity analysis of a 1D cerebral circulation model" at the World Congress of Biomechanics in Dublin Ireland on 8-12 July 2018	[Policy Makers], [Industry], [Scientific Community (higher education, Research)]	100
Zainab Altai (USFD) gave a talk on "Investigating a possible mechanism of humeral fracture in non-ambulant children" at the World Congress of Biomechanics in Dublin Ireland on 8-12 July 2018	[Policy Makers], [Industry], [Scientific Community (higher education, Research)]	100
Francesc Levrero-Florencio (UOXF) gave a talk on "Effect of Fibre and Sheetlet Distribution on Physiological Models for Heart Contraction" at the World Congress in Computational Mechanics 2018 in New York USA on 22-27 July 2018	[Policy Makers], [Industry], [Scientific Community (higher education, Research)]	100
Peter Coveney (UCL) gave a talk on "Scalability of Computational Medicine applications within CompBioMed" at the VPH2018 Conference in Zaragoza Spain on 5-7 September 2018	[Scientific Community (higher education, Research)], [Industry]	100
Blanca Rodriguez (Oxford) gave a talk on "Human In Silico Drug Trials with Multiscale Models of the Heart" at the VPH2018 Conference in Zaragoza Spain on 5-7 September 2018	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney (UCL) gave a talk on "Verification, validation and uncertainty quantification: the role of force fields" at the Daresbury Lab Workshop "Forcefields: Status, challenges & vision" on 28 January 2019	[Scientific Community (higher education, Research)]	20
Peter Coveney (UCL) gave a talk on "Accurate, precise and reliable predictions from modelling and simulation using high performance computers?" at the EMMC expert meeting on the Verification and Validation of computational models, Manchester, UK, on 17 January 2019	[Scientific Community (higher education, Research)]	30

Peter Coveney (UCL) gave a talk on "Computer Science and Healthcare" at the 11th Siemens Technology and Innovation Council meeting in Washington D.C. on 10 December 2018	[Scientific Community (higher education, Research)], [Industry]	30
Hugh Martin (CBK) gave a talk on CompBioMed at the FocusCoE Kick Off meeting in Frankfurt Germany on 20-21 February 2019	[Scientific Community (higher education, Research)]	50
Peter Coveney gave a talk on "High throughput binding affinity predictions enabled through heterogeneous workflows at the emerging exascale" at the workshop on "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications" in the Netherlands on 28-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	20
Joao Damas (Accellera) gave a talk on "Containerization for Reproducible Deployment of Biomedical Applications and Workflows in Diverse Computing Infrastructures" at the workshop on "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications" in the Netherlands on 28-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	20
Mariano Vasquez gave a talk at the workshop on "Container Technologies in Cloud and High Performance Computing Research and Commercial Applications" in the Netherlands on 28-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	20
Peter Coveney (UCL) gave a talk on "Personalised medicine" at the event "Simulation-based Science for Health" in Amsterdam on 12-14 September 2019	[Scientific Community (higher education, Research)], [Industry]	30
Stefan Doerr (UPF) and José Jimenez (UPF) presented a poster on "ACEMD-ai: Ab-initio machine learning calculations of small molecules quantum energies and forces" at the 2018 Workshop on Free Energy Methods, Kinetics and MSMs in Drug Design in Boston USA on 14-18 May 2018	[Scientific Community (higher education, Research)]	30
Stefan Doerr (UPF) and José Jimenez (UPF) presented a poster on "Deep Learning based protein-ligand relative affinity prediction" at the 2018 Workshop on Free Energy Methods, Kinetics and MSMs in Drug Design in Boston USA on 14-18 May 2018	[Scientific Community (higher education, Research)]	50
Joao Damas (Accellera) gave a talk on "Reproducible Deployment in Diverse Computing Infrastructures" at the CompBioMed Containerisation Meeting in Amsterdam Netherlands on 28-29 May 2019	[Scientific Community (higher education, Research)], [Industry]	20
Joao Damas (Accellera) gave a talk on "PlayMolecule: bridging the gap between researchers and biomedical applications in diverse computing" at the CompBioMed All-Hands Meeting 2019 in Oxford UK on 29-30 April 2019	[Scientific Community (higher education, Research)], [Industry]	30
Natalia Jimenez (ATOS) gave a Keynote Presentation on "Big Data and Artificial Intelligence in the Development of Vaccines" at the GSK Innovation Workshop in Brussels Belgium on 5 December 2018	[Industry]	40
Alfonso Santiago (BSC) gave a talk promoting CompBioMed at the Integratead heat workshop in Bad Herrenalb Germany on 15-17 May 2019	[Scientific Community (higher education, Research)]	40
David Wright (UCL) presented, planned and coded for the INSPIRE project hackathon, which took place in New York USA on 11-15 February 2019	[Scientific Community (higher education, Research)]	10
Gavin Pringle (EPCC) showed the Virtual Humans film at the Latin American Introductory School on Parallel Programming and Parallel Architecture for High Performance Computing in Mexico on 12-23 Feb 2018	Scientific Community (research)	60
Herman van Vlijmen (Janssen) gave a talk on "Predicting Activity Cliffs with Free-Energy Perturbation" at the CompBioMed All Hands Meeting in Oxford UK on 29 April 2019	[Scientific Community (higher education, Research)], [Industry]	30
Herman van Vlijmen (Janssen) gave a talk on "Utility of simulation methods from an industry perspective" at the UK QSAR meeting in Cambridge UK on 4 April 2019. http://ukqsar.org/index.php/2019/01/10/ukqsar-spring-2019-cambridge/	[Scientific Community (higher education, Research)], [Industry]	50
Herman van Vlijmen (Janssen) gave a talk on "Prediction of Activity Cliffs Using FEP+ and Gromacs FEP" at the BioExcel Alchemical Free Energy Workshop in Göttingen Germany on 27-28 May 2019. http://pmx.mpibpc.mpg.de/workshop_alchemistry2019/index.html	[Scientific Community (higher education, Research)], [Industry]	30
Robin Richardson (UCL) gave a talk on "Development of HemeLB and adaptation to the clinic" at the UKCOMES HemeLB Meeting in London UK on 29 May 2019	[Scientific Community (higher education, Research)]	30

Robin Richardson (UCL) gave a talk on "Performance optimization and multiscale modelling with HemeLB" at the Royal Society in London UK on 6 November 2018	[Scientific Community (higher education, Research)]	30
Robin Richardson (UCL) gave a talk on "Multiscale Modelling for Cerebral Blood Flow" at the Lorentz Center Workshop on Multiscale Modelling in Leiden Netherlands on 16-18 April 2018	[Scientific Community (higher education, Research)]	30
Robin Richardson (UCL) gave a lecture and demo on "Simple magnetic drug targeting simulations with HemeLB" at an MPI training course on 4 September 2018	[Scientific Community (higher education, Research)]	30
Robin Richardson (UCL) gave a demonstration of the Binding Affinity Calculator at the European HPC Summit Week 2018 in Ljubljana Slovenia on 28 May 2018	[Scientific Community (higher education, Research)], [Industry]	15
Blanca Rodriguez (Oxford) gave an invited seminar on "Human In Silico Trials in Pharmacology and Cardiology" during an Invited seminar at the Department of Biomedical Engineering at King's College London in London UK in May 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Virtual Physiological Human Summer School in Barcelona Spain in June 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Blanca Rodriguez (Oxford) gave an invited talk on "Human In Silico Trials in Pharmacology and Cardiology" at the Joint Research Centre Summer School in Alternative Approaches to Animal Testing in Ispra Italy in June 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Elisa Passini (Oxford) gave a Computer Science Masterclass on "Computing meets Biology" at a Computer Science Masterclass at The Royal Institution in London UK in June 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
Gabor Zavodszky (UvA) gave an invited talk on "How do Red Blood Cells and Platelets move in our Arteries? The circulatory system of the Virtual Human" at JMBC 2019 in Delft Netherlands on 17 May 2019	[Scientific Community (higher education, Research)], [Industry]	50
Gabor Zavodszky (UvA) gave an invited talk on "The virtual artery - A multiscale model for vascular pathophysiology" at the MultiScale Workshop in the Lorentz Center in Leiden Netherlands on 16-20 April 2018	[Scientific Community (higher education, Research)], [Industry]	50
Ruth Aris (BSC) gave a talk on "HPC computational modeling on supercomputers: Biomedical applications and the CompBioMed project" at HelloAI Summer School in Barcelona on 18-21 June 2018	[Scientific Community (higher education, Research)]	30
Peter Coveney (UCL) showed the CompBioMed "Virtual Humans" film at the LRZ event "Next-Gen HPC - The Path to Exascale: Artificial Intelligence & Personalized Medicine" in Garching on 29-30 June 2018	[Scientific Community (higher education, Research)]	30
ATOS promoted CompBioMed during a GSK Innovation Workshop in Brussels on 5 December 2018	[Industry]	40
Natalia Jimenez (ATOS) gave a talk on "Challenges and opportunities in Life Sciences" at the ELIXIR Bioinformatics Suppliers Forum in London on 7 May 2019	[Scientific Community (higher education, Research)], [Industry]	30
Janssen and Acellera sponsored the 2018 Workshop on "Free Energy Methods, Kinetics and Markov State Models in Drug Design" in Boston USA on 14-18 May 2018	[Scientific Community (higher education, Research)], [Industry]	30
Gavin Pringle (EPCC) gave a talk on CompBioMed at the PRACE CoE FET-HPC EXDCI Workshop in Brühl Germany on 30 October 2018	[Scientific Community (higher education, Research)]	30
Emily Lumley (UCL) gave a talk on CompBioMed Dissemination, Training and Links with Industry, discussing the Virtual Humans Video at the PRACE CoE FET-HPC EXDCI Workshop in Brühl Germany on 30 October 2018	[Scientific Community (higher education, Research)]	30
Alexander Patronis (UCL) gave a talk on "Preparing Initialisation for Extreme-scale Simulation" at the "HemeLB: cardiovascular modelling and simulation in UKCOMES" Workshop in London UK on 29-30 May 2019	[Scientific Community (higher education, Research)]	30
Jon McCullough (UCL) gave a talk on "Self-coupling of HemeLB: Recent developments towards simultaneous arterial-venous modelling" at the "HemeLB: cardiovascular modelling and simulation in UKCOMES" Workshop in London UK on 29-30 May 2019	[Scientific Community (higher education, Research)]	30
Alfons Hoekstra, UvA, gave an Invited lecture on "Multiscale Modelling in Vascular (patho)physiology" at a CWI Scientific Computing Seminar	[Scientific Community (higher education, Research)]	20

Peter Coveney (UCL) met with representatives at the Istituto Italiano di Tecnologia (including the Computational mOdeling of NanosCaE and bioPhysical sysTems lab) in Genova Italy to discuss CompBioMed on 18 July 2018	[Scientific Community (higher education, Research)]	10
Peter Coveney (UCL) and Dieter Kranzlmüller (LRZ) met with Dr Christiane Druml at the Josephinum in Austria to discuss CompBioMed and potential collaborations on 23 October 2018	[General Public], [Other]	3
Peter Coveney (UCL) sat on the Scientific Advisory Board for the BioExcel CoE, including for the BioExcel AHM on 20-21 November 2018	[Scientific Community (higher education, Research)]	30
Peter Coveney (UCL) gave a talk on "Personalised medicine in drug discovery and treatment" at the Newton Dinner for the elite of the Science Museum's donors on 12 February 2019	[General Public], [Medias], [Investors]	100
Andrea Townsend-Nicholson (UCL) and Clint Davies-Taylor (Dassault Systèmes) gave presentations at "Sense About Science's Evidence Week at Parliament 2019" at the UK House of Parliament, Upper Waiting Hall on 26 June 2019	[Policy makers], [Medias], [General Public]	50
Andrea Townsend-Nicholson (UCL) gave a talk at "UCL Biochemistry Open Day Research Talks" in London UK on 28-29 June 2019	[General Public]	700
Xavier Vigouroux (ATOS) was a speaker at the Birds of a Feather BOF on "The Computational Biomedicine Community and the HPC Industry: working together to advance personalised medicine" at ISC 2018 in Frankfurt Germany on 27 June 2018	[Industry], [Scientific Community (higher education, Research)], [General Public]	40
Cyril Mazauric (ATOS) was a speaker at the Birds of a Feather BOF on "Personalised medicine and the HPC industry" at ISC 2019 in Frankfurt Germany on 19 June 2019	[Industry], [Scientific Community (higher education, Research)], [General Public]	40
Cyril Mazauric (ATOS) and Natalia Jimenez (ATOS) gave a technical talk at the Atos Scientific Community Meeting in Paris France on 19-20 February 2019	[Industry]	120
Natalia Jimenez (ATOS) gave an Industry Talk on "Challenges and opportunities in Life Sciences" at the Elixir Bioinformatics Supplier Forum in London UK on 7 May 2019	[Industry]	50
Jazmin Aguado-Sierra (BSC) gave a seminar on "Computers Simulating the heart: How close are we to recreating physiology?" at the Cardiovascular Seminar Series, Division of Cardiovascular Sciences, University of Manchester in Manchester UK on 2 May 2019	[Scientific Community (higher education, Research)]	25
Jazmin Aguado-Sierra (BSC) gave a talk on "HPC Cardiovascular Simulations using Alya Red: Cardiac Resynchronisation Therapy (Preliminary Results)" at the CompBioMed AHM 2019 in Oxford UK on 29-30 April 2019	[Scientific Community (higher education, Research)]	30
Alfonso Santiago (BSC) was a panel member on "Democratizing HPC & AI, Startups Scale up with Cloud Native" at Kubecon in Barcelona Spain on 20-23 May 2019	[Scientific Community (higher education, Research)], [Industry]	150
Alfonso Santiago (BSC) gave a talk on "A verification and validation process for a fluid-electro-mechanical model of the human heart" at the VECMA AHM in Amsterdam Netherlands on 9-10 May 2019	[Scientific Community (higher education, Research)]	30
Marco Verdicchio (SURFsara) gave a presentation on "Personalised Medicine & the HPC industry" at ISC 2019 in Frankfurt Germany on 21-25 June 2019	[Scientific Community (higher education, Research)], [Industry]	25
Elisa Passini (Oxford) gave a Webinar on "Human in silico drug trials to provide digital evidence on pro-arrhythmic cardiotoxicity" at the US National Academies of Sciences, Engineering and Medicine in Washington DC USA in May 2019	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	30
The Virtual Humans film was presented by Alfons Hoekstra (UvA) during the event "Bessensap" in the Netherlands on 15 June 2018	[Medias], [Scientific Community (higher education, Research)]	400
Marco Viceconti (USFD) gave a talk on "Do virtual patients see electric Doctors?" to patients and carers at the public launch of the Sheffield NIHR Biomedical Research Centre in neurodegenerative Disease on 14 Dec 2017. http://sheffieldbrc.nihr.ac.uk/public-launch-event/	[Clinicians], [General Public]	100
Marco Viceconti (USFD) showed the Virtual Humans film in a talk during the Insigneo Showcase on 3 May 2018. https://insigneo.org/event/insigneo-showcase-2018/	[Clinicians], [Policy makers], [Investors], [Scientific Community (higher education, Research)]	300

Oxford ran several sessions on computer simulations during Cardiology meetings as part of the European Society of Cardiology Working Group in e-cardiology with Enrico Gianluca Caiati. This included a session on "The future of computer modelling in heart disease" given by Blanca Rodriguez at ESC Congress 26-30 August 2017	[Scientific Community (higher education, Research)], [Medical Students], [Clinicians]	50
EPCC showed the Virtual Humans film at the Bayes Centre VIP launch at the University of Edinburgh in Edinburgh UK on 10 October 2018	[Policy makers], [Investors], [Scientific Community (higher education, Research)]	50
LifeTec Group presented a poster about AngioSupport at the Materials Technology (MaTe) Institute on 13 December 2018	[Scientific Community (higher education, Research)]	20
Jazmin Aguado (BSC) presented the Virtual Humans video and distributed CompBioMed flyers at the Cardiovascular Seminar Series at the Division of Cardiovascular Sciences, University of Manchester in Manchester UK on 2nd May 2019	[Scientific Community (higher education, Research)]	30
ATOS promoted CompBioMed during an ATOS Scientific Community Meeting in Paris France on 19-20 February 2019	[Scientific Community (higher education, Research)], [Industry]	50
ATOS promoted CompBioMed during a ATOS Tech Days in Paris France, which was also transmitted as a webinar on 16-17 May 2019	[Scientific Community (higher education, Research)], [Industry]	60
Alfons Hoekstra (UvA) and Peter Coveney (UCL) gave a lecture and debate on "Your digital twin: closer than you think" at the UvA University Day. https://alumni.uva.nl/en/services/university-day/en-your-digital-twin.html	[General Public]	100
Alfons Hoekstra (UvA) gave a talk on "The virtual artery, a multiscale model for vascular physiology – progress and examples" at the 5th International Conference on Computational & Mathematical Biomedical Engineering (CMBE17) in Pittsburgh USA on 10-12 April 2017	[Scientific Community (higher education, Research)], [Industry]	100
Alberto Marzo and Ana Paula Narata (USFD) presented the video "Pipeline Embolization Device: Visualization of the blood flow on an aneurysm" at LINCC2019 in The Louvre Paris in June 2019	[Clinicians], [Medical Students], [Industry], [Scientific Community (higher education, Research)]	400
Sauro Succi showed the Virtual Humans film at the event "Master in HPC" at the International Centre for Theoretical Physics in Trieste Italy on 14 Feb 2019	[Scientific Community (higher education, Research)]	30

9.8 Other

Description of Activity	Audience(s) (see above table)	No. of People
Gavin Pringle (EPCC) publicised the CompBioMed Conference to all Archer users in 6 mailings in the ARCHER News and Training Opportunities mailing list and news page on 16 April to 21 May 2019. http://www.archer.ac.uk/about-archer/news-events/	[Scientific Community (higher education, Research)]	48,000
EPCC listed CompBioMed2 details in UoE's College Research Committee report on 17 May 2019	[Scientific Community (higher education, Research)]	50
Bettine van Willigen and Tim van den Boom (LifeTec Group) demoed AngioSupport for the Amsterdam Medical Center in Amsterdam Netherlands on 4 April 2019	[Clinicians]	6
Bettine van Willigen and Tim van den Boom (LifeTec Group) demoed AngioSupport for the Catharina Hospital Eindhoven in Eindhoven Netherlands on 23 May 2019	[Clinicians], [Medical Students]	15
Elisa Passini (Oxford) gave a live interview for the Matthew Wright Show on talkRADIO on 14 June 2019	[General Public], [Medias]	30,000
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to the Director - Institute for Computational Biomedicine, Weill Cornell Medical College, and Englander Institute for Precision Medicine in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	2

Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Chief Business Officer - New York Genome Center in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Managing Director - Biolabs in New York USA in September 2018	[Industry]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Executive Director - Institute of Computational Medicine, NYU Langone Health in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Academic Partnerships - Broad Institute of Harvard and MIT in Boston USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Chief Operating Officer - CIMIT Boston in Boston USA in September 2018	[Industry]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Manager - Cambridge Innovation Center in Boston USA in September 2018	[Industry]	2
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Associate Director (Research) - Massachusetts General Hospital Center for Computational and Integrative Biology, Harvard University in New York USA in September 2018	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) gave an Introductory Presentation of CompBioMed and an Invitation to join CompBioMed as Associate Partner, to Director R&D - Mitra Biotech in Boston USA in September 2018	[Industry]	3
Paul Best (CBK) participated in the Technical Meeting on Coordinator Models, Inference Algorithms Group at the Broad Institute of Harvard and MIT in USA in April 2019	[Scientific Community (higher education, Research)] [Clinicians]	1
Paul Best (CBK) participated at a Guest Lecture on "Machine Learning Strategies in the Genome and the Phenome – Toward a Better Understanding of Complex Traits" at "Five Points Lecture Series, New York Genome Center" in New York USA in September 2018	[Scientific Community (higher education, Research)], [Clinicians], [Industry]	50
Gavin Pringle (EPCC) showed the Virtual Humans video during the two 'HPC for Medics' course in London on 7th Dec 2017	[Medical Students], [Clinicians]	20
Gavin Pringle (EPCC) showed the Virtual Humans video during the two 'HPC for Medics' course in London on 8th Dec 2017	[Medical Students], [Clinicians]	20
Gavin Pringle (EPCC) showed the Virtual Humans video during the 'HPC for Bioscientist' in London on 7th March 2018	[Scientific Community (higher education, Research)]	20
USFD regularly speak to the the clinical researchers that are embedded in the Insigneo institute, who then talk at clinical conferences about the use of in silico medicine.	[Clinicians]	20
CompBioMed featured in the elnraCentral press release sent around by email on "Seven new Service Providers join elnraCentral service catalogue" on 19 November 2018	[Scientific Community (higher education, Research)], [Industry]	100
Alfons Hoekstra (Uva) presented the Virtual Humans film to pupils aged 16/17 in 3 schools in Amsterdam on 3 November 2018	[General Public]	90
Sauro Succi showed the Virtual Humans film at three schools around Italy in 2018 and 2019	[General Public]	100
Alberto Marzo (USFD) presented the Virtual Humans film to 15 Year 4 undergraduate students in Mechanical Engineering at the University of Sheffield on 1 February 2018	[Scientific Community (higher education, Research)]	15
Alberto Marzo (USFD) presented the Virtual Humans film to 100 Year 1 undergraduate students in Bioengineering at the University of Sheffield on 1 November 2018	[Scientific Community (higher education, Research)]	100
Alberto Marzo (USFD) presented the Virtual Humans film to 15 Year 4 undergraduate students in Mechanical Engineering at the University of Sheffield on 1 February 2019	[Scientific Community (higher education, Research)]	15

ATOS promoted CompBioMed during an ATOS Tech Talk Webinar on 3 October 2018	[Industry]	60
ATOS promoted CompBioMed during a People in Motion Webinar on 11 October 2018	[Industry]	70
ATOS promoted CompBioMed during a roundtable discussion at ISUM (International Supercomputing Conference in Mexico) in Mexico on 26-29 March 2019	[Scientific Community (higher education, Research)], [Industry]	30
SkeleDock & Kdeep on the CompBioMed Playmolecule platform won the Drug Design Data Resource (D3R) Grand Challenge 4 - an annual, international competition which offers several tasks considered to be of great pharmaceutical interest, on 4 April 2019	[Scientific Community (higher education, Research)], [Industry]	50
Elisa Passini (Oxford) won the International 3Rs Prize for computer modelling that predicts human cardiac safety better than animal studies, on 12 March 2018	[Scientific Community (higher education, Research)], [Industry]	50
UCL won the 11th IEEE International Scalable Computing Challenge (SCALE 2018) at the IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing (CCGrid) 2018 held in Washington DC, on 1-4 May 2018	[Scientific Community (higher education, Research)], [Industry]	200
A paper by Alfons Hoekstra (UvA) and Gábor Závodszy (UvA) on "Red blood cell and platelet diffusivity and margination in the presence of cross-stream gradients in blood flows" was awarded the cover image in Physics of Fluids on 12 March 2019	[Scientific Community (higher education, Research)], [Industry]	200
Emily Lumley (UCL) produced and distributed 4 editions of the printed CompBioMed Newsletter	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	400
Emily Lumley (UCL) produced and distributed 8 editions of the CompBioMed e-Newsletter	[Scientific Community (higher education, Research)], [Industry]	800
USFD wrote about CompBioMed's involvement at Evidence Week at Parliament in Insigneo's Newsletter in June 2019.	[Scientific Community (higher education, Research)], [Industry]	140
BAC, EnsembleMD, and CBK were mentioned in the "Hartree Centre Phase 1 & 2 Baseline Evaluation" Report on 1 October 2018, aimed at the UK Government to demonstrate the value and contribution of Hartree expertise has on UK research and innovation.	[Policy makers]	50
Bettine van Willigen and Tim van den Boom (LifeTec Group) won first prize for their poster on "Clinical decision tool: AngioSupport" at the BME research day in Eindhoven Netherlands on 2 April 2019.	[Scientific Community (higher education, Research)]	100