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CO	Confidential, only for members of the consortium (including the Commission Services)	
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1 Version Log

Version	Date	Released by	Nature of Change
V0.1	08/10/2021	Hugh Martin	First Draft
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2 Contributors

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3 Definition and Acronyms

Acronyms	Definitions
BSC	Barcelona Supercomputing Centre
CBMC19	CompBioMed Conference 2019
CBMC21	CompBioMed Conference 2021
CoE	Centre of Excellence
cPPP	Contractual Public Private Partnership
CPU	Core Processing Unit
CT2S	Computerised Tomography to Strength
CWI	Centrum Wiskunde & Informatika
DICE	Data Infrastructure Capacity for EOSC
DXA	Dual-energy X-ray Absorptiometry

EOSC	European Open Science Cloud
EsD	Exascale Demonstrators
EU	European Union
EU	European Union
FAQ	Frequently Asked Questions
HPC	High Performance Computing
HTC	High Throughput Computing
IP	Intellectual Property
ISW	In Silico World
JCIM	Journal of Chemical Information and Modelling
JCTC	Journal of Chemical Theory and Computation
KPI	Key Performance Indicator
LEXIS	Large-scale Execution for Industry and Society
LRZ	Leibniz Supercomputing Centre
MPI	Message Passing Interface
SME	Small and Medium Enterprise
UCL	University College London
UNIBO	University of Bologna
UQ	Uncertainty Quantification
USA	Unites States of America
USFD	University of Sheffield
UvA	University of Amsterdam
WHO	World Health Organisation
WP	Work Package

4 Public Summary

This deliverable, D1.5 “Report on Dissemination and Innovation”, is a report on dissemination and innovation activities produced by the CompBioMed Centre Excellence between the start of the second phase (1 October 2019) and the 25th month (30 October 2021) of its second phase.

5 Introduction

Computational methods, based on human biology, are reaching maturity in the biomedical domain, rendering predictive models of health and disease increasingly relevant to clinical practice by providing a personalised aspect to treatment. 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.

Dissemination and outreach have played a major and crucial role in the first 25 months of CompBioMed2 and will continue to do so. We have promoted the Centre of Excellence’s (CoEs) outcomes (publications, codes, education & training, best practices, events, activities) to stakeholders, in particular targeting our four major stakeholder groupings: academia, industry, clinical/medical, and the general public.

This deliverable describes our extensive dissemination activities in the first 25 months of CompBioMed2, reaching massive numbers of people, far beyond what this CoE has been able to achieve prior to this period. During a particularly challenging time due to the global coronavirus pandemic, our dissemination activities were adjusted to fit the moment. This allowed CompBioMed2 to take advantage of unique dissemination opportunities, leading to far-reaching dissemination which is demonstrated by the statistics of our outreach in this period.

Training and engagement are substantial aspects of the Centre’s overall dissemination activities. However, those two specific aspects are dealt with in WP6 and will not be reported here. For training and engagement activities in this period, please refer to D6.3 “Final Report on Engagement”, and D6.5 “Final Report on Training Activities” which will be published in M44 (May 2023) and M46 (July 2023) respectively.

CompBioMed2 has produced and will continue to produce innovations that require innovation management. This deliverable describes the work and framework in monitoring, capturing, and guiding new and existing innovations during the first 25 months of the project.

Incubation activities are a key part of innovation management; however, these are dealt with in WP5. For incubation activities in this period, please refer to D5.2 “Advanced Report on Biomedical Applications” which will be published in M26 (November 2021) of the project.

6 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 first 25 months of CompBioMed2, the consortium produced a substantial 281 separate dissemination activities. These activities include:

- 112 Peer-Reviewed Publications
- 130 CompBioMed YouTube Videos
- 523 Tweets
- 77 LinkedIn posts
- 8 Events organised
- 151 Participations at events
- 4 Booths

along with additional activities, as described throughout this section. In this section, we describe our dissemination campaign in the first 25 months of the project.

6.1 Impact of the Coronavirus Pandemic on Dissemination Activities

The coronavirus pandemic, which started in early 2020, has been met with sweeping non-pharmaceutical interventions, colloquially known as lockdowns (encompassing stay-at-home orders, curfews, quarantines, cordons sanitaires and similar societal restrictions). This has obviously had substantial impact on the dissemination activities of a scientific research centre of excellence, affecting 19 of the first 25 months of CompBioMed2. Any dissemination activities involving person-to-person interactions in the same space have largely been wiped out, instead placing a heavy emphasis on online, TV, and Radio activities, in particular, online activities.

While there were substantial plans for in-person events during CompBioMed2 (see Section 6.4.1), it was found that most were possible to convert to an online format, including the second edition of the CompBioMed Conference. The result is that talks, posters, booths, workshops, and conferences continued to take place during the pandemic, but in virtual formats.

Virtual events comprise a significant amount of the activities described in this deliverable, these introduce both positives and negatives.

On the negative side, the loss of person-to-person interactions in the same location has reduced the amount of discussion and connections made during events. The virtual format does not lend itself well to discussion, neither during allocated discussion segments, nor informally between sessions. There are ways to try to regain these interactions, as we attempted for CompBioMed Conference 21 (CBMC21, see Section 6.4.1), but they can never be fully regained.

Additionally, there is a notable drop in engagement from participants in virtual events. Naturally, attendees can fit competing virtual commitments in and around the virtual events, and frequently do so. Without being at the location of the event for the duration of it, participants can drop in and out of events at will, leading to many of them only tuning in for specific parts that they are most interested in. Furthermore, even when tuned in they are free to pay as much or as little attention as they choose. There are methods to improve engagement, as we attempted with CBMC21, but again it is not possible to reach the engagement levels of in-person events.



On the positive side, it is very easy to attend virtual events; there is no need for international travel, no need to clear multiple days in one's diary, and there is no or little cost in attending. In the early days of lockdown, we and others noted a rise in attendance at virtual events compared to what was anticipated (at the peak, upwards of 4-fold higher than expectations), likely due to the aforementioned reasons. However, in the more recent days of the pandemic, attendance numbers at virtual events have waned from their peak, perhaps due to a decreasing appetite for events in such a format. Nonetheless, it continued to be possible to get healthy attendance at virtual events.

In general, a major opportunity that CompBioMed2 was able to take full advantage of was the fervent media and general public interest in coronavirus related research. Being a biomedical project with several strands of research related to tackling the pandemic, we were able to capture the attention of some enormous television, print, and online media companies. The result is that we were able to reach tens of millions more people with our dissemination activities while the interest was at its peak. Interest in coronavirus research has waned somewhat since the early months of the pandemic, but it still remains high and is something that we plan to continue to take advantage of moving forward.

6.2 Dissemination Materials

In this section, we describe the dissemination materials that were produced and/or harnessed in the first half of the project. The strategy shows a wide-reaching approach to peer reviewed publications that target Academia, Industry, and the Clinic, while popularised publications target the General Public in addition to those same groups. Our video content has gained attention, with a fast building YouTube following keen on our content such as recorded talks/webinars, as well as our continuing dissemination campaign surrounding the Virtual Humans film produced in CompBioMed1. Meanwhile, our newsletters, posters, and other materials have kept a steady flow of dissemination into the world throughout the first 25 months of the project.

6.2.1 Publications

In this section we summarise peer-reviewed popularised publication outputs

Peer Reviewed Publications

The CompBioMed CoE has published 112 peer-reviewed publications since the start of CompBioMed2 (see deliverable D3.6 from CompBioMed1 for publications prior). These are listed in Appendix 10.1, and are also listed on the CompBioMed website along with summaries of each paper¹. The summaries help visitors from all backgrounds to understand the work being done in CompBioMed.

In the first 25 months of CompBioMed2, we achieved an output of 4.5 publications per month on average, which continues the excellent publication output seen in the second half of CompBioMed1 (4.6 publications per month on average). This high level of output contrasts greatly to the output in the first half of CompBioMed1, which was 1.3 publications per month. This demonstrates a clear and substantial benefit to CompBioMed2 being the second phase of a project, rather than being a project that is starting from scratch, allowing the project to hit the ground running from the off.

The publications have been impactful, as shown in Table 1 below, there are 6 notable papers that have achieved high Altmetric scores. Altmetric assigns a score based on instances of the publication in question

¹ <https://www.compbiomed.eu/media-social/publications-2/>



appearing in news articles, blog posts, Wikipedia, social media, and so on. Once scores are in the 20's and above, they are in the top 5% of all publications tracked by Altmetric, so the figures in the table represent substantial traction and interest in these papers.

Table 1: CompBioMed2 publications with high Altmetric scores

No.	Publication Title	Citation	Altmetric
1	Coarse graining molecular dynamics with graph neural networks	B. E. Husic, N. E. Charron, D. Lemm, J. Wang, A. Pérez, M. Majewski, A. Krämer, Y. Chen, S. Olsson, G. de Fabritiis, F. Noé and Cecilia Clementi, J. Chem. Phys. 153, 194101 (2020), DOI: 10.1063/5.0026133	36
2	Dual Transcriptomic and Molecular Machine Learning Predicts all Major Clinical Forms of Drug Cardiotoxicity	Polina Mamoshina, Alfonso Bueno-Orovio, and Blanca Rodriguez, Front Pharmacol., 11: 639 (2020) DOI: 10.3389/fphar.2020.00639	45
3	The Impact of Uncertainty on Predictions of the CovidSim Epidemiological Code	W. Edeling, H. Arabnejad, R. Sinclair, D. Suleimenova, K. Gopalakrishnan, B. Bosak, D. Groen, I. Mahmood, D. Crommelin and P. Coveney, Nat Comput Sci, 1, 128–135 (2021), DOI: 10.1038/s43588-021-00028-9	52
4	TorchMD: A Deep Learning Framework for Molecular Simulations	S. Doerr, M. Majewski, A. Pérez, A. Krämer, C. Clementi, F. Noe, T. Giorgino, and G. De Fabritiis, J. Chem. Theory Comput., 17, 4, 2355–2363 (2021), DOI: 10.1021/acs.jctc.0c01343	59
5	A Deep Learning Pipeline to Automate High-Resolution Arterial Segmentation with or without Intravenous Contrast	Chandrashekar, Anirudh, Ashok Handa, Natesh Shivakumar, Pierfrancesco Lapolla, Raman Uberoi, Vicente Grau, and Regent Lee, Annals of Surgery, (2020), DOI:10.1097/SLA.0000000000004595	152
6	The 'Digital Twin' to enable the vision of precision cardiology	Corral-Acero J, Margara F, Marciniak M, Rodero C, Loncaric F, Feng Y, Gilbert A, Fernandes JF, Bukhari HA, Wajdan A, Martinez MV, Santos MS, Shamohammedi M, Luo H, Westphal P, Leeson P, DiAchille P, Gurev V, Mayr M, Geris L, Pathmanathan P, Morrison T, Cornelussen R, Prinzen F, Delhaas T, Doltra A, Sitges M, Vigmond EJ, Zacur E, Grau V, Rodriguez B, Remme EW, Niederer S, Mortier P, McLeod K, Potse M, Pueyo E, Bueno-Orovio A, Lamata P., Eur Heart J., 41(48):4556-4564 (2020), DOI:10.1093/eurheartj/ehaa159	163

Popularised Publications

In the second half of the project, ComoBioMed2 research featured in 33 substantial popularised publications, either online or in print. Each article is listed in Appendix 10.2. On this front, we have taken substantial advantage of media interest in both digital twins and in coronavirus research. This has resulted in many major publications featuring our work, reaching tens of millions of people; substantially beyond the audience sizes that we were able to reach in CompBioMed1. Below are listed some of the larger publications:

- Futura Sante
- Il Sole 24ORE
- Daily Telegraph
- Suddeutsche Zeitung
- The Sun
- AOL
- Daily Mail
- Yahoo! Actualités
- Yahoo! News
- The Evening Standard
- Irish Examiner
- Newsweek
- Reformatorisch Dagblad
- Sky News
- Gulf News
- BBC Science Focus

We have attempted to give rough estimates of the potential exposure that these publications have achieved, in some cases they are reliable circulation figures, others are estimates calculated considering the monthly visitors to each website (data available on similarweb.com) and estimating that up to 1/10th of visitors may have seen our article. As each article is in place for longer than a single month this may underestimate the overall reach of the article, but this gives us an idea of the scale of audiences that we are reaching. Using this method, the result is a cumulative figure of 68,553,207 people. This shows that we are reaching tens of millions of people with our popularised publications alone.



Figure 1: Screenshot of Nature article on our coronavirus

Figure 1: Screenshot of Nature article on our coronavirus



Figure 3: CompBioMed2 WIRED IT article on digital twins

research, which was widely distributed in Italian and English.

Nature published an article on "Simulating the pandemic: What COVID forecasters can learn from climate models"², which discussed the CompBioMed's CovidSim UQ work that featured in a separate Nature Computational Science publication (DOI: 10.1038/s43588-021-00028-9), on 13 November 2020. The Nature article achieved a massive Altmetric score of 184.

In the same issue of *Nature Computational Science* that contained the publication of our CovidSim UQ work, the W.H.O. published a paper on "Quantifying the uncertainty of CovidSim"³ that further discussed our paper. The W.H.O. article itself has achieved an Altmetric score of 30.

The Italian version of WIRED magazine published an article titled "Il gemello Virtuale"⁴ on CompBioMed's virtual human work. The magazine has substantial reach, and the article garnered the attention of WIRED UK who are now working on a similar article.

Italian newspaper *Il Sole 24ORE*'s associated magazine *Platinum Aziende & Protagonisti* published an article on "High performance computing and machine learning to defeat the pandemic" concerning CompBioMed coronavirus

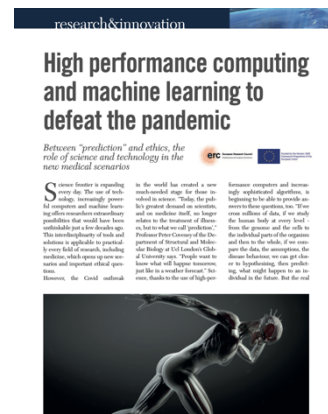


Figure 2: Il Sole 24ORE's article on CompBioMed2 coronavirus research

6.2.2 Newsletters

In CompBioMed2, we release regular print- and e-Newsletters that 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. During CompBioMed2 we have produced and disseminated 3 print- and 2 e-newsletters.

6.2.3 Posters

While the pandemic put a halt to in-person events—the usual venue for poster presentations—there were a number of virtual events that supported presentation of virtual posters. These usually involved some kind of chat feature that allowed participants to interact with the poster presenters. Our own CBMC21 conference took this approach, and 8 posters were presented there. In the first half of CompBioMed2, 9 CompBioMed posters were presented at various other events. These are listed among the items in Appendix **Error! Reference source not found.**

² <https://www.nature.com/articles/d41586-020-03208-1>

³ Leung, K., Wu, J.T. Quantifying the uncertainty of CovidSim. *Nat Comput Sci* **1**, 98–99 (2021). DOI: 10.1038/s43588-021-00031-0

⁴ Wired IT, Vol 96, Spring 2021 Health Edition, ISSN 2035-7397

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

6.2.4 Other materials

Due to the pandemic, there were no opportunities of note where we might have handed out our usual physical dissemination materials such as CompBioMed branded stress toys, stickers, and leaflets. We will resume activities involving these in the second half of the project.

6.2.5 Film, Video, and Television

In this section we discuss film, video, and television activities during the first 25 months of CompBioMed2. The activities are listed in Appendix 10.3.

The CompBioMed YouTube Channel

CompBioMed2 continued to heavily leverage its video output as it did in CompBioMed1. As one might expect, online videos performed well in the pandemic in terms of views. By the end of CompBioMed1, the Computational Biomedicine YouTube channel⁶ had released 81 videos, amassing 13,687 views and 202 subscribers. By month 25 of CompBioMed2, the YouTube channel had released 130 videos, amassing 45,305 total channel views and 813 subscribers. While around 50 videos were released on the YouTube channel in both the second period of CompBioMed1 and the first 25 months of CompBioMed2, there was a much greater rise in views and subscribers during the first 25 months of CompBioMed2. This demonstrates our growing traction and momentum, as well as the increased appeal of CompBioMed to the media and general public due to our coronavirus research, along with a greater consumption of online content during lockdowns. Figure 4 shows the trends in the growth of the YouTube channel since the start of CompBioMed1, showing exponential growth as people increasingly elect to follow and view our video content.

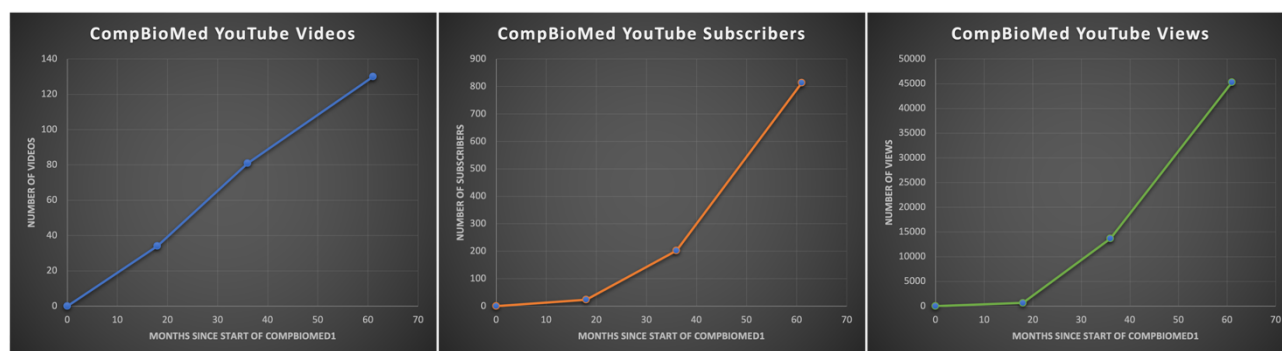


Figure 4: CompBioMed YouTube growth trends since the start of CompBioMed1. The data points were captured at months 18 (halfway through CBM1), 36 (end of CBM1), and 61 months (25 months into CompBioMed2).

The Virtual Humans Video

The Virtual Humans film produced in CompBioMed1 remains our most popular single item on the YouTube channel, having amassed 12,662 views alone (about 2-8 times more than any other CompBioMed YouTube video, and about 2-4 times other CoEs' most viewed content). 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

⁶ https://www.youtube.com/channel/UCUilfmesH_psiArXT3xcppA/featured
PU

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.

The dissemination campaign for the video was substantial and is dealt with in detail in CompBioMed1 deliverable D.3.6. However, the dissemination of the video has continued into CompBioMed2, as shown in Appendix 10.9 which lists 38 instances of dissemination showing the full film or using clips/assets from the film. This includes major popularised publications such as *Il Sole 24ORE*, *WIRED Italy*, *Futura Sante*, *Euronews*, and *Yahoo! Actualités*, reaching a roughly estimated 18.5 million people.

Television appearances

Peter Coveney and Andrea Townsend-Nicholson appeared on the EuroNews Futuris Programme, on a piece about "Virtual Humans to map the future of major surgery" on 10 September 2020, the piece ran multiple times throughout the day. Euronews reaches 150 million viewers each month, with a reach of 430 million households in total.

Roger Highfield mentioned CompBioMed COVID-19 research on the BBC *Today* Programme, in the week of March 23rd, 2020, as well as on BBC Newshour on the BBC World Service on 25 March. Likewise, Peter Coveney appeared on BBC NEWS World Service on a piece on "Supercomputers seeking solutions for Covid-19", on 18 April 2020.

6.3 Online Presence

In this section, we describe CompBioMed's online presence in the first 25 months of CompBioMed2, covering the social media and website presence that has been deployed. The strategy shows a social media campaign designed to focus on the effective platforms of Twitter, LinkedIn, 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.

6.3.1 Social Media

CompBioMed2's social media activity in the first 25 months is listed in Appendix 10.4. We have elected to focus our social media efforts only on platforms that our experience has shown to be effective (in terms of achieving reach and traction) in scientific research projects, namely YouTube, LinkedIn, and Twitter.

Our efforts on LinkedIn⁷ are relatively recent, having not featured in CompBioMed1. Already, however, we have posted 77 times, amassing 191 followers and 6,787 impressions. This demonstrates that LinkedIn is a valuable addition to our social media activity.

On Twitter, the official CompBioMed account⁸ now has 1,294 total tweets, with 523 tweets of those being tweeted in the first 25 months of CBM2. The account has 1,265 followers, with 538 of those following in the first 25 months of CBM2. The twitter account has achieved 510,449 total impressions the number of times a user is served a Tweet in timeline or search results), with 180,129 of those occurring in the first 25 months of CBM2. These statistics demonstrate the great reach that a well followed twitter account can achieve, Twitter's suitability for the social media activity of scientific research projects, and the benefits of funding the second phase of a project compared to starting a project from scratch. The trends in these

⁷ <https://www.linkedin.com/company/compbiomed/>

⁸ https://twitter.com/bio_comp



numbers since the start of CompBioMed1 are shown in Figure 5, showing steady growth as people continue to elect to follow and view our twitter content.

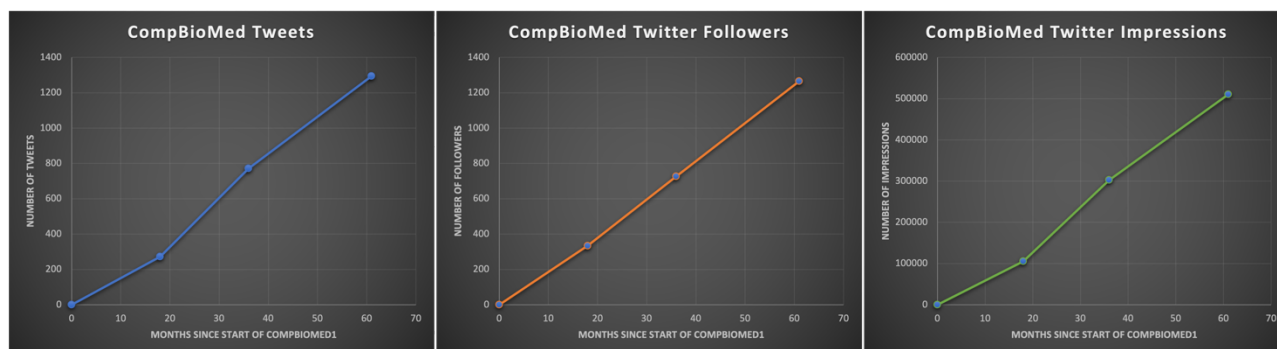


Figure 5: CompBioMed Twitter account growth trends since the start of CompBioMed1. The data points were captured at months 18 (half way through CBM1), 36 (end of CBM1), and 61 months (25 months into CompBioMed2).

For our YouTube activity, please see Section 6.2.5, which covers the activity and statistics of the CompBioMed YouTube account.

A selection of extremely well followed social media accounts posted about CompBioMed. On Twitter this included @NaturePortfolio and @Nature, @skynews, @Newsweek, @irishexaminer, @The_MRC, and @breakingnewsie. On Facebook, this included the Nature Facebook account. These heavy hitting accounts have racked up millions of impressions. Impressions from external accounts can't be measured precisely, but they can be estimated based on the number of followers of each account.

6.3.2 Websites

In this section, we describe changes and improvements to the CompBioMed website, the new CompBioMed Conference 2021 website, and other website activity.

The CompBioMed Website

In CompBioMed2, we have of course benefitted hugely from having already developed the project website in CompBioMed1. The website was fine-tuned over the course of the Centre's first phase and continued into CompBioMed2 as a fully featured hub for the project. We do, of course, continue to update it, not just in terms of news, events, service updates, training etc., but also adding new areas and functionality on the website when needed. For instance, we created the CompBioMed coronavirus portal⁹, which describes our various threads of work, activity, collaborations, and resources related to coronavirus research. We also added the scalability support portal¹⁰, offering free support to improve the scalability of computational biomedicine solutions with high performance computers. More information on the service pages of the website can be found in D4.2, published at the same time as this deliverable (M25 – October 2021)

In terms of website traffic, the CompBioMed website's 165 pages has seen 139,405 visitors in total, up from 109,908 visitors at the end of CBM1. The website has received 252,687 visits, up from 199,669 visits at the end of CBM1. Trends are difficult to track across the projects since Google's tracking algorithm changed substantially in September 2018, rendering it impossible to interpret trends that cross that date.

⁹ <https://www.compbioimed.eu/compbioimed-and-coronavirus/>

¹⁰ <https://www.compbioimed.eu/compbioimed-scalability-channel/>

The CompBioMed Conference Website

The CompBioMed Conference 2021 took place virtually in September 2021 and is described in Section 6.4.1. In terms of the conference website¹¹, which is relevant to this section, we collaborated with the conference service vFairs to produce an attractive website to provide conference and registration information, the agenda, an FAQ, details on sponsors, and a link to the virtual conference itself. This expires 1 month after the conference, so will no longer be active, but we plan to migrate all the information over to the previous CompBioMed Conference website in November 2021.

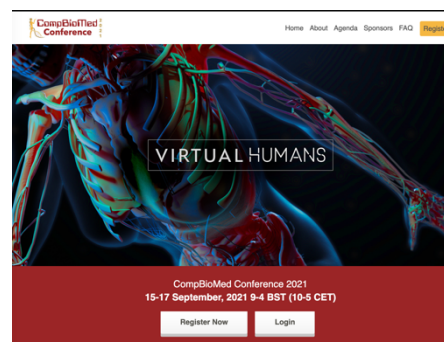


Figure 6: Main page of the CBMC21 website

Other Website Activity

In addition to the CompBioMed-owned websites, there was also plenty of dissemination activity occurring on external websites. Appendix 10.5 lists the activity in the second half of the project on external websites (other than the popularised publication activity already listed in Appendix 10.2). These include posts on partner and associate partner websites such as LRZ, CWI, the Science Museum, EPCC and so forth.

6.4 Events

In this section, we describe the various events that CompBioMed2 organised and those in which they participated. We strongly leveraged our active consortium, giving talks and presenting posters at a vast number of events that targeted all our stakeholders (discussed further in Section 6.6). We also organised a number of events/aspects within events, including the major CompBioMed Conference in September 2021.

6.4.1 Event Organisation

In Appendix 10.6, the events organised by the CompBioMed consortium in the first 25 months of CBM2 are listed. These include:

- A "WP3 Meeting on Machine Learning meets Modelling and Simulation Methods" 16-17 March 2020
- A meeting on "Best practices to handle sensitive data and access to European-level tools for data management" at Sensitive Data Management and EUDAT Services on 29 March 2020
- WP5 organised a workshop on Incubator Activities, which took place virtually on 26th May 2020
- A meeting on "Advanced HPC usage and parallel computing" at Cluster Computing for Computational Science on 3 and 10 December 2020
- A HiPEAC conference 2021 workshop on "The HPC CoE services and applications" on 20 January 2021
- A thematic session organised with FocusCoE, BioExcel and PerMedCoE on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference on 4 May 2021
- A meeting on "CPU parallel programming in HPC facilities" at MPI and OpenMP in Scientific Software Development on 9 and 11 June 2021
- CompBioMed Conference 2021 (CBMC21), held on 15-17 September 2021

Some highlights from this list are described below.

¹¹ <https://cbmc21.vFairs.com/>

Workshop on Machine Learning meets Modelling and Simulation Methods

WP3 organised a workshop on Machine Learning meets Modelling and Simulation Methods¹² on 16-17 March 2020. CompBioMed2 was constructed with a dedicated work package on the emerging topic of machine learning and artificial intelligence with a focus on high performance data analytics required for these approaches. This workshop was an opportunity for certain Core and Associate Partners working on this topic to gather and discuss current progress and the possibilities and needs to advance this burgeoning field. The meeting was due to take place in person at Leibniz Supercomputing Centre (LRZ) in Munich but was at the last minute taken online as the pandemic took hold. Whilst it was challenging to convert the meeting into a virtual one at very short notice, it was nonetheless successful.

Workshop on Incubator Activities

WP5 organised a workshop on Incubator Activities¹³, which took place virtually on 26th May 2020 to kick-off the Incubator activities involved in WP5. The meeting was originally intended to be held in person in Amsterdam but was moved to a virtual format due to the onset of the pandemic. The workshop addressed subjects including:

- The Long-term sustainability of the CompBioMed Centre of Excellence
- Business opportunities with HPC
- Research on the Impact of HPC on healthcare in terms of quality and business model
- Spinning out from academia: commercialising research applications

It also featured guest talks from Amsterdam Business School, ConceptionX, ACE Incubator, VPH institute, Oncoradiomics, Quantib, LifeTec Group, ELEM Biotech, Zapata, and Deep Learning Partnership.

The CompBioMed Conference 2021

Following the successful inaugural edition of the CompBioMed Conference in 2019, we produced a follow up 3-day conference on 15-17 September 2021. The 2019 edition of the conference was an in-person event in London, but due to the pandemic, the 2021 edition was converted to a virtual event.

As discussed in Section 6.1, virtual events inherently possess substantial positives compared to in-person events, but also significant negatives. In order to attempt to offset the negative aspects in terms of reduced participant interaction and participant engagement, we opted to use the virtual conference platform vFairs. This service attempts to re-create some of the aspects of an in-person conference: virtual lobbies, auditoriums, poster sessions, exhibition booths, as well as chat functions (networking areas, booth and poster chat functions). Furthermore, the vFairs service offers a leaderboard functionality that rewards attendees with points for participating in various parts of the conference, and the winners are awarded real prizes at the end of the conference.

¹² <https://www.compbioimed.eu/machine-learning-meets-modelling-and-simulation-methods/>

¹³ <https://www.compbioimed.eu/incubator-activities-meeting/>



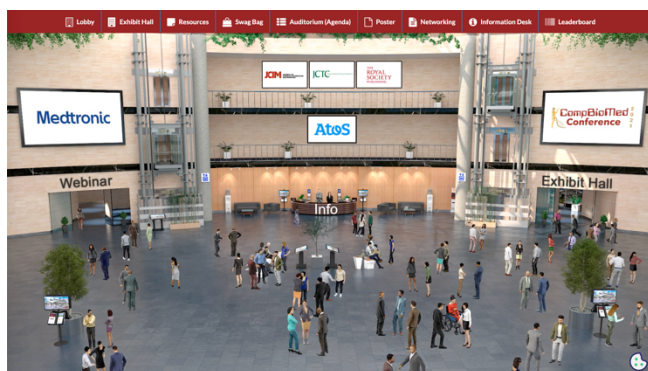


Figure 8: CBMC21 vFairs Lobby

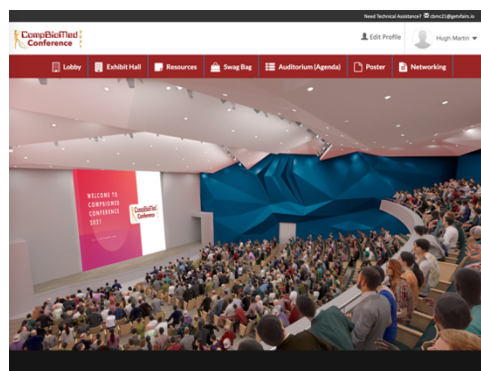


Figure 7: CBMC21 vFairs Auditorium

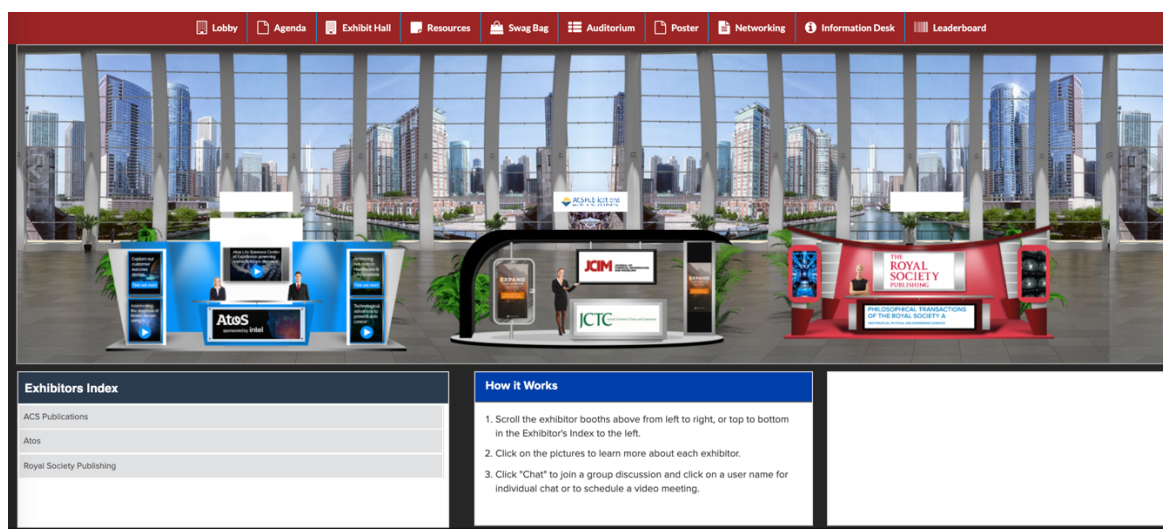


Figure 9: CBMC21 vFairs Booths

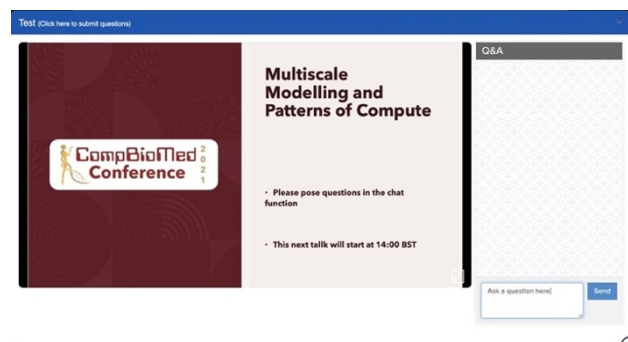


Figure 10: CBMC21 vFairs presentation interface with Q&A

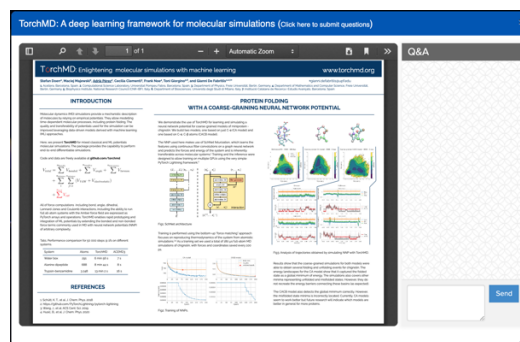


Figure 11: CBMC21 vFairs Poster interface with Q&A

Through these features, the hope was to drive up participation and engagement. This was indeed observed, with participation and interactions with booths and posters notably increasing once the attendees were informed of the features, prizes, and methods required to win them. Nonetheless, the level of participation and interaction did not approach the levels that one typically finds in an in-person event.

The talks at the event followed 3 computational biomedicine themes, and sessions on specific subjects were held under each theme. The sessions covered all manner of subjects across computational biomedicine, as follows:

Biomedical Applications

- PerMedCoE: Modelling and simulation for the interpretation of single-cell data
- Molecular Medicine & Drug Discovery
- Organ Modelling and Simulation

Methodology

- Multiscale Modelling & Patterns of Compute
- Building the Virtual Human
- On the path to the Exascale and Validation, Verification and Uncertainty Quantification
- The role of Quantum Computing in biomedicine

Technology and Outreach

- Imaging & Visualisation (with additional Verification, Validation and Uncertainty Quantification talk)
- Accelerating the Adoption of *in silico* Trials
- From desktop to HPC and beyond in the clinic
- Improving Trust in Computational Tools
- Public Awareness, Training and Education including Public Policy

The event was sponsored by Atos, Medtronic, JCTC, JCIM, The Royal Society Publishing, and UKCOMES.

In total there were 185 Registered Attendees, which is a little less than the 200 attendees seen at CBMC19. Attendees were charged €40, €50 or €60 depending on whether they were a student and if they registered before the early bird cut-off date. There were 77 Presentations across 3 days, most were pre-recorded and played at the specified slot with the speaker present to answer questions in the chat, but some talks were delivered live. Talks were kept available to registered participants on the vFairs portal for 1 month and are soon due to be placed on the CompBioMed YouTube channel, they will also be available on compbiomed-conference.org. There were 8 posters and 3 sponsor booths at the event.

As discussed in Section 6.1, user engagement at virtual events is notoriously low. One method we harnessed to improve this was to track participant engagement using in-built vFairs features, then award points to those actions, and display a leaderboard in the conference portal. The 3 highest scores each won prizes, and indeed this seemed to spur on increased engagement such as questions being asked at posters and booths.

Overall, our experience with the virtual conference on vFairs was a positive one, with strong participation, a great selection of talks covering many aspects of computational biomedicine, and a relatively low cost compared to an in-person event. Virtual events may never fully close the gap on in-person events in certain areas, but they also hold the aforementioned advantages.

6.4.2 Event Participation

Even though the pandemic caused the cancellation of many events and prevented in-person events for most of the period, the CompBioMed consortium was extremely active in the first 25 months of CompBioMed2 in terms of event participation. Appendix 10.7 shows the full listing of event participation, which includes keynote presentations, invited talks, talks, posters, meetings, booths, and panel discussions. In total, a considerable 151 event participations were recorded during this period across 61 major events (listed below) among other smaller events and occurrences. The events ranged from conferences, workshops, seminars, webinars, birds-of-a-feather, meetings, and sessions. They targeted all of CompBioMed's stakeholders: academia, industry, clinicians, the general public, policy makers, medias, PU



customers, and investors. For more on the targeting of specific types of stakeholders, see Section 6.6. Below are the 61 major events that the CompBioMed consortium participated in during the period:

1. Supercomputing 2019 (SC)
2. FRAME 18th Annual Lecture 2019
3. American Heart Association Meeting 2019
4. International Conference on Pattern Recognition and Machine Intelligence 2019
5. NeurIPS 2019
6. IBSA Foundation Forum 2019
7. Invitational Conference for European Medical Associations 2019
8. BioFIT 2019
9. SURFsara Super Day 2019
10. International Perspective Meeting at the Clara Angela Foundation 2019
11. Supercomputing 2020 (SC)
12. International Supercomputing Conference 2020 (ISC)
13. European Community on Computational Methods in Applied Sciences 2020 (ECCOMAS)
14. European Society of Cardiology 2020
15. TRM Forum 2020
16. Innovation in Cardiovascular Interventions 2020 (ICI)
17. Computing in Cardiology 2020
18. Virtual Physiological Human 2020 (VPH)
19. The Statistical Atlases and Computational Modeling of the Heart Workshop 2020 (STACOM)
20. International Symposium on Biomedical Imaging 2020 (ISBI)
21. AI4Science 2020
22. EuroScience Open Forum 2020 (ESOF)
23. OpenEye Conference 2020
24. UKCOMES Winter Symposium 2020
25. Reliability and Reproducibility in Computational Science 2020
26. EC Stakeholder Workshop 2020
27. CECAM workshop on the Importance of Being H.P.C. Earnest 2020
28. Soapbox Science 2020
29. Insigneo Winter Symposium 2020
30. EuroHPC Summit Week 2021
31. International Supercomputing Conference 2021 (ISC)
32. Conference on Coupled Problems in Science and Engineering 2021 (COUPLED)
33. Mechanistic Machine Learning and Digital Twins for Computational Science, Engineering & Technology 2021 (MMLDT-CSET)
34. BSC Severo Ochoa Doctoral Symposium 2021
35. International Symposium on Computer Methods in Biomechanics and Biomedical Engineering 2021 (CMBBE)
36. European Society of Biomechanics 2021 (ESBiomech)
37. International Conference on Computational Science 2021 (ICCS)
38. Heart Rhythm Society Meeting 2021
39. Functional Modelling and Imaging of the Heart Conference 2021
40. Functional Modelling and Imaging of the Heart Conference 2021
41. European Heart Rhythm Association Annual Workshop 2021
42. Intel Dev Summit 2021
43. The European Federation of National Associations of Orthopaedics and Traumatology First European Consensus Conference 2021 (EFORT)
44. CompBioMed Conference 2021 (CBMC21)



45. Biomedical Engineering Conference 2021 (BioMedEng)
46. Platform for Advanced Scientific Computing 2021 (PASC)
47. IEEE International Conference on Biomedical And Health Informatics Jointly Organised with the 17th IEEE-EMBS International Conference on Wearable and Implantable Body Sensor Networks 2021 (IEEE BHI-BSN 2021)
48. Global CIO Forum 2021
49. Cambridge New Therapeutics Forum 2021
50. Bioinformatics Granada 2021
51. Atos Innovation week 2021
52. LRZ Results Workshop 2021
53. European Network on High-performance Embedded Architecture and Compilation 2021 (HiPEAC)
54. InSilc Workshop: In Silico Clinical Trials Concepts and Adoption 2021
55. La Medicina in Silico in Italia: Uno Sguardo Prospettico 2021
56. ExCALBUR Workshop III: Towards Exascale Simulation of Integrated Engineering Systems 2021
57. Next-Generation CFD: Cutting-Edge Applications, Advanced Modelling and Machine Learning Seminar Showcase 2021
58. ExCALBUR Workshop V: Data Visualisation and Data Flows 2021
59. EuroCC Greece Chapter Meeting 2021
60. Insist All-hands Meeting 2021
61. Bilateral Italy-South Africa Meeting “Civilian and Defence Applications of Artificial Intelligence, Big Data and High Performance Computing” 2021

6.5 Other Dissemination

This section addresses instances of dissemination that did not easily fit into the categories in the previous sections. These instances are listed in Appendix 10.8. These include award ceremonies, notable circulations on mailing lists, internal publications within partners, booklet appearances, external publications that mention CompBioMed, and so forth.

6.6 Targeted Activity

The dissemination activity in CompBioMed was targeted towards all its stakeholders, be it academics, industry personnel, clinicians, or the general public. The academic and industrial backgrounds of the CompBioMed consortium naturally mean that these groups of stakeholders are often targeted. In total, 214 items of dissemination activity (shown across Appendix 10) included the scientific community as targets, while 195 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, as well as HPC underrepresented and EU13 countries.

6.6.1 General Public

In total there were 85 activities that were inclusive of the general public as target audiences. While smaller in number than those targeting the scientific community and industry, the activities targeting the general public were by far the heaviest hitting in terms of people reached. By our estimations, these activities reached 122,904,245 people. Whilst this figure is an estimate it indicates that these activities reached



millions of people perhaps over 100M, the vast majority of these (perhaps 90%) were the general public. These activities are covered well in Sections 6.2.1, 6.2.5, and 6.3.1, largely involving popularised publications (68,553,207), video & television (34,034,537), website (125,218), and social media activity (20,305,918).

In CompBioMed1 we had great success reaching the general public with our Virtual Humans IMAX film, and indeed the film featured in many of our heavy-hitting activities in CompBioMed2. We plan to recreate this success again in the second period of CompBioMed2 with another IMAX film, due for completion in 2022, see Section 6.8 for more details.

6.6.2 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. WP6 has a dedicated task on “Expanding CompBioMed Medical Student Training Programme” which conducts activities in training medical students in HPC for computational biomedicine. Deliverable D6.5: “Final Report on Training Activities” will describe these activities. Beyond that, it was important that CompBioMed raised awareness of Computational Biomedicine more broadly to clinicians and medical students across Europe and the world, through targeted dissemination activity.

Across the various dissemination activities listed in Appendix 10, 78 activities were targeted at the clinical domain in the first 25 months of CompBioMed2. Among them are our consortium’s participation in the following clinically relevant events:

1. American Heart Association Meeting 2019
2. Invitational Conference for European Medical Associations 2019
3. Innovation in Cardiovascular Interventions 2020 (ICI)
4. European Society of Cardiology 2020
5. TRM Forum 2020
6. Computing in Cardiology 2020
7. Insigneo Winter Symposium 2020
8. Virtual Physiological Human 2020 (VPH)
9. International Symposium on Biomedical Imaging 2020 (ISBI)
10. The European Federation of National Associations of Orthopaedics and Traumatology First European Consensus Conference 2021 (EFORT)
11. CompBioMed Conference 2021 (CBMC21)
12. IEEE International Conference on Biomedical And Health Informatics Jointly Organised with the 17th IEEE-EMBS International Conference on Wearable and Implantable Body Sensor Networks 2021 (IEEE BHI-BSN 2021)
13. Functional Modelling and Imaging of the Heart Conference 2021
14. European Heart Rhythm Association Annual Workshop 2021
15. Heart Rhythm Society Meeting 2021
16. Functional Modelling and Imaging of the Heart Conference 2021
17. Cambridge New Therapeutics Forum 2021
18. InSilico Workshop: In Silico Clinical Trials Concepts and Adoption 2021
19. La Medicina in Silico in Italia: Uno Sguardo Prospettico 2021

At our own CompBioMed Conference 2021, several of the sessions were particularly relevant to people from the clinic as well as medical students, these sessions are listed below:

- Organ Modelling and Simulation



- Building the Virtual Human
- Imaging & Visualisation
- Accelerating the Adoption of *in silico* Trials
- From desktop to HPC and beyond in the clinic
- Improving Trust in Computational Tools
- Public Awareness, Training and Education including Public Policy

Of the 185 attendees at CBMC21, 4 attendees were from the clinical domain, as well as one of the plenary speakers, Lucile Houyel. While this demonstrates that we are bringing clinicians into our activities, it also reflects the difficulties in appealing to clinicians and medical students, which is why pro-active efforts (like those described in this section, and our medical student training programme) are required to break into the domain.

As covered in CompBioMed1 deliverables, we continue to have and update a dedicated section¹⁴ of the website designed to present information most relevant to clinical visitors.

In CompBioMed1 we had great success using the Virtual Humans IMAX film to appeal to clinicians. We plan to recreate this success again in the second period of CompBioMed2 with another IMAX film, due for completion in 2022, see Section 6.8 for more details.

6.6.3 Other H2020 Projects and CoEs

We share the view of the European Commission that its 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 EC funded projects that CompBioMed has undertaken.

FocusCoE

FocusCoE is a Coordination and Support Action for the HPC CoEs. CompBioMed works closely with FocusCoE in several of its work packages:

- **WP2 - The HPC CoE General Assembly**
WP2 established HPC3 (HPC CoE Council), which is the CoE General Assembly. HPC3 discusses, makes decisions on, and takes actions on matters relevant to all HPC CoEs. CompBioMed sits on HPC3 as an active member.
- **WP3 - CoE-Industry Interaction**
This work package works toward developing the interaction between the CoEs and the industry with the aim to increase the impact of the CoE effort on the competitiveness of European companies. CompBioMed has worked with FocusCoE WP3 through:
 - Disseminating successful collaborations between CoEs and industry, and by sharing those among all CoEs, FocusCoE WP3 aimed at identifying good collaboration practices, i.e. procedures and approaches that were found particularly effective and beneficial for the companies and CoEs involved. For CompBioMed in particular, the outcomes of its collaboration with Janssen Pharmaceutica were featured.
 - Featuring in Industry Surveying, in part to raise awareness about the CoEs' services to industry.
 - Sectorial events. These are events in the various industrial sectors that are relevant to the CoEs for the purpose of showcasing their work and growing networks in the relevant sectors. CompBioMed participated in Biofit 2019, which took place in Marseille on 10-11

¹⁴ <https://www.compbioimed.eu/home/clinical-users/>



December 2019. CompBioMed will also participate in Medica 2021, due to take place on 15-18 November 2021.

- A Best Practices Booklet. This is the product of the collective experiences of the CoEs in sectorial events, offering a guide on how to successfully organise event participation and maximize gains from that participation.

- **WP4 - Training**

This work package coordinated training and training services across the CoEs. In FocusCoE WP4, CompBioMed:

- Listed their training events on the FocusCoE hpccoe.eu training registry.
- Participated in the FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 5 November 2020
- Participated in the second FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 21 January 2021

- **WP5 - Promoting EU HPC CoEs**

The main goal of this work package is to promote CoE success stories and provide an overview on all exploitable results, making sure that FocusCoE helps to build the European HPC CoEs “brand”, rather than being a brand itself. Working with WP5, CompBioMed:

- Had its news and twitter feeds appear on the FocusCoE hpccoe.eu website
- Had its services listed on the FocusCoE hpccoe.eu website
- Collaborated with FocusCoE, BioExcel and PerMedCoE during a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HIPEAC conference on 4 May 2021
- Co-organised a workshop with FocusCoE, EXCELLERAT, EoCoE, ChEESE, HiDALGO, BioExcel, at the HIPEAC conference 2021 on "The HPC CoE services and applications" on 20 January 2021
- Featured in the FocusCoE News Flash (an email sent to the CoE mailing list)

POP

CompBioMed has long been collaborating with POP CoE to bring HemeLB to the exascale. Our work with them is described in previous dissemination deliverables. Activity in the current period includes:

- CompBioMed worked with POP on the presentation "Readying HemeLB and SCEMa Codes for Exascale with POP and E-CAM Centres of Excellence" at PASC21, on 7 July 2021
- POP, FocusCoE, and CompBioMed held a booth at BioFIT 2019 in Marseille on 10-11 December 2019
- At Supercomputing 2020, POP carried out the following activities relating to CompBioMed:
 - The POP CoE ran a half day tutorial on "Practical Hybrid Parallel Application Performance Engineering" involving HemeLB in collaboration with CompBioMed, including a case study demonstrating measurements of HemeLB on SuperMUC-NG and JUWELS/V100.
 - The corresponding POP assessment report was also accepted by the ProTools workshop and was presented.
 - Brian Wylie from the POP CoE published his presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB in collaboration with CompBioMed.
 - Brian Wylie from the POP CoE disseminated a printable cube showing a Score-P summary measurement of HemeLB application execution on 32 JUWELS/V100 compute nodes with 129 MPI processes and 128 GPUs.
 - Brian Wylie from the POP CoE gave a presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB.



E-CAM

CompBioMed has long been collaborating with E-CAM CoE, working with HemeLB. Our work with them is described in previous dissemination deliverables. Activity in the current period includes:

- CompBioMed worked with POP AND E-CAM on the presentation "Readying HemeLB and SCEMa Codes for Exascale with POP and E-CAM Centres of Excellence" at PASC21
- E-CAM's work with HemeLB of CompBioMed featured in FocusCoE newsletter #9
- E-CAM posted an article on "February Module of the Month: ALL library implementation in HemeLB, a CoE collaboration"

BioExcel, PerMedCoE, EXCELLERAT, EoCoE, ChEESE, HiDALGO

Activities with other CoEs in the current period include:

- CompBioMed collaborated with FocusCoE, BioExcel and PerMedCoE during a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference 2021.
- A video of CompBioMed's collaboration with FocusCoE, BioExcel and PerMedCoE was posted on the HiPEAC Youtube channel. It was a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference 2021.
- CompBioMed co-organised a workshop with FocusCoE, EXCELLERAT, EoCoE, ChEESE, HiDALGO, BioExcel, at the HiPEAC conference 2021 on "The HPC CoE services and applications".

EOSC Hub

CompBioMed has been contributing the provision of services on the EOSC-hub service catalogue. The following CompBioMed services are now listed on the EOSC Hub:

- The CompBioMed Training portal
- CompBioMed Scalability Support
- CompBioMed Software Hub
- CompBioMed Visitor Programme
- CompBioMed HPC Allocations
- CompBioMed Incubator Registry

Each of these services are displayed on the EOSC portal with detailed contents including description of each service, entry point of the service, the point of contact, and the definition of the conditions and agreement that apply to each of the services.

Innovation Radar

CompBioMed codes were listed on the EU funded Innovation Radar¹⁵ website. Innovation Radar is a European Commission initiative to identify high potential innovations and innovators in EU-funded research and innovation projects. Their goal is to allow every citizen, public official, professional and businessperson to discover the outputs of EU innovation funding and give them a chance to seek out innovators. The website lists CompBioMed codes Alya, HemeLB, HemoCell, OpenBF, Palabos-Vertebroplasty simulator, Palabos – Flow Diverter Simulator, BAC, HTMD, Playmolecule, Virtual Assay, CT2S, and Insigneo Bone Tissue Suite.

EuroCC

Andrea Townsend-Nicholson (UCL) gave a talk on "Introducing CompBioMed for HPC for the Greek Health & Life Sciences Sector" at the EuroCC Greece Chapter meeting 2021.

¹⁵ <https://www.innoradar.eu/innovation/38359>



In Silico World

The In Silico World (ISW) project launched in 2021. CompBioMed and ISW disseminate to each other to make use of their collective networks, and they collaborate on running a joint scalability slack channel for scalability support (see deliverable D6.1 for more information).

6.6.4 EU13 and HPC Underrepresented Countries

The CompBioMed Centre of Excellence is targeting HPC underrepresented and EU13 countries in its activities, primarily through our network of partners and via events.

Our Associate Partner network contains a growing list of partners from HPC-poor and EU13 countries:

- PSNC – Poznan Supercomputing and Networking Center, Poland
- Zayed University, United Arab Emirates
- Pozlab, Poland
- The Academic Computer Centre Cyfronet AGH, Poland
- Sano, Poland
- KINDI, Centre for Computing Research, Qatar
- Institute of Molecular Biology, National Academy of Sciences, Armenia
- DiaVita, Bulgaria
- Qatar Robotic Surgery Centre (QRSC), Qatar
- Russian-Armenian University, Armenia

We are also in talks with Sven Loncaric, Croatia Data Centre of Excellence to bring them in as an associate partner.

Our original intention with CBMC21 was for it to be held in Greece to encourage participation from EU13 and HPC underrepresented countries, but the pandemic forced us to take the event online. Nonetheless, we expended a great deal of effort in identifying contacts in EU13 and HPC underrepresented countries that might take an interest in our activities in computational biomedicine, finding 212 in total. We have been disseminating our webinars, CBMC21 activity and other activity to these contacts. At CBMC21 we had talks from EU13 and HPC underrepresented countries:

- Luca Meacci, Universidade de São Paulo
- Alya Arabi, United Arab Emirates University
- Marek Kasztelnik, ACC Cyfronet AGH
- Benjamin Csippa, Budapest University of Technology and Economics
- Bartosz Bosak, Poznan Supercomputing and Networking Center

The CBMC21 attendees were from all over the globe, including the following EU13 and HPC underrepresented countries: Poland, Czech Republic, Hungary, Pakistan, Brazil, United Arab Emirates, Turkey, Armenia, Aruba, Zimbabwe, Bangladesh, India, Congo Kinshasa, Philippines, Colombia, Sierra Leone, Mexico.

Our intention remains to hold a major event such as the third CompBioMed Conference in an EU13 or HPC underrepresented country.



As mentioned in the previous section, Andrea Townsend-Nicholson (UCL) gave a talk on “Introducing CompBioMed for HPC for the Greek Health & Life Sciences Sector” at the EuroCC Greece Chapter meeting 2021. We will continue to engage with EuroCC and NCCs.

6.7 Metrics and Key Performance Indicators

Various metrics have been posted throughout this deliverable, below are some key metrics:

- Number of activities of all kinds - 281
- Number of events participated in - 61
- Number of attendees at our organised events (not including training events) - 515
- Number of publications - 112
- Publication Altmetrics – 6 publications above an Altmetric of 30
- Website stats and social media stats - 53,018 website views, 6,787 LinkedIn impressions, 180,129 Twitter impressions, 45,305 YouTube views
- Estimated sizes of audiences reached – estimated 123,108,000 people reached

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

- 1) **KPI:** Number of publications in peer-reviewed international journals (or computational conference proceedings) that acknowledge the support of CompBioMed
Target: 6 publications by M24
Result: Achieved, 112 publications by M25
- 2) **KPI:** Number CompBioMed2 dissemination events attended by 50 or more people
Target: 2 events by M24
Result: Achieved, 5 events with attendance of 50 or more people by M25
- 3) **KPI:** Number of companies engaged
Target: 5 companies engaged by M24
Result: Achieved, 5 new companies added as associate partners by M25

6.8 Future Dissemination Plans

Originally, we planned to create an IMAX film in the first two years of CompBioMed2 that would demonstrate our Centre’s research and describe Computational Biomedicine generally, in the context of how it can aid patients and the general public. It would be a follow up to the hugely successful Virtual Humans film produced in CompBioMed1, which we disseminated very widely to all manner of audiences in different contexts and continue to do so to this day. This plan for a follow-up film was adjusted due to the pandemic, since in-person screenings of the film were a key component to its success, and in-person events are only now starting to return after widespread lockdowns. Additionally, the keen media and general public focus on pandemics has created an opportunity to make the film themed on the role of computational biomedicine in fighting the pandemic.

The pandemic themed video is now due for completion in September 2022, alongside a number of in-person screenings to the general public.

Other upcoming plans include:

- CompBioMed will participate in Medica 2021, collaborating with other CoEs, due to take place on 15-18 November 2021.
- Andrea Townsend-Nicholson (UCL) will be participating in the Sense about Science event in London targeting policy makers, in November 2021.
- Jazmin Aguado-Sierra (BSC) will be at the clinician-heavy event called Health Tech: Digital Health: Remote Monitoring in San Diego, CA, December 2-4, 2021.
- CompBioMed will be at the Heart Rhythm Society's HRX conference in San Diego in September 2022.
- Andrea Townsend-Nicholson (UCL) is participating in filming with Russian TV channel "Friday!" on a piece on virtual humans that will broadcast on the TV channel, featuring our Virtual Humans video.

In general, with lockdowns easing across the globe, in the second half of CompBioMed2 we hope to return to participating in and organising many in-person events once again. In person events are slowly starting to appear, such as the upcoming Medica 2021, Sense about Science, Health Tech: Digital Health: Remote Monitoring, and Heart Rhythm Society's HRX conference, with many being hybrid events that offer both in person and virtual access.

7 Innovation

The need to identify and realise the potential of new technologies, and maximise their impact is of paramount importance in CompBioMed2. Central to this is close collaboration with our user community. We have built a substantial network of collaborators since the beginning of CompBioMed1 in 2016, the majority of whom have become Associate Partners of the project, meaning their engagement with our funded core partners is more longstanding. Our network of industrial partners ranges from global pharmaceutical companies to start-ups and SMEs. Since the end of CompBioMed1, seven new industrial Associate Partners have joined the project, including six SMEs, a result of greater awareness of the project from dissemination efforts.

There is significant innovation potential within the CoE, this is due in part to the large number of private companies who have participated in, and collaborated with the project, as associate and funded partners. We have sought to capture and realise the potential of this in several directions, including opportunities which have arisen in the commercial sector, and the exploitation of High-Performance Computing (HPC) and High-Throughput Computing (HTC) to develop better and faster solutions than were previously possible. We have also increased our focus on the development and adaptation of applications for the emerging exascale, and further aligned some existing activities along the same trajectory. Innovations identified in CompBioMed1 have been further developed within the incubator activity managed in WP5, new innovations, which have come from both scientific trials and implementation of the CompBioMed knowledge base services, including medical training and services provided by our HPC centre partners to facilitate wider use of resources. The commercialisation of computational biomedicine and its applications have also become the subject of PhD research at the University of Amsterdam, in collaboration with CompBioMed core partners.

Dialogue was established early within CompBioMed2 with the wider contractual Public Private Partnership (cPPP) for HPC and the newly formed EuroHPC actors to ensure that the approach to Innovation Management in CompBioMed aligns with the overall strategic objectives of the cPPP, synergistic benefits of co-exploitation with other CoEs, and Exascale Demonstrators (EsDs) as they evolve, lessons are learned for the establishment of best practice methods for successful innovation across CoEs. Additionally, the lead beneficiary of CompBioMed (UCL) is a core partner in the support action FocusCoE; they have used their



presence to lead the formulation of several best practice documents on Innovation Management and Sustainability, and ensured the activities of CompBioMed align with the common innovation activities undertaken by FocusCoE, and other CoEs, where applicable.

7.1 Innovation within CompBioMed 2

7.1.1 Deliverables

The first innovation deliverable (D1.5 - Innovation Plan) was generated in Month 7 of CompBioMed2 and detailed the framework for managing innovation. It built upon the innovation infrastructure developed during CompBioMed1. Resources are provided to support researchers in the capture and exploitation of innovations, and to consider the societal, educational, and commercial possibilities available, and their capability to exploit the innovation through resources of their parent organisation. These include regular reviews of exploitation plans within the project and setting-up and maintaining a register of innovation incubator activities and a formal IP register, which records background, foreground and related third party IP, the same basic infrastructure is adopted in CompBioMed2. The latest table showing the capture of CompBioMed products and services is listed in Appendix 10.11.

7.1.2 Management Review

Innovation management activities are designed to promote entrepreneurial opportunities within the research activities, from invention through to exploitation, and are coordinated across all work packages as a transverse function. Representatives from WP1 attend WP meetings and WP leaders meeting to identify new inventions, products and services that arise in the course of normal research activities, to bring into the outlined innovation management process.

7.1.3 Innovation in the core work programme

There was considerable activity within the core work programme towards the exploitation of software and services developed in the first iteration of the project (CompBioMed1), this was used to formulate the work programme for CompBioMed2, shaping the work packages to develop and mature those applications and HPC services which are necessary to scale up for use at the exascale.

The principal work to enable full exploitation of our software applications is embedded in the core work programme through the CoE's incubation activities in WP5, where application codes developed in CompBioMed1 are nurtured and developed for use outside of the CoE. These routes will be both open-source releases and commercial offerings, where appropriate. Task 5.3 ('Preparing Content for External Use and Commercialisation') assesses the benefits and potential for impact of each application and the best approach from within and beyond the project.

There are similar activities embedded in the data service work packages, although these are somewhat less mature than the software applications that were intensively developed during CompBioMed1. As the project progresses there will be more experience of these services, and plans will be developed for the best route for their subsequent exploitation. Progress will be reported in the deliverables from those work packages in due course.

The same processes are being applied to new products and services emerging in CompBioMed2. Examples of those identified so far in CompBioMed2 include: new data transfer infrastructures developed in collaboration with DICE (Data Infrastructure Capacity for EOSC) and LEXIS (Large-scale Execution for PU



Industry and Society), for intense data transfer across HPC centre and data staging; an automated benchmark environment for code testing, code execution, analysis and postprocessing; code scalability support to increase the quality of code output; materials relating to courses for the introduction of student and professional medics to high performance computing and *in silico* research; and an e-Seminar series with 18 instalments to date (as of October 6 2021) covering a wide range of topics in computational biomedicine¹⁶.

7.2 Research into innovation process in computational biomedicine and applicability to CoE

PhD research within the Business School of the University of Amsterdam (UvA), which is co-sponsored by Atos, funded partner of the CoE, is using a case study from CompBioMed to explore the business case for the use of *in silico* biomedical research more widely in a clinical capacity.

The research carried out to date has been a use case of CT2S (see Appendix 10.11), which is a workflow to provide accurate estimations of human bone strength, currently used in clinical research but targeted for greater uptake. The research has included cost-effectiveness analysis of CT2S, an osteoporosis screening tool, to gather evidence for clinical adoption; this research has been carried out as a collaboration between University of Sheffield (USFD) and University of Bologna (UNIBO). The preliminary results from this study were presented at CompBioMed Conference 2021 and are now in preparation for submission to a peer-reviewed journal. In the study, cost effectiveness analysis was carried out to compare CT2S to a conventional screening tool (DXA) and a no screening scenario for post-menopausal women in the Netherlands, across a range of cost and screening intervals. Results across all age groups indicated that screen in any form has long term cost benefits, and that CT2S offers further cost benefits over conventional screening methods, particularly for those in the highest age groups in the study. Ongoing work includes the deployment of the CT2S code on HPC machines at SURF and cost analysis to compare this with other public cloud systems.

Planned future work in this domain will include an in-depth study into the cost and benefit of *in silico* trials using the 'BoneStrength' application, an expansion of CT2S under development at UNIBO, and comparison to equivalent *in vivo* trials, potentially building a business case for more general update of *in silico* methods.

7.3 Future Innovation Management Plans

Throughout the remaining duration of the project, the approach developed through the first and second phases of the project, and summarised in this deliverable, will be taken. There will be a continuation of attendance at WP meetings by WP1 representatives, and further capture of innovation, products and services to determine if further support and advice to originators is required. New products and services, and innovations arising from activities in CompBioMed2 will be further developed within the framework of the IP registry and incubator activities. New inventions, products and services arising from the research activities in the project, will be disseminated through available channels once the assessment of IP potential has been carried out and necessary steps have been taken to protect those which are commercially exploitable. Completion of the PhD research at UvA, it is hoped, will bring greater attention to the project from those with commercial interest in the medical and pharmaceutical industry.

¹⁶ <https://www.compbioimed.eu/events-2/>



8 Risk Management

The following possible sources of risks have been identified:

- a) **Pandemic related lockdowns restricting travel and social distancing measures may continue or be re-introduced, impacting CompBioMed in-person meetings and events.**

Probability	High
Impact	High
Risk Assessment	High
Mitigation	During the coronavirus pandemic we have become accustomed to running meeting and events in a virtual format, allowing them to proceed regardless of lockdowns or social distancing measures. Even large-scale events such as CompBioMed Conference 2021 were held online, demonstrating that all types of meetings and event can be converted to a virtual format. At the time of writing, in-person events are returning, and we are participating in them. However, we remain ready to adjust to virtual formats at even short notice, and factor this into our preparations.

- b) **Even with lockdowns and social distancing eased, people may feel reluctance to travel to and attend meetings and events in person, resulting in reduced attendance/participation.**

Probability	High
Impact	Medium
Risk Assessment	Medium
Mitigation	A solution to mitigate this risk, which is increasingly common during the period that lockdowns and social distance measures are easing, is the introduction of hybrid approaches to meetings and events, where attendees are given the option to attend in person or online. There is an appetite in the population to return to normality, and that drives people to attend meetings and events in person, but there is also a section of the population who remain reluctant to travel. Online/in-person hybrid events provide a solution for everyone, allowing healthy participation at meetings and events. This can either be done by allowing video/audio dial in options, streaming options, or video/audio recording and then later posting the video/audio online. The best approach depends on the type and scale of meeting.

9 Conclusions

There was a substantial amount of dissemination activity in the course of the first 25 months of CompBioMed2. The actions of the CompBioMed consortium have met and gone beyond the plans laid out in the dissemination action plan and the project's description of work. We adapted quickly and effectively to the challenges that the pandemic presented our dissemination work.

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, far beyond what we have been able to achieve prior to this period. The project's dissemination KPIs were met and exceeded.

In terms of innovation, we will continue to monitor CompBioMed2 innovations, capturing them and providing guidance using the established framework for innovation management.

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



10 Appendices

The appendices below list individual instances of dissemination activity categorised into activity types.

10.1 CompBioMed Publications

No.	Publication Title	Citation
1	Conformational Searching with Quantum Mechanics	Matthew Habgood, Tim James, Alexander Heifetz, Quantum Mechanics in Drug Discovery, 2114, DOI: 10.1007/978-1-0716-0282-9_14
2	From digital hype to analogue reality: Universal simulation beyond the quantum and exascale eras	Peter V. Coveney, Roger R. Highfield, Journal of Computational Science, 46, DOI: 10.1016/j.jocs.2020.101093
3	Ensemble-Based Steered Molecular Dynamics Predicts Relative Residence Time of A 2A Receptor Binders	Andrew Potterton, Fouad S. Hussein, Michelle W. Y. Southey, Mike J. Bodkin, Alexander Heifetz, Peter V. Coveney, Andrea Townsend-Nicholson, Journal of Chemical Theory and Computation, 15/5, 10.1021/acs.jctc.8b01270
4	Characterising GPCR–ligand interactions using a fragment molecular orbital-based approach	Alexander Heifetz, Tim James, Michelle Southey, Inaki Morao, Matteo Aldeghi, Laurie Sarrat, Dmitri G Fedorov, Mike J Bodkin, Andrea Townsend-Nicholson, Current Opinion in Structural Biology, 55, DOI:10.1016/j.sbi.2019.03.021
5	Are CT-Based Finite Element Model Predictions of Femoral Bone Strengthening Clinically Useful?	Marco Viceconti, Muhammad Qasim, Pinaki Bhattacharya, Xinshan Li, Current Osteoporosis Reports, 16/3, DOI: 10.1007/s11914-018-0438-8
6	The effect of boundary and loading conditions on patient classification using finite element predicted risk of fracture	Zainab Altai, Muhammad Qasim, Xinshan Li, Marco Viceconti, Clinical Biomechanics, 68, DOI: 10.1016/j.clinbiomech.2019.06.004
7	Identifying the start of a platelet aggregate by the shear rate and the cell-depleted layer	B. J. M. van Rooij, G. Závodszy, V. W. Azizi Tarkalooeyeh, A. G. Hoekstra, Journal of The Royal Society Interface, 16/159, DOI:10.1098/rsif.2019.0148
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9	Location-Specific Comparison Between a 3D In-Stent Restenosis Model and Micro-CT and Histology Data from Porcine In Vivo Experiments	P. S. Zun, A. J. Narracott, C. Chiastra, J. Gunn, A. G. Hoekstra, Cardiovascular Engineering and Technology, 10/4, 10.1007/s13239-019-00431-4
10	Application of the ESMACS Binding Free Energy Protocol to a Multi-Binding Site Lactate Dehydrogenase A Ligand Dataset	David W. Wright, Fouad Hussein, Shunzhou Wan, Christophe Meyer, Herman van Vlijmen, Gary Tresadern, Peter V. Coveney, Advanced Theory and Simulations, 3/1, 10.1002/adts.201900194
11	Continuum model for flow diverting stents in 3D patient-specific simulation of intracranial aneurysms	Sha Li, Bastien Chopard, Jonas Latt, Journal of Computational Science, 38, 10.1016/j.jocs.2019.101045
12	DeltaDelta neural networks for lead optimization of small molecule potency	José Jiménez-Luna, Laura Pérez-Benito, Gerard Martínez-Rosell, Simone Sciabola, Rubben Torella, Gary Tresadern, Gianni De Fabritiis, Chemical Science, 10/47, DOI: 10.1039/c9sc04606b
13	Drug-induced shortening of the electromechanical window is an effective biomarker for in silico prediction of clinical risk of arrhythmias	Passini, E., Trovato, C., Morissette, P., Sannajust, F., Bueno-Orovio, A., & Rodriguez, B. (2019). British journal of pharmacology, 176(19), 3819–3833. https://doi.org/10.1111/bph.14786
14	Improving the clinical understanding of hypertrophic cardiomyopathy by combining patient data, machine learning and computer simulations: A case study	Lyon, A., Mincholé, A., Bueno-Orovio, A., & Rodriguez, B. (2019). Morphologie : bulletin de l'Association des anatomistes, 103(343), 169–179. https://doi.org/10.1016/j.morpho.2019.09.001
15	High arrhythmic risk in antero-septal acute myocardial ischemia is explained by increased transmural reentry occurrence	Martinez-Navarro, H., Mincholé, A., Bueno-Orovio, A., & Rodriguez, B. (2019). Scientific reports, 9(1), 16803. https://doi.org/10.1038/s41598-019-53221-2
16	Blinded In Silico Drug Trial Reveals the Minimum Set of Ion Channels for Torsades de Pointes Risk Assessment	Zhou, X., Qu, Y., Passini, E., Bueno-Orovio, A., Liu, Y., Vargas, H. M., & Rodriguez, B. (2020). Frontiers in pharmacology, 10, 1643. https://doi.org/10.3389/fphar.2019.01643
17	The ‘Digital Twin’ to enable the vision of precision cardiology	Corral-Acero J, Margara F, Marciniak M, Rodero C, Loncaric F, Feng Y, Gilbert A, Fernandes JF, Bukhari HA, Wajdan A, Martinez MV, Santos MS, Shamohammadi M, Luo H, Westphal P, Leeson P, DiAchille P, Gurev V, Mayr M, Geris L, Pathmanathan P, Morrison T, Cornelussen R, Prinzen F, Delhaas T, Doltra A, Sitges M, Vigmond EJ, Zaccar E, Grau V, Rodriguez B, Remme EW, Niederer S, Mortier P, McLeod K, Potse M, Pueyo E, Bueno-Orovio A, Lamata P., Eur Heart J., 41(48):4556-4564 (2020), DOI:10.1093/eurheartj/ehaa159
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22	Human biventricular electromechanical simulations on the progression of electrocardiographic and mechanical abnormalities in post-myocardial infarction	Wang, Z. J., Santiago, A., Zhou, X., Wang, L., Margara, F., Levro-Florencia, F., Das, A., Kelly, C., Dall'Armellina, E., Vazquez, M., & Rodriguez, B. (2021), 23(23 Suppl 1), i143–i152, DOI:10.1093/europace/evaa405
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32	A 2-Step Deep Learning Method with Domain Adaptation for Multi-Centre, Multi-Vendor and Multi-Disease Cardiac Magnetic Resonance Segmentation	Acero, Jorge Corral, Vaanathi Sundaresan, Nicola Dinsdale, Vicente Grau, and Mark Jenkinson, In International Workshop on Statistical Atlases and Computational Models of the Heart, 196-207 (2020), DOI:10.1007/978-3-030-68107-4_20
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55	The effect of protein mutations on drug binding suggests ensuing personalised drug selection	S. Wan, D. Kumar, V. Ilyin, U. Al Homsy, G. Sher, A. Knuth, P. V. Coveney, Sci. Rep., 11, 13452 (2021), DOI: 10.1038/s41598-021-92785-w
56	Tutorial applications for Verification, Validation and Uncertainty Quantification using VECMA toolkit	D. Suleimenova, H. Arabnejad, W. N. Edeling, D. Coster, O. O. Luk, J. Lakhilvi, V. Jancaskas, M. Kulczewski, L. Veen, D. Ye, P. Zun, V. Krzhizhanovskaya, A. Hoekstra, D. Crommelin, P. V. Coveney, D. Groen, J. Comput. Sci., 53, 101402 (2021), DOI: 10.1016/j.jocs.2021.101402
57	In-silico human electro-mechanical ventricular modelling and simulation for drug-induced pro-arrhythmia and inotropic risk assessment	F. Margara, Z. J. Wang, F. Levrero-Florencio, A. Santiago, M. Vázquez, A. Bueno-Orovio and B. Rodriguez, Progress in Biophysics and Molecular Biology, 159, 58-74 (2021), DOI: 10.1016/j.pbiomolbio.2020.06.007
58	When We Can Trust Computers (and When We Can't)	P. V. Coveney and R. R. HighfieldPhil. Trans. R. Soc. A., 379, 20200409 (2021), DOI: 10.1098/rsta.2020.0067
59	Finite element analysis informed variable selection for femoral fracture risk prediction	M. Taylor, M. Viceconti, P. Bhattacharya, X. Li, Journal of the Mechanical Behavior of Biomedical Materials, 118, 104434 (2021) DOI: 10.1016/j.jmbbm.2021.104434
60	Evaluation of patient tissue selection methods for deriving equivalent density calibration for femoral bone quantitative CT analyses	C. Winsor, X. Lib, M. Qasim, C. R. Henaka, P. J. Pickhardt, H. Ploeg, M. Viceconti, Bone, 143 (2021) DOI: 10.1016/j.bone.2020.115759
61	TorchMD: A Deep Learning Framework for Molecular Simulations	S. Doerr, M. Majewski, A. Pérez, A. Krämer, C. Clementi, F. Noe, T. Giorgino, and G. De Fabritiis, J. Chem. Theory Comput., 17, 4, 2355–2363 (2021), DOI: 10.1021/acs.jctc.0c01343
62	Uncertainty Quantification in Classical Molecular Dynamics	S. Wan, R. C. Sinclair and P. V. Coveney, Phil. Trans. R. Soc. A, 379, 20200082 (2021), DOI: 10.1098/rsta.2020.0082
63	The influence of external electric fields on proton transfer tautomerism in the guanine-cytosine base pair	A. Gheorghiu, P. V. Coveney and A. A. Arabi, Phys. Chem. Chem. Phys. 23, 6252-6265 (2021), DOI: 10.1039/D0CP06218A
64	The Impact of Uncertainty on Predictions of the CovidSim Epidemiological Code	W. Edeling, H. Arabnejad, R. Sinclair, D. Suleimenova, K. Gopalakrishnan, B. Bosak, D. Groen, I. Mahmood, D. Crommelin and P. Coveney, Nat Comput Sci, 1, 128–135 (2021), DOI: 10.1038/s43588-021-00028-9
65	TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing	M. Bieniek, A. Bhati, S. Wan and P. V. Coveney, J. Chem. Theory Comput., 17, 2, 1250–1265 (2021), DOI: 10.1021/acs.jctc.0c01179
66	Pharmaceutical Industry—Academia Cooperation	A. Heifetz, P. V. Coveney, D. G. Fedorov, I. Morao, T. James, M. Southey, K. Papadopoulos, M. J. Bodkin, A. Townsend-Nicholson, in: Mochizuki Y., Tanaka S., Fukuzawa K. (eds) Recent Advances of the Fragment Molecular Orbital Method, Springer, Singapore (2021), DOI: 10.1007/978-981-15-9235-5_15
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68	Guiding Medicinal Chemistry with Fragment Molecular Orbital (FMO) Method	A. Heifetz, T. James, M. Southey, M. J. Bodkin, S. Bromidge, Quantum Mechanics in Drug Discovery. Methods in Molecular Biology, vol. 2114, 37-48 (2020) DOI: 10.1007/978-1-0716-0282-9_3
69	Accurate Scoring in Seconds with the Fragment Molecular Orbital and Density-Functional Tight-Binding Methods	I. Morao, A. Heifetz, D. G. Fedorov, Quantum Mechanics in Drug Discovery. Methods in Molecular Biology, vol. 2114, 143-148 (2020) DOI: 10.1007/978-1-0716-0282-9_9
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73	Characterizing Protein-Protein Interactions with the Fragment Molecular Orbital Method	A. Heifetz, V. Sladek, A. Townsend-Nicholson, D. G. Fedorov, In: Quantum Mechanics in Drug Discovery, part of Methods in Molecular Biology, vol. 2114, 187-205 (2020), DOI: 10.1007/978-1-0716-0282-9_13
74	Characterizing Rhodopsin-Arrestin Interactions with the Fragment Molecular Orbital (FMO) Method	A. Heifetz, A. Townsend-Nicholson, Methods Mol Biol. 2114:177-186 (2020) DOI: 10.1007/978-1-0716-0282-9_12
75	Analyzing GPCR-Ligand Interactions with the Fragment Molecular Orbital (FMO) Method	A. Heifetz, T. James, M. Southey, I. Morao, D. G. Fedorov, M. J. Bodkin, A. Townsend-Nicholson, In: Quantum Mechanics in Drug Discovery, part of Methods in Molecular Biology, vol. 2114, 163-175 (2020), DOI: 10.1007/978-1-0716-0282-9_11
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80	Hydrodynamic Resistance of Intracranial Flow-Diverter Stents: Measurement Description and Data Evaluation	B. Csispa, D. Gyürki, G. Závodszy, I. Szikora and G. Paál, Cardiovascular Engineering and Technology 11, 1–13 (2020) DOI: 10.1007/s13239-019-00445-y
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84	AdaptiveBandit: A Multi-armed Bandit Framework for Adaptive Sampling in Molecular Simulations	A. Pérez, P. Herrera-Nieto, S. Doerr, and G. De Fabritiis, J. Chem. Theory Comput. 16, 7, 4685–4693 (2020) DOI: 10.1021/acs.jctc.0c00205
85	Coarse graining molecular dynamics with graph neural networks	B. E. Husic, N. E. Charron, D. Lemm, J. Wang, A. Pérez, M. Majewski, A. Krämer, Y. Chen, S. Olsson, G. de Fabritiis, F. Noé and Cecilia Clementi, J. Chem. Phys. 153, 194101 (2020), DOI: 10.1063/5.0026133
86	SkeleDock: A Web Application for Scaffold Docking in PlayMolecule	A. Varela-Rial, M. Majewski, A. Cuzzolin, G. Martínez-Rosell and Gianni De Fabritiis, J. Chem. Inf. Model. 60, 6, 2673–2677 (2020), DOI: 10.1021/acs.jcim.0c00143
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91	Coupling one-dimensional arterial blood flow to three-dimensional tissue perfusion models for in silico trials of acute ischaemic stroke	R. M. Padmos, T. I. Józsa, W. K. El-Bouri, P. R. Konduri, S. J. Payne and A. G. Hoekstra, J R Soc Interface Focus, 11, 20200082 (2020), 10.1098/rsfs.2020.0082
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94	Electrophysiological and anatomical factors determine arrhythmic risk in acute myocardial ischaemia and its modulation by sodium current availability	H. Martinez-Navarro, X. Zhou, A. Bueno-Orovio and B. Rodriguez, J R Soc Interface Focus, 11, 20200082 (2020), 10.1098/rsfs.2020.0082
95	The EurValve model execution environment	M. Bubak, K. Czechowicz, T. Gubała, D. R. Hose, M. Kasztelnik, M. Malawski, J. Meizner, P. Nowakowski and S. Wood, J R Soc Interface Focus, 11, 20200082 (2020), 10.1098/rsfs.2020.0082
96	Analysis of mechanotransduction dynamics during combined mechanical stimulation and modulation of the extracellular-regulated kinase cascade uncovers hidden information within the signalling noise	G. Ascolani, T. M. Skerry, D. Lacroix, E. Dall’Ara and A. Shuaib, J R Soc Interface Focus, 11, 20200082 (2020), 10.1098/rsfs.2020.0082
97	Deep medical image analysis with representation learning and neuromorphic computing	N. Getty, T. Brettin, D. Jin, R. Stevens and F. Xia, J R Soc Interface Focus, 11, 20200082 (2020), 10.1098/rsfs.2020.0082
98	Computational biomedicine. Part I: molecular medicine – Introduction	S. Wan, A. Potterton, F. S. Hussein, D. W. Wright, A. Heifetz, M. Malawski, A. Townsend-Nicholson and P. V. Coveney, J R Soc Interface Focus, 10, 20190128 (2020), DOI: 10.1098/rsfs.2020.0047
99	Hit-to-lead and lead optimization binding free energy calculations for G protein-coupled receptors	S. Wan, A. Potterton, F. S. Hussein, D. W. Wright, A. Heifetz, M. Malawski, A. Townsend-Nicholson and P. V. Coveney, J R Soc Interface Focus, 10, 20190128 (2020), DOI: 10.1098/rsfs.2019.0128
100	On the faithfulness of molecular mechanics representations of proteins towards quantum-mechanical energy surfaces	G. König and S. Riniker, J R Soc Interface Focus, 10, 20190121 (2020), DOI: 10.1098/rsfs.2019.0121
101	How quickly can we predict trimethoprim resistance using alchemical free energy methods?	P. W. Fowler, J R Soc Interface Focus, 10, 20190141 (2020), DOI: 10.1098/rsfs.2019.0141
102	Large-scale binding affinity calculations on commodity compute clouds	S. J. Zasada, D. W. Wright and P. V. Coveney, J R Soc Interface Focus, 10, 20190133 (2020), DOI: 10.1098/rsfs.2019.0133
103	Rapid, accurate, precise and reproducible ligand–protein binding free energy prediction	S. Wan, A. P. Bhati, S. J. Zasada and P. V. Coveney, J R Soc Interface Focus, 10, 20200007 (2020), DOI: 10.1098/rsfs.2020.0007
104	The influence of base pair tautomerism on single point mutations in aqueous DNA	A. Gheorghiu, P. V. Coveney and A. A. Arabi, J R Soc Interface Focus, 10, 20190120 (2020), DOI: 10.1098/rsfs.2019.0120
105	Quantum computing using continuous-time evolution	V. Kendon, J R Soc Interface Focus, 10, 20190143 (2020), DOI: 10.1098/rsfs.2019.0143
106	Educating and engaging new communities of practice with high performance computing through the integration of teaching and research	A. Townsend-Nicholson, J R Soc Interface Focus, 10, 20200003 (2020), DOI: 10.1098/rsfs.2020.0003
107	Sensitivity analysis of a strongly-coupled human-based electromechanical cardiac model: Effect of mechanical parameters on physiologically relevant biomarkers	F. Levrero-Florencio, F. Margara, E. Zacur, A. Bueno-Orovio, Z. J. Wang, A. Santiago, J. Aguado-Sierra, G. Houzeaux, V. Grau, D. Kay, M. Vázquez, R. Ruiz-Baier, B. Rodriguez, Computer Methods in Applied Mechanics and Engineering, 361 (2020) DOI: 10.1016/j.cma.2019.112762
108	The influence of red blood cell deformability on hematocrit profiles and platelet margination	B. Czaja, M. Gutierrez, G. Závodszy, D. de Kanter, A. Hoekstra, O. Eniola-Adefeso, PLoS Comput Biol, 16(3): e1007716, 2020, DOI: 10.1371/journal.pcbi.1007716

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110	Lattice-Boltzmann interactive blood flow simulation: Sensitivity analysis of a strongly-coupled human-based electromechanical cardiac model: Effect of mechanical parameters on physiologically relevant biomarkers on pipeline	S. S. Esfahani, X. Zhai, M. Chen, A. Amira, F. Bensaali, J. AbiNahed, S. Dakua, G. Younes, A. Baobeid, R. A. Richardson and P. V. Coveney, Int J CARS 15, pp. 629–639, 2020, DOI: 10.1007/s11548-020-02120-3
111	Hemoglobin Acceleration and Visualization for Cerebral Aneurysms	S. S. Esfahani, X. Zhai, M. Chen, A. Amira, F. Bensaali, J. AbiNahed, S. Dakua, G. Younes, R. A. Richardson and P. V. Coveney, 2019 IEEE International Conference on Image Processing (ICIP) Taipei, Taiwan, pp. 1376–1380, 2020, DOI: 10.1109/ICIP.2019.8803712
112	Accuracy and Precision of Alchemical Relative Free Energy Predictions With and Without Replica-Exchange	S. Wan, G. Tresadem, L. Perez-Benito, H. van Vlijmen, P. V. Coveney, Advanced Theory and Simulations, 3(1), 1900195, 2020, DOI: 10.1002/adts.201900195

10.2 Popularised Publications

No.	Description of Activity	Audience(s) (see above table)	No. of People
1	Daniele Tartarini (USFD) published an article on "ExaHyPE's OpenMP GPGPU Port—Lessons Learned" Online Article on peano-framework on 30 July 2020 http://www.peano-framework.org/wp-content/uploads/2020/08/GPGPU_Lessons_Learned.pdf	[Scientific community], [General Public]	50
2	Elisa Passini (Oxford) and CompBioMed featured in an article on "Is the end of animal testing in sight?" that featured in E&T, Engineering & Technology on The Institution of Engineering and Technology (IET) website on 10 December 2019 https://eandt.theiet.org/content/articles/2019/12/is-the-end-of-animal-testing-in-sight/	[Scientific Community (higher education, Research)], [Industry], [General Public]	625,000
3	UCL CompBioMed coronavirus research featured in The Daily Telegraph print newspaper in an article titled "Supercomputers aid the search for a cure", on 7 April 2020	[General Public] [Medias]	2,300,000
4	UCL CompBioMed coronavirus research featured on The Telegraph website (telegraph.co.uk) in the article "Your smartphone could help fight coronavirus while you sleep", on 8 April 2020 https://www.telegraph.co.uk/technology/2020/04/08/smartphone-could-help-fight-coronavirus-sleep/	[General Public] [Medias]	2,000,000
5	UCL CompBioMed coronavirus research featured in The Sun in an article titled "Hi-Tech Hunt", on 7 April 2020	[General Public] [Medias]	2,600,000
6	UCL CompBioMed coronavirus research featured in the ITV News article "Scientists using world's most powerful supercomputers to tackle coronavirus", on 7 April 2020. https://www.itv.com/news/2020-04-07/scientists-using-worlds-most-powerful-supercomputers-to-tackle-coronavirus	[General Public] [Medias]	200,000
7	UCL CompBioMed research featured in the Dail Mail article "Scientists are using the world's most powerful supercomputers to speed up the development of treatments for the deadly coronavirus", on 21 July 2020 https://www.dailymail.co.uk/sciencetech/article-8192785/Worlds-powerful-supercomputers-used-speed-coronavirus-treatment.html	[General Public] [Medias]	2,000,000
8	UCL CompBioMed research featured in the Irish Examiner article on "Scientists using world's most powerful supercomputers to tackle coronavirus", on 7 April 2020 http://www.irishexaminer.com/breakingnews/world/scientists-using-worlds-most-powerful-supercomputers-to-tackle-coronavirus-992578.html?utm_source=dlvr.it&utm_medium=twitter	[General Public] [Medias]	200,000
9	Tech Central (techcentral.co.za) published the article "How supercomputers are being used to tackle Covid-19" featuring CompBioMed coronavirus research, on 7 April 2020 https://techcentral.co.za/how-supercomputers-are-being-used-to-tackle-covid-19/97145/	[Scientific Community (higher education, Research)], [Industry], [General Public]	40,000
10	BBC Science Focus (sciencefocus.com) published the article "Coronavirus: supercomputers drafted in to detect potential treatments" featuring CompBioMed coronavirus research, on 7 April 2020 https://www.sciencefocus.com/news/coronavirus-supercomputers-drafted-in-to-detect-potential-treatments/	[Scientific Community (higher education, Research)], [Industry], [General Public]	200,000
11	The Evening Standard published the article "Supercomputers speed up search for a treatment" that featured CompBioMed coronavirus research, on 7 April 2020	[General Public] [Medias]	1,200,000
12	CompBioMed coronavirus research featured in a Newsweek article on "How Supercomputers Are Being Used to Win the Fight Against Coronavirus" on 14 April 2020 https://www.newsweek.com/supercomputers-coronavirus-covid19-research-science-vaccine-treatment-white-house-1497719	[General Public] [Medias]	5,000,000
13	CompBioMed coronavirus research featured in an online Süddeutsche Zeitung article on "Bis der Supercomputer anschlägt", on 9 April 2020 https://www.sueddeutsche.de/digital/coronavirus-pandemie-medikamente-supercomputer-forschung-1.4870862?reduced=true	[General Public] [Medias]	5,000,000
14	CompBioMed coronavirus research featured in a print Süddeutsche Zeitung article on "Rechnen mit Molekülen", on 8 April 2020 https://www.sueddeutsche.de/digital/coronavirus-pandemie-medikamente-supercomputer-forschung-1.4870862?reduced=true	[General Public] [Medias]	330,000
15	CompBioMed coronavirus research featured in an AOL article on "Scientists using world's most powerful supercomputers to tackle coronavirus", on 6 April 2020 https://www.aol.co.uk/news/2020/04/06/scientists-using-worlds-most-powerful-supercomputers-to-tackle/?guccounter=1&guce_referrer=aHR0cHM6Ly93d3cudWNsLmFjLnVrLw&guce_referrer_sig=AQAAAFnoXf8TbLpsn4wYvYvOiu_jBISlHzyD2Wbnp92X9jhe7aLDRhigcISVUyKcAGhuHUhEm3xZEEERbafnWZDtCiVgMNIopCrISOMVTOkhkBNAAewvZ8GjmN_IsTzDtU6YUPt7Z_6hKoGESDGAykwutufLnvYackBrGwmlc8h	[General Public] [Medias]	10,000,000



16	Sky News published an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" that featured CompBioMed coronavirus research, on 3 June 2020	[General Public] [Medias]	7,500,000
17	Yahoo! News posted an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" featuring CompBioMed coronavirus research, on 3 June 2020 https://uk.news.yahoo.com/pandemic-1-7-million-unknown-viruses-potential-infect-022600763.html	[General Public] [Medias]	10,000,000
18	Gulf News posted an article on "Going Viral: Day 67 Under COVID-19 Lockdown" featuring CompBioMed coronavirus research, on 4 June 2020 https://gulfnews.com/world/europe/going-viral-day-67-under-covid-19-lockdown-1.1591246048978	[General Public]	2,000,000
19	Science Business posted an article on "UCL researchers are using the world's most powerful supercomputers to tackle COVID-19" featuring CompBioMed coronavirus research on 7 April 2020 https://sciencebusiness.net/network-updates/ucl-researchers-are-using-worlds-most-powerful-supercomputers-tackle-covid-19	[Scientific Community (higher education, Research)], [Industry], [General Public]	5,000
20	EuroNews posted an article on "Virtual humans to map the future of major surgery" featuring CompBioMed research, on 10 September 2020 https://www.euronews.com/2020/08/24/digital-doppelgangers-to-map-the-future-of-major-surgery	[General Public] [Medias]	2,600,000
21	Futura Sante posted an article titled "In video: your digital avatar will serve as a medical guinea pig" featuring CompBioMed research, the Virtual Humans film, and the Euronews video, on 29 August 2020, https://www.futura-sciences.com/sante/actualites/medecine-video-votre-avatar-numerique-servira-cobaye-medical-82637/	[General Public] [Medias]	1,400,000
22	Playtech.ro posted an article titled "Oamenii de știință vor să îți creeze un geamă virtual, iar motivul e cât se poate de îmbucurător" featuring CompBioMed research, and the Virtual Humans Film, on 26 August 2020	[General Public] [Medias]	1,000,000
23	Yahoo! Actualités posted an article titled "In video: meeting with the digital avatar, virtual double of your body" leading to the Futura Sante article, on 26 August 2020 https://fr.news.yahoo.com/vid%C3%A9o-rencontre-l-avatar-num%C3%A9rique-103000487.html?guccounter=1&guce_referrer=aHR0cHM6Ly93d3cuZ29vZ2xlLnNvbS8&guce_referrer_sig=AQAAAN6cw55soN4gKBUSVuOk7vxXfqHpqD4azwq7X01t6wXXKie4l-h0cFtmEWdpUUrQXctjpnq1VBUqW7LMx04q61YPBBd9p3UgtNVJWYz2r-n5FclNou1m8nalJQeFTzq4C00RSotuxx1AdxOeUq-NHl2hG4HDz9sJwGFwJAMq2W4W	[General Public] [Medias]	2,000,000
24	Nacional Neovisni News Magazin posted an article titled "Koncept virtualnog pacijenta i dalje koristan zdravstvenim radnicima" covering CompBioMed research, on 25 August 2020 https://www.nacional.hr/koncept-virtualnog-pacijenta-ce-dalje-biti-koristan-zdravstvenim-radnicima/	[General Public]	80,000
25	iPro Up posted an article titled "Biomedicina: así funcionan los "gemelos humanos virtuales" que prometen salvar miles de vidas en los próximos años" featuring CompBioMed research and the Virtual Humans film,	[General Public]	80,000
26	Ziarul de Iasi posted an article titled "Oamenii de știință vor să îți creeze un geamă virtual. Ai accepta?" linking to the playtech.ro article featuring CompBioMed research and the Virtual Humans film, on 26 August 2020	[General Public]	150,000
27	UCL Alumni Magazine posted an article on CompBioMed's coronavirus research, in October 2020	[Scientific Community (higher education, Research)]	200
28	Reformatorisch Dagblad published an article on "Supercomputer brengt patiënt virtueel in beeld" featuring CompBioMed research, on 4 November 2020 https://www.rd.nl/artikel/884377-supercomputer-brengt-patient-virtueel-in-beeld	[General Public], [Medias]	160,000
29	Nature published an article on "Simulating the pandemic: What COVID forecasters can learn from climate models" on CompBioMed's CovidSim UQ work, on 13 November 2020 https://www.nature.com/articles/d41586-020-03208-1	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	3,000,000
30	WIRED IT (Italy) published an article titled "Il gemello Virtuale" on CompBioMed's virtual human work, on 16 March 2021. Wired IT, Vol 96, Spring 2021 Health Edition, ISSN 2035-7397	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	6,300,000
31	Il Sole 24ORE's (Italy) associated magazine "Platinum Aziende & Protagonisti" published an article on "High performance computing and machine learning to defeat the pandemic" concerning CompBioMed coronavirus research, on 19 July 2021	[General Public], [Medias]	382,112
32	PCMag UK posted an article on "Welcome to the Virtual Humans Factory" featuring CompBioMed research, on 8 April 2021 https://uk.pcmag.com/health-fitness/132648/welcome-to-the-virtual-humans-factory	[General Public]	200,000
33	EPCC posted an article titled "Creating Virtual Humans" about CompBioMed2 and CBMC21 in the EPCC News Publication, in Summer 2021 https://issuu.com/epccedinburgh/docs/epcc_news_89_web	[Scientific Community (higher education, Research)], [Industry]	845

10.3 Film, Video, and Television

No.	Description of Activity	Audience(s) (see above table)	No. of People
34	Peter Coveney and Andrea Townsend-Nicholson (UCL) appeared on the EuroNews Futuris Programme, on a piece about "Virtual Humans to map the future of major surgery", on 10 September 2020, the piece ran multiple times throughout the day	[General Public], [Medias]	7,000,000
35	Roger Highfield (Science Museum) mentioned CBM COVID-19 research on the BBC Today Programme, in the week of March 23rd 2020	[General Public], [Medias]	7,000,000
36	Roger Highfield (Science Museum) mentioned CBM COVID-19 research on BBC Newshour (BBC Sounds) on the BBC World Service on 25 March	[General Public], [Medias]	10,000,000



	https://www.bbc.co.uk/sounds/play/w172wq5849yy557		
37	Peter Coveney (UCL) appeared on BBC NEWS World Service on a piece on "Supercomputers seeking solutions for Covid-19", on 18 April 2020 https://www.bbc.co.uk/programmes/w3csz97r	[General Public], [Medias]	10,000,000
38	Andrea Townsend-Nicholson (UCL) and Cristin Merritt appeared on the Turbulence at the Exascale podcast: Women in HPC on 11 February 2021 https://www.youtube.com/watch?v=ycgC6ppTO_Q	[Scientific Community (higher education, Research)], [Industry], [General Public]	101
39	Peter Coveney's (UCL) talk on "Supercomputing, COVID-19 and the Transformation of Medicine" at ISC 2020, featuring CompBioMed coronavirus and other research, was posted on the ISC Group Videos Youtube channel on 6 July 2020 https://youtu.be/1iFGfpdp_Gg	[Scientific Community (higher education, Research)], [Industry], [General Public]	437
40	The Primeur Magazine Youtube channel posted a video titled "Peter Coveney explains the HPC and Supercomputing support for COVID-19 research in Europe" about Peter Coveney's (UCL) talk at ISC 2020, on 29 Jun 2020 https://www.youtube.com/watch?v=AHb4llzFDQw&t=4s	[Scientific Community (higher education, Research)], [Industry], [General Public]	55
41	The Euronews Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 24 August 2020 https://www.youtube.com/watch?v=1gU1N_YwC4	[General Public], [Medias]	615
42	The Euronews Next Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 24 August 2020 https://youtu.be/yeCCHuQeEPU	[General Public], [Medias]	1,512
43	The Digital EU Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 31 August 2020 https://youtu.be/8DrE3dD-ywQ	[General Public], [Medias]	97
44	Wouter Edeling (CWI) of the VECMA project posted a video seminar of the CompBioMed CovidSim UQ work on Youtube, on 10 June 2021 https://www.youtube.com/watch?v=HzNeByTh74E	[Scientific Community (higher education, Research)], [Industry], [General Public]	12
45	A video of CompBioMed's collaboration with FocusCoE, BioExcel and PerMedCoE was posted on the HiPEAC Youtube channel. It was a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference 2021. The video was posted on 7 May 2021 https://www.youtube.com/watch?v=CNa2j7HAXmU	[Scientific Community (higher education, Research)], [Industry]	90
46	Emily Lumley (UCL) posted 49 videos on the CompBioMed YouTube channel	[Scientific Community (higher education, Research)], [Industry], [Industry], [General Public]	31,618

10.4 Social Media

No.	Description of Activity	Audience(s) (see above table)	No. of People
47	SURF tweeted on 20 April about the MPI/OpenMP course on 9-11 June https://twitter.com/SURF_onderzoek/status/1384416777032118272	[General Public]	1,619
48	EPCC posted on the EPCC Blog about CompBioMed2 and the CompBioMed21 conference, in July 2021 https://www.epcc.ed.ac.uk/blog/2021/07/compbio-med-creating-virtual-humans	[Scientific Community (higher education, Research)], [Industry], [General Public], [Policy makers], [Customers], [Other]	100
49	Roger Highfield tweeted about his article "CORONAVIRUS: WHAT WE KNOW (AND DON'T KNOW) ABOUT THE VIRUS" featuring CompBioMed on 25 March 2020	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	17,600
50	The eResearch UCL Twitter account, @eResearch_UCL, tweeted about the article "Using the world's most powerful supercomputers to tackle COVID-19" featuring CompBioMed research, on 16 April 2020	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	3,299
51	The Irish Examiner twitter account, @irishexaminer, tweeted about UCL CompBioMed research featured in the article on "Scientists using world's most powerful supercomputers to tackle coronavirus", on 7 April 2020 https://twitter.com/irishexaminer/status/1247302702826020865?s=20	[General Public], [Medias]	222,900
52	The twitter account @breakingnewsie tweeted about the Irish Examiner article on "Scientists using world's most powerful supercomputers to tackle coronavirus", on 7 April 2020 https://twitter.com/breakingnewsie/status/1247302703010594818?s=20	[General Public], [Medias]	76,000
53	The Newsweek Twitter account, @Newsweek, tweeted about CompBioMed coronavirus research on 14 April 2020 https://twitter.com/Newsweek/status/1250118124353007616	[General Public], [Medias]	3,400,000
54	Andy Grant (Atos) posted on LinkedIn about CompBioMed coronavirus research on 15 Apr 2020	[Scientific Community (higher education, Research)], [Industry], [General Public]	3,026
55	The Sky News twitter account, @skynews, tweeted about an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" featuring CompBioMed Coronavirus Research, on 3 June 2020 https://twitter.com/SkyNews/status/1268008281676697600?s=20	[General Public], [Medias]	7,300,000
56	LRZ posted a news item on linkedin featuring CompBioMed and the Euronews piece, on 26 August 2020 https://www.linkedin.com/posts/leibniz-supercomputing-centre_virtual-humans-to-map-the-future-of-major-activity-6704676553021771776-t4-K/	[Scientific Community (higher education, Research)], [Industry]	1,170
57	ET Works (@etnetworks) tweeted about a Roger Highfield (Science Museum) webinar on "Tomorrow's Technology Today" in which he presented the Virtual Humans, on 12 November 2020	[Scientific Community (higher education, Research)], [Industry], [General Public]	250
58	Nature (@NaturePortfolio) tweeted about CompBioMed's CovidSim UQ work on 13 November 2020 https://twitter.com/NaturePortfolio/status/1327383050913771521?s=19	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	2,200,000

		Public]	
59	Nature (@Nature) tweeted about CompBioMed's CovidSim UQ work on 13 November 2020 https://twitter.com/Nature/status/1327305419405090816?s=20	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	2,100,000
60	Nature (@Nature) tweeted about CompBioMed's CovidSim UQ work on 16 November 2020 https://twitter.com/Nature/status/1327305419405090816?s=20	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	2,100,000
61	Nature (@Nature) tweeted about CompBioMed's CovidSim UQ work on 17 November 2020 https://twitter.com/Nature/status/1327305419405090816?s=20	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	2,100,000
62	The Nature facebook page posted on facebook about CompBioMed's CovidSim UQ work on 13 November 2020 https://www.facebook.com/nature/posts/10158183838268167	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	514,198
63	The Medical Research Council, @The_MRC, tweeted Roger Highfield's blog on Virtual Pandemics featuring CompBioMed's CovidSim UQ work, on 23 November 2020 https://twitter.com/The_MRC/status/1330818479235211265?s=20	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	76,400
64	LRZ posted a news item on linkedin featuring CompBioMed, in January 2021 https://www.linkedin.com/posts/leibniz-supercomputing-centre_the-advancement-of-hpc-towards-exascale-computing-activity-6757614656090583040-RiJe/	[Scientific Community (higher education, Research)], [Industry]	1,170
65	Krishnakumar Gopalakrishnan (UCL) posted on linkedin about the CompBioMed CovidSim UQ work, in February 2021 https://www.linkedin.com/posts/krishnakumargopalakrishnan_the-impact-of-uncertainty-on-predictions-activity-6770000461920653312-yGVm/	[Scientific Community (higher education, Research)], [Industry]	50
66	LRZ posted a news item on linkedin concerning CompBioMed research, in June 2021 https://www.linkedin.com/posts/leibniz-supercomputing-centre_digitaltwin-research-v2c-activity-6813382842039447552-SPfn/	[Scientific Community (higher education, Research)], [Industry]	1,170
67	Gavin Pringle (EPCC), Emily Lumley (UCL), Marc Derquennes posted an article titled "CompBioMed is joining the LEXIS Project Open Call" on linkedin on 30 March 2021 https://www.linkedin.com/pulse/compbiomed-joining-lexis-project-open-call-marc-derquennes	[Scientific Community (higher education, Research)], [Industry], [General Public], [Policy makers], [Customers], [Other]	50
68	Emily Lumley (CBK) posted 77 posts on the CompBioMed LinkedIn page https://www.linkedin.com/company/compbiomed/	[Scientific Community (higher education, Research)], [Industry], [General Public]	6,787
69	Emily Lumley (CBK) tweeted 523 times on the CompBioMed Twitter account https://twitter.com/bio_comp	[Scientific Community (higher education, Research)], [Industry], [General Public]	180,129

10.5 Websites

No.	Description of Activity	Audience(s) (see above table)	No. of People
70	SURF posted an article on "Working towards virtual humans in the CompBioMed project" on the SURF website https://www.surf.nl/en/working-towards-virtual-humans-in-the-compbiomed-project	[General Public]	100
71	Roger Highfield (Science Museum) posted a blog article on "CORONAVIRUS: WHAT WE KNOW (AND DON'T KNOW) ABOUT THE VIRUS" on the Science Museum Group Blog on 23 March 2020. https://www.sciencemuseumgroup.org.uk/blog/coronavirus-science-what-we-know-and-dont-know-about-the-virus/	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
72	UCL posted an article on "Using the world's most powerful supercomputers to tackle COVID-19" on the UCL website, featuring CompBioMed coronavirus research, on 7 April 2020. https://www.ucl.ac.uk/news/supercomputers	[Scientific Community (higher education, Research)]	500
73	Roger Highfield (Science Museum) posted a blog article on "UP CLOSE WITH CORONAVIRUS" which linked to CompBioMed coronavirus research, on 13 April 2020 https://www.sciencemuseumgroup.org.uk/blog/up-close-with-coronavirus/	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
74	Roger Highfield (Science Museum) posted a blog article on "CORONAVIRUS: QUEST FOR A CURE" featuring CompBioMed coronavirus research, on 4 May 2020 https://www.sciencemuseumgroup.org.uk/blog/coronavirus-quest-for-a-cure/	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
75	Gauss Centre for Supercomputing (GCS) posted an article on "GCS Centres Support Research to Mitigate Impact of COVID-19 Pandemic" featuring CompBioMed coronavirus research, on 11 May 2020 https://www.gauss-centre.eu/news/research-highlights/article/gcs-centres-support-research-to-mitigate-impact-of-covid-19-pandemic/	[Scientific Community (higher education, Research)], [Industry], [Industry]	100
76	Roger Highfield (Science Museum) posted a blog article on "CORONAVIRUS: FROM ANTIBODIES TO VACCINES" featuring CompBioMed coronavirus research, on 1 June 2020, https://www.sciencemuseumgroup.org.uk/blog/coronavirus-from-antibodies-to-vaccines/	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
77	UCL posted a news item on "Supercomputers can increase predictions' accuracy" featuring CompBioMed coronavirus research, on 3 June 2020 https://www.ucl.ac.uk/news/headlines/2020/jun/supercomputers-can-increase-predictions-accuracy	[Scientific Community (higher education, Research)]	500
78	SpiritFM posted an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" featuring CompBioMed coronavirus research, on 3 June 2020 https://www.spiritfm.net/news/national-news/3115619/after-the-pandemic-17-million-unknown-viruses-have-potential-to-infect-humans/	[General Public]	100
79	PirateFM posted an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" featuring CompBioMed coronavirus research, on 3 June 2020 https://www.piratefm.co.uk/news/uk-news/3115617/after-the-pandemic-17-million-unknown-viruses-have-potential-to-infect-humans/	[General Public]	100

80	Simple News posted an article on "After The Pandemic: 1.7 million unknown viruses have potential to infect humans" featuring CompBioMed coronavirus research, on 3 June 2020 https://simplenews.co.uk/uk/after-the-pandemic-1-7-million-unknown-viruses-have-potential-to-infect-humans/	[General Public]	2,000
81	Al Khaleej Today posted an article on "Going Viral: Day 67 Under COVID-19 Lockdown" featuring CompBioMed coronavirus research, on 4 June 2020 https://al-khaleejtoday.net/international/108676/Going-Viral-Day-67-under-COVID-19-lockdown.html	[General Public]	5,000
82	LRZ posted an article on "Simulating the Human" featuring CompBioMed coronavirus and other research, on 31 March 2020 https://www.lrz.de/presse/ereignisse/2020-03-31_Simulating-the-Human/	[Scientific Community (higher education, Research)], [Industry]	20,000
83	ARCHER posted new on their website about "'covid-sim" COVID-19 pandemic modelling tool available on ARCHER" on 29 April and 6 May 2020	[Scientific Community (higher education, Research)]	100
84	iatranshumanisme.com posted an article titled "Virtual humans: the future of surgical procedures" featuring CompBioMed research and the Virtual Humans film on 28 August 2020 https://iatranshumanisme.com/2020/08/28/humains-virtuels-le-futur-des-interventions-chirurgicales/	[Scientific Community (higher education, Research)], [Industry], [General Public]	100
85	Patient Numérique posted an article titled "La médecine personnalisée passe-t-elle par les "jumeaux numériques"?" featuring CompBioMed research and the Virtual Humans film, on 31 August 2020 https://www.patientnumerique.com/actus/actualites/2020/08/la-medecine-personnalisee-passe-t-elle-par-les-jumeaux-numeriques/	[General Public]	200
86	Daily Factline posted an article titled "Virtual Humans Assist In Mapping The Future Of Major Surgery" featuring CompBioMed research, on 7 September 2020 https://dailyfactline.com/virtual-humans-assist-in-mapping-the-future-of-major-surgery/	[General Public]	200
87	ECH Alliance posted an article titled "Virtual humans to map the future of major surgery" featuring CompBioMed research and the Virtual Humans Film, on 3 September 2020	[General Public]	200
88	Roger Highfield (Science Museum) posted a blog article on "CORONAVIRUS: Virtual Pandemics" featuring CompBioMed CovidSim UQ research, on 12 November 2020, https://www.sciencemuseumgroup.org.uk/blog/coronavirus-virtual-pandemics/	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
89	CWI posted an article titled "MULTIPLE SIMULATIONS BEST FOR COVID-19 PREDICTIONS" on CompBioMed CovidSim UQ work, on 13 November 2020 https://www.cwi.nl/news/2020/multiple-simulations-best-for-covid-19-predictions	[Scientific Community (higher education, Research)], [Industry]	10,000
90	CWI posted an article titled "Multiple simulations best for Covid-19 predictions" on CompBioMed CovidSim UQ work, on 13 November 2020 https://www.ucl.ac.uk/news/2020/nov/multiple-simulations-best-covid-19-predictions	[Scientific Community (higher education, Research)], [Industry]	500
91	UvA posted an article on "Methods known from climate science can make Covid-19 models more robust" on the UvA website, concerning the CompBioMed CovidSim UQ work, on 19 November 2020 https://www.uva.nl/en/shared-content/faculteiten/en/faculteit-der-natuurwetenschappen-wiskunde-en-informatica/news/2020/11/methods-known-from-climate-science-can-make-covid-19-models-more-robust.html?origin=ilqjCjLURfmNjNlVykWRcg&cb&cb	[Scientific Community (higher education, Research)]	1,000
92	Roger Highfield (Science Museum) posted a blog article on "CORONAVIRUS: CAN AI SOLVE FUTURE PANDEMICS?" featuring CompBioMed coronavirus research, on 17 December 2020, https://www.sciencemuseumgroup.org.uk/blog/coronavirus-can-ai-solve-future-pandemics/?utm_source=Twitter&utm_medium=Organic%20Link&utm_campaign=L%20AP%20Science%20Museum%20Group%20Blog%2017/12/2020	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	5,000
93	EPCC posted an article "CompBioMed: creating virtual humans" on the EPCC website, on 22 Jul 2021 https://www.epcc.ac.uk/blog/2021/07/compbio-med-creating-virtual-humans	[Scientific Community (higher education, Research)], [Industry]	100
94	A dedicated website was created for the CompBioMed code TIES (thermodynamic integration with enhanced sampling) http://www.ties-service.org	[Scientific Community (higher education, Research)], [Industry]	50
95	E-CAM's work with HemeLB of CompBioMed featured in FocusCoE newsletter #9, in March 2021 https://www.hpccoe.eu/?mailpoet_router&endpoint=view_in_browser&action=view&data=WzcsImE4OTM3ZDdlMDNjMlIsMjcwLDA5MV0	[Scientific Community (higher education, Research)], [Industry]	100
96	E-CAM posted an article on "February Module of the Month: ALL library implementation in HemeLB, a CoE collaboration" on 26 February 2021, https://www.e-cam2020.eu/all-library-implementation-in-hemelb-a-coe-collaboration/	[Scientific Community (higher education, Research)], [Industry]	100
97	HemeLB featured in FocusCoE Newsletter #5 in July 2020, https://www.hpccoe.eu/?mailpoet_router&endpoint=view_in_browser&action=view&data=WzMsImZlODE2NWFiMTVMlIsMTAsImI2YjYxZiIsMywXQ	[Scientific Community (higher education, Research)], [Industry]	100
98	CompBioMed listed several CompBioMed services on the EOSC-hub platform, in November 2020	[Scientific Community (higher education, Research)], [Industry]	100
99	Innovation Radar listed CompBioMed software on their platform - Alya, HemeLB, HemoCell, OpenBF, Palabos-Vertebroplasty simulator, Palabos – Flow Diverter Simulator, BAC, HTMD, Playmolecule, Virtual Assay, CT2S, Insigneo Bone Tissue Suit https://www.innoradar.eu/innovation/38359	[Industry]	100
100	FocusCoE disseminated CompBioMed success stories through their WP3 activities including CompBioMed's work with Janssen Pharmaceutica, which also appears on the hpccoe.eu website https://www.hpccoe.eu/success-stories/	[Industry]	100
101	CompBioMed coronavirus research appeared on the FocusCoE hpccoe.eu page "How EU projects work on supercomputing applications to help contain the corona virus pandemic" https://www.hpccoe.eu/2020/12/07/how-eu-projects-work-on-supercomputing-applications-to-help-contain-the-corona-virus-pandemic/	[Scientific Community (higher education, Research)], [Industry]	100
102	CompBioMed's news and twitter feeds appear on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/compbio-med-2/	[Scientific Community (higher education, Research)], [Industry]	100
103	CompBioMed's services are listed on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/technological-offerings-of-the-eu-hpc-coes-3/	[Scientific Community (higher education, Research)], [Industry]	100
104	Three of CompBioMed's use cases appear on the FocusCoE hpccoe.eu website	[Scientific Community (higher education, Research)], [Industry]	100

	https://www.hpccoe.eu/use-cases/	Research]], [Industry]	
105	CompBioMed's training events have appeared on the FocusCoE hpccoe.eu training registry https://www.hpccoe.eu/coe-training-calendar/	[Scientific Community (higher education, Research)], [Industry]	100
106	CompBioMed featured in the ETP4HPC Handbook of European HPC Projects, 31 August 2021 https://www.etp4hpc.eu/pujades/files/European%20HPC%20Handbook%202021%20final.pdf	[Scientific Community (higher education, Research)], [Industry]	100
107	Emily Lumley (UCL) published CompBioMed newsletter No. 9 in February 2020 https://www.compbioimed.eu/wp-content/uploads/2020/02/newsletter9_v1.1.pdf	[Scientific Community (higher education, Research)], [Industry]	50
108	Emily Lumley (UCL) published CompBioMed newsletter No. 10 in August 2020 https://www.compbioimed.eu/wp-content/uploads/2020/07/newsletter10_v1.3.pdf	[Scientific Community (higher education, Research)], [Industry]	50
109	Emily Lumley (UCL) published CompBioMed newsletter No. 11 in January 2021 https://www.compbioimed.eu/wp-content/uploads/2021/01/newsletter11_final.pdf	[Scientific Community (higher education, Research)], [Industry]	50
110	Emily Lumley (CBK) published 36 new pages on the CompBioMed website https://www.compbioimed.eu/	[Scientific Community (higher education, Research)], [Industry], [Clinics], [General Public]	53,018

10.6 Organisation of Events

No.	Description of Activity	Audience(s) (see above table)	No. of People
111	CompBioMed Conference 2021 (CBMC21) was held on 15-17 September 2021 https://cbmc21.vfairs.com/ and www.compbioimed-conference.org	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	185
112	SURF organised a meeting on "Advanced HPC usage and parallel computing" at Cluster Computing for Computational Science on 3 and 10 December 2020 https://www.surf.nl/en/agenda/online-course-cluster-computing-for-computational-science	[Scientific Community (higher education, Research)], [Industry]	65
113	SURF organised a meeting on "Best practices to handle sensitive data and access to European-level tools for data management" at Sensitive Data Management and EUDAT Services on 29 March 2020 https://www.surf.nl/en/agenda/training-sensitive-data-management-and-eudat-services	[Scientific Community (higher education, Research)], [Industry], [General Public]	30
114	SURF organised a meeting on "CPU parallel programming in HPC facilities" at MPI and OpenMP in Scientific Software Development on 9 and 11 June 2021 https://events.prace-ri.eu/event/1185/	[Scientific Community (higher education, Research)], [Industry]	35
115	David Wifling and Gerald Mathias (LRZ) organised a "WP3 Meeting on Machine Learning meets Modelling and Simulation Methods" 16-17 March 2020 https://www.compbioimed.eu/machine-learning-meets-modelling-and-simulation-methods/	[Scientific Community (higher education, Research)], [Industry]	30
116	David Wifling (LRZ), Marco Verdicchio (SURF) and Gavin Pringle (EPCC) organised a HiPEAC conference 2021 workshop with FocusCoE, EXCELLERAT, EoCoE, ChEESE, HiDALGO, and BioExcel on "The HPC CoE services and applications" on 20 January 2021 https://www.hpccoe.eu/events/1972/	[Scientific Community (higher education, Research)], [Industry]	50
117	CompBioMed collaborated with FocusCoE, BioExcel and PerMedCoE during a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference on 4 May 2021	[Scientific Community (higher education, Research)], [Industry]	50
118	WP5 organised a workshop on Incubator Activities, which took place virtually on 26th May 2020 https://www.compbioimed.eu/incubator-activities-meeting/	[Scientific Community (higher education, Research)], [Industry]	20

10.7 Participation in Events

No.	Description of Activity	Audience(s) (see above table)	No. of People
120	Andrea Townsend-Nicholson (UCL), Andrew Narracott (USFD), Cristin Merritt gave a talk on "Demystifying the Dark Arts of HPC - Introducing Biomedical Researchers to Supercomputers" at SC20 State of the Practice on 17 November 2020 https://sc20.supercomputing.org/presentation/?id=sotp104&sess=sess288	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	370
121	Andrea Townsend-Nicholson (UCL) presented a poster on "Educating and engaging new communities of practice with high performance computing through the integration of teaching and research" at EuroHPC Summit Week 2021 on 23 March 2021 https://team.swapcard.com/exhibitor/RXhoaWJpdG9yXzMwMzkxNA==/details	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	103
122	Andrea Townsend-Nicholson (UCL) gave a BoF on "HPC and You - A student BoF on enjoying a career and community in HPC" at ISC '21, on 29 June 2021 https://app.swapcard.com/event/isc-high-performance-2021-digital/planning/UGxhbm5pbmdfNDQ0NjY0	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	82
123	Andrea Townsend-Nicholson (UCL) presented a poster on "Medics on HPC: Bringing Supercomputing to the Next Generation of Healthcare Practitioners" at ISC '21, on 30 June 2021	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	82
124	David Oks (BSC) gave a talk on "Numerical Performance Assessment of Different FSI Non-Boundary Conforming Methods" at ECCOMAS 2020 on 11-15 January 2021 https://virtual.wccm-eccomas2020.org/	[Scientific Community (higher education, Research)], [Industry]	3,000
125	David Oks (BSC) gave a talk on "Parallel Fluid-Structure Interaction Model for Bioprosthetic Aortic Valve Replacements" at ICI 2020 on 5-6 December 2020 https://cbset.org/ici-meeting-2020/	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	3,000
126	David Oks (BSC) gave a talk on "In-silico Analysis of Materials and Eccentricity in Aortic Valve	[Scientific Community (higher education, Research)], [Industry]	300

	Replacements" at COUPLED 2021 on 14-16 June 2021 https://coupled2021.cimne.com/	Research]]	
127	David Oks (BSC) gave a talk on "Influence of Transcatheter Aortic Valve Replacements on Coronary Flow: a Fluid-Structure Interaction Analysis" at MMLDT-CSET 2021 on 26-29 September 2021 https://coupled2021.cimne.com/	[Scientific Community (higher education, Research)], [Industry]	50
128	David Oks (BSC) gave a talk on "A One-Dimensional Finite Element Model for Human Circulatory Systems" at 6th BSC Severo Ochoa Doctoral Symposium on 7-9 September 2021 https://upcommons.upc.edu/handle/2117/166636	[Scientific Community (higher education, Research)]	105
129	Alfonso Santiago (BSC) gave a keynote talk on "Numerical models as regulatory evidence: gathering credibility evidence through VVUQ" at CMBBE21 on 7-9 September 2021 https://upcommons.upc.edu/handle/2117/166636 https://program.m-anage.com/cmbbe2021/en-US/ProgramSearch/Program/?searchstring%3D%26programid%3D98696%26pProgramGrade%3DAll%26pHideLogin%3DFalse%26pHidePersonal%3DFalse%26pShowPrivate%3DFalse&sa=D&source=calendar&ust=1631353433522827&usg=AOvVaw2B1Ns1ia2z9QemHOT4dxaP	[Scientific Community (higher education, Research)], [Industry]	200
130	Jazmin Aguado-Sierra (BSC) gave a talk on "Cardio-Vascular COVID" at PRACE Days 2021 at EuroHPC Summit Week, 22-26 March 2021 https://app.swapcard.com/event/eurohpc-summit-week-2021/planning/UGxhbm5pbmdfMzM2ODU1	[Scientific Community (higher education, Research)], [Industry]	50
131	Christian Spieker (UvA) gave a talk on "Detailed Blood Cell Flow Mechanics In Curved Vessel Geometry" at ESB 2021 on 13 July 2021 https://esbiomech.org/conference/wp-content/uploads/sites/3/2021/07/ESB2021_booklet.pdf	[Scientific Community (higher education, Research)]	24
132	Max van der Kolk (UvA) gave talk "des-ist: A Simulation Framework to Streamline Event-Based In Silico Trials" at ICCS 2021, on 16-18 June 2021 https://doi.org/10.1007/978-3-030-77967-2_53	[Scientific Community (higher education, Research)], [Industry]	20
133	Gabor Zavodszky (UvA) gave invited talk on "Current scaling limits of a large-scale cellular blood flow simulation" at CMBBE2021 on 7-9 September 2021	[Scientific Community (higher education, Research)]	40
134	Elisa Passini (Oxford) gave a talk on "In Silico investigation of arrhythmia mechanisms in hypertrophic cardiomyopathy" at the Heart Rhythm Society Meeting, USA, in July 2021	[Scientific Community (higher education, Research)], [Clinicians]	200
135	Blanca Rodriguez (Oxford) gave a Keynote talk on "Enabling Precision Medicine through the Digital Twin and In Silico Trials" at the Functional Modelling and Imaging of the Heart conference, in June 2021	[Scientific Community (higher education, Research)], [Clinicians]	200
136	Blanca Rodriguez (Oxford) gave a talk on "Machine Learning Approaches to ECG Interpretation" at European Society of Cardiology, Amsterdam/Virtual, in August 2020	[Scientific Community (higher education, Research)], [Clinicians]	100
137	Lei Wang gave a talk on "Effects of fibre orientation on electrocardiographic and mechanical functions in a computational human biventricular model" at the Functional Modelling and Imaging of the Heart conference, in June 2021	[Scientific Community (higher education, Research)], [Clinicians]	100
138	Zhinuo Jenny Wang (Oxford) gave a talk on "Post myocardial infarction ionic remodelling promotes repolarisation dispersion and electrocardiogram abnormalities in acute and chronic stages" at European Heart Rhythm Association Annual Workshop/Virtual, in April 2021	[Scientific Community (higher education, Research)], [Clinicians]	100
139	Blanca Rodriguez (Oxford) gave a talk on "Extending in silico trials for cardiac contractility" at TRM meeting, Lugano, Switzerland 2019, in December 2020	[Scientific Community (higher education, Research)], [Clinicians]	50
140	Blanca Rodriguez (Oxford) gave a talk on "Artificial Intelligence for Cardiac Pharmacology" at ACP international conference, Virtual, 2020, in October 2020	[Industry], [Clinicians]	100
141	Blanca Rodriguez (Oxford) gave a CompBioMed symposium at University of Davis, CA, USA in February 2020	[Scientific Community (higher education, Research)]	30
142	Blanca Rodriguez (Oxford) gave a keynote talk on "Human In Silico Trials in Pharmacology and Cardiology" at Annual lecture for the FRAME organisation, on 17 October 2019	[General Public]	40
143	Blanca Rodriguez (Oxford) gave a talk on "Enabling Precision Medicine through the Digital Twin and In Silico Trials" at Computing in Cardiology, Virtual, in September 2020	[Scientific Community (higher education, Research)]	100
144	Blanca Rodriguez (Oxford) gave a talk on "Mechanisms of calcium alternans" at American Heart Association Meeting, in November 2019	[Scientific Community (higher education, Research)], [Clinicians]	100
145	Jon McCullough (UCL) gave a talk on "A comparison of capillary bed representations in 3D, human-scale blood flow simulations" at VPH2020 on 26 August 2020	[Scientific Community (higher education, Research)], [Industry], [Medical Students], [Clinicians]	100
146	Jon McCullough (UCL) gave a talk on "3D Blood Flow for the Virtual Human with HemeLB: Steps Towards the Exascale" at EuroHPC Summit Week 2021 on 25 March 2021	[Scientific Community (higher education, Research)], [Industry]	50
147	Jon McCullough (UCL) gave a talk on "Visualization of human-scale blood flow simulation using Intel OSPRay Studio on SuperMUC-NG" at ISC21 - Intel Dev Summit at 23 June 2021	[Scientific Community (higher education, Research)], [Industry]	100
148	Jon McCullough (UCL) gave a talk on "Taking blood flow simulation towards the exascale with HemeLB" at CMBBE21 at 9 September 2021	[Scientific Community (higher education, Research)], [Industry]	75
149	Vicente Grau (Oxford) gave a talk on "Optimized Rigid Motion Correction from Multiple Non-simultaneous X-Ray Angiographic Projections" at International Conference on Pattern Recognition and Machine Intelligence, on 17 Dec 2019	[Scientific Community (higher education, Research)], [Industry]	200
150	Vicente Grau (Oxford) gave a talk on "A 2-Step Deep Learning Method with Domain Adaptation for Multi-Centre, Multi-Vendor and Multi-Disease Cardiac Magnetic Resonance Segmentation" at Miccai - STACOM workshop, at 1 September 2020	[Scientific Community (higher education, Research)], [Industry]	150
151	Vicente Grau (Oxford) gave a talk on "Biventricular Surface Reconstruction From Cine Mri Contours Using Point Completion Networks" at ISBI Conference on 1 April 2020	[Scientific Community (higher education, Research)], [Industry]	800
152	Marco Viceconti (UNIBO) was rapporteur for In Silico Trials consensus statements at the EFORT First European Consensus Conference, on 22 June 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians], [Civil Society], [Policy makers], [Medias], [Investors]	200
153	Marco Viceconti (UNIBO) was plenary Keynote as winner of the ESB Huiskes Medal for career achievement, he gave a talk on "How I see the future of MSK computational biomechanics" on 13 July 2021 https://esbiomech.org/conference/esb2021/	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	200
154	Marco Viceconti (UNIBO) gave a podium presentation on "CLINICAL VALIDATION FOR REGULATORY QUALIFICATION OF IN SILICO TRIALS METHODOLOGIES" at the 26th conference of the European Society of Biomechanics on 14 July 2021	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	100



	https://esbiomech.org/conference/esb2021/		
155	Antonino Amedeo La Mattina (UNIBO) gave a podium presentation on "Towards in silico phase III clinical trials for osteoporosis drugs: cohort expansion with anatomic statistical atlas" at 26th conference of the European Society of Biomechanics on 14 July 2021 https://esbiomech.org/conference/esb2021/	[Scientific Community (higher education, Research)], [Industry], [Medical Students]	100
156	Gianni De Fabritiis (UPF) gave an invited talk on "From symbolic to neural network potentials in molecular simulations" at AI4Science, on 8 July 2020 https://ai4science-amsterdam.github.io/events2/	[Scientific Community (higher education, Research)] [Industry]	30
157	Gianni De Fabritiis (UPF) gave an invited talk on "Reinforcement learning strategy in the Unity obstacle challenge" at Neurips, on 14 December 2019 https://nips.cc/Conferences/2019	[Scientific Community (higher education, Research)] [Industry]	50
158	Gianni De Fabritiis (UPF) gave a keynote talk on "Can we machine learn chemistry and drug discovery?" at the IBSA Foundation Forum, on 9 October 2019 http://www.ibsa-foundation.org/en/activities/forums/how-artificial-intelligence-can-change-the-pharmaceutical-landscape	[Scientific Community (higher education, Research)] [Industry]	50
159	Xinshan Li (USFD) gave a talk on "A finite element investigation of the positioning of Arabidopsis cerclage pessary in the prevention of spontaneous preterm birth" at CBMC21 on 25-27 September 2019	[Scientific Community (higher education, Research)] [Industry], [Clinicians]	50
160	Xinshan Li (USFD) gave a talk on "Femoral neck loading during gait cycle using coupled musculoskeletal-finite element modelling approach" at BioMedEng conference on 6-7 September 2021	[Scientific Community (higher education, Research)] [Industry], [Clinicians]	150
161	Alfons Hoekstra (UvA) gave a CompBioMed talk on "The Virtual Physiological Human" at "Celebration of the past, the present and the future", an invitational conference for European Medical Associations in Amsterdam, Netherlands on 6-7 November 2019	[Clinicians]	25
162	Gabor Zavodszky (UvA) gave a talk showing the Virtual Humans film at "Celebration of the past, the present and the future", an invitational conference for European Medical Associations in Amsterdam, Netherlands on 6-7 November 2019	[Clinicians]	25
163	Peter Coveney (UCL) was a panelist discussing digital twins on the session "I Love Biology. Why Don't Biologists Love Theory?" at PASC21 online, on 5 July 2021	[Scientific Community (higher education, Research)], [Industry]	200
164	Peter Coveney gave a talk on "Readying HemeLB and SCeMa Codes for Exascale with POP and E-CAM Centres of Excellence" at PASC21 online, on 7 July 2021 https://pasc21.pasc-conference.org/program/schedule/presentation/?id=msa142&sess=sess142	[Scientific Community (higher education, Research)], [Industry]	200
165	Peter Coveney's (UCL) gave a talk on "Supercomputing, COVID-19 and the Transformation of Medicine" at ISC 2020 Digital, featuring CompBioMed coronavirus and other research on 22-25 June 2020	[Scientific Community (higher education, Research)], [Industry]	200
166	Marco Viceconti (UNIBO) chaired a session on Pathophysiology at VPH2020 on 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
167	Marco Viceconti (UNIBO) chaired a session on Clinical: neuro-musculo-skeletal at VPH2020 on 28 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
168	Peter Coveney (UCL) gave a talk on "Computational chemistry to analyse drug-protein interaction for COVID-19" featuring CompBioMed coronavirus research at VPH2020 on 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
169	Jazmin Aguado-Sierra (BSC) gave a talk on "In Silico study of cardiotoxicity of antimalarial drugs" featuring CompBioMed coronavirus research at VPH2020 on 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
170	Benjamin Czaja (UvA) presented a poster on "The influence of flowing Red Blood Cells on Wall Shear Stress in a Diabetic Retinal Microaneurysm" at VPH2020 on 26 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
171	Claudia Mazza (USFD) presented a poster on "Gait and balance impairment in people with multiple sclerosis across different levels of disability" at VPH2020 on 26 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
172	Ivan Benemerito (USFD) presented a poster on "1D modelling of blood flow through elastic networks of catheterised arteries" at VPH2020 on 26 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
173	Claudia Mazza (USFD) chaired a session on Clinical: monitoring & connected health at VPH2020 on 26 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
174	Alfons Hoekstra (UvA) chaired a session on Methods: multiscale modelling at VPH2020 on 27 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
175	Shunzhou Wan (UCL) gave a talk on "Accurate ligand selectivity prediction for G protein-coupled receptors" featuring CompBioMed coronavirus research at VPH2020 on 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
176	Gabor Zavodszky (UvA) gave a talk on "Scale-bridging from cellular blood flow to continuum level using a statistical approach" featuring CompBioMed coronavirus research at VPH2020 on 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
177	Marco Viceconti (UNIBO) gave a keynote talk on "Predicting muscle activation patterns in pathological subjects" featuring CompBioMed coronavirus research at VPH2020 on 27 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	200
178	Sauro Succi from IIT presented at the EuroScience Open Forum (ESOF) and discussed CompBioMed, in Trieste, Italy, on 4-10 July 2020, https://www.ildeno.it/cern-big-data-e-modelli-matematici-per-trovare-una-cura-contro-il-covid/	[Scientific Community (higher education, Research)], [Industry]	100
179	Pavel Zun (UvA) gave a talk on "The StentValid Collection and Validation of a Multiscale Model of In-Stent Restenosis" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
180	Raymond Padmos (UvA) gave a talk on "A Multiscale Model of Cerebral Perfusion During Acute Ischaemic Stroke with Collaterals" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
181	Remy Petkantchin (UNIGE) gave a talk on "Lattice-Boltzmann Fibrinolysis" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
182	Raimondas Galvelis (Acellera) gave a talk on "ACEMD 4: protein-ligand complex simulations with a hybrid method of neural network potential and molecular mechanics" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
183	Ioannis Zacharoudiou (UCL) gave a talk on "Development and performance comparison of a HemeLB GPU code for human-scale blood flow simulation" at CBMC21 on 15-17 September	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50



	2021		
184	Elisabeth Mayer (LRZ) gave a talk on "Visualization of Human-Scale Blood Flow Simulation using Intel OSPRay Studio on SuperMUC-NG" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
185	Daniele Tartarini (USFD) gave a talk on "pFIRE a parallel Framework for biomedical Image Registration" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
186	Jon McCullough gave a talk on "Human-Scale Vascular Simulation with HemeLB – Progress towards the Virtual Human" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
187	Crispin Keable (Atos) gave a talk on "The Value of Exascale" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
188	Ivan Benemerito (USFD) gave a talk on "Identification of biomarkers for distal perfusion following an ischaemic event" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
189	Guillaume Hautbergue (BSC) gave a talk on "Innovation in Medical Education: Using high performance computing to share mixed methods research projects across Medical Schools" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
190	Mateusz K. Bieniek and Alex Wade (UCL) gave a talk on "WebTIES: Relative Binding Free Energies based on Dual Topology with support for OpenMM / NAMD 3 within a Web Portal" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
191	Agastya Bhati (UCL) gave a talk on "Large scale systematic relative binding free energy study of ligand-protein interactions: a first application of the TIES toolkit" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
192	Andrea Townsend-Nicholson (UCL) gave a talk on "Creating a community of practice in computational biomedicine: optimising training delivery to maximise user engagement" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
193	Shunzhou Wan (UCL) gave a talk on "Evaluation and Characterization of Potential SMYD3 Inhibitors" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
194	Oscar Camara (UPF) gave a talk on "Joint project-based training of medical, biology and engineering students on data science and computational models in biomedicine" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
195	Art Hoti (UCL) gave a talk on "A long-timescale, ensemble study of SARS-CoV-2 protein-ligand interactions" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
196	Peter Coveney (UCL) gave a talk on "Building the Virtual Human: From where we are now to where we aspire to be" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
197	Shunzhou Wan (UCL) gave a talk on "Energetic and Structural Insights into the Inhibitors of SARS-CoV-2 Main Protease from Repurposing Drug Libraries" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
198	Jazmin Aguado-Sierra (BSC) gave a talk on "Computational Modeling of Ischemia, Myocardial Infarction and Hypokalemia in a Human Heart Model Demonstrate High Fidelity between Clinical Data and Simulation" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
199	Marco Viceconti (UNIBO) gave a talk on "Models Vs. Experiments: a theoretical framing as a foundation for Good Simulation Practices" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
200	Christian Spieker (UvA) gave a talk on "Novel Application Motivated Advanced Boundary Conditions for Cellular Blood Flow Simulations" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
201	Antonino Amedeo La Mattina and Alma Mater Studiorum (UNIBO) gave a talk on "Synthetic Cohorts for Osteoporosis Drug Phase III Clinical Trials: Cohort Generation from Anatomic Statistical Atlas" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
202	Paula Domínguez Gómez (UPF) gave a talk on "Sensitivity analysis to haemodynamic boundary conditions in human coronary arteries" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
203	Yue Hao gave a talk on "Investigation of Flow Patterns in a 2D Thrombus Based on Porosity Data" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
204	David Oks (BSC) gave a talk on "In-silico fluid-structure interaction analysis of the effect of eccentricity on the performance of bioprosthetic aortic valve replacements" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
205	Roberta De Michele (UNIBO) gave a talk on "Innovation adoption: the role of a Community of Practice" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
206	Bastien Chopard (UNIGE) gave a talk on "Anomalous platelets transport in a shear flow of blood" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
207	Adria Perez (UPF) presented a poster on "Enlightening molecular simulations with machine learning" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
208	Qian Goh (USFD) presented a poster on "Texture Analysis for Detecting Placenta Abnormality During Pregnancy" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
209	Alex Wade (UCL) presented a poster on "Controlling Aleatoric Error in Protein-ligand Binding Free Energy Calculation and Comparing Uncertainty Across Molecular Dynamics Engines" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
210	Mat Bieniek (UCL) presented a poster on "TIES 20: RBFE with a Flexible Superimposition Algorithm and Partial Ring Morphing" at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
211	ATOS hosted a booth at CBMC21 on 15-17 September 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
212	Emily Lumley (UCL) hosted a CompBioMed booth at the ESBiomech 2021 conference on 11-14 July 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
213	Peter Coveney (UCL) gave a talk on "Reproducibility in computational science" at an invited talk at Supercomputing Conference 2019 (SC19), Gaithersburg, MD, USA, 17 November 2019	[Scientific Community (higher education, Research)], [Industry]	50
214	Peter Coveney (UCL) gave a talk on "The Role of Theory, Modelling and Simulation in the Emergence of Life" invited talk, Winter Retreat, Brixen, Italy, 17-20 February 2020.	[Scientific Community (higher education, Research)], [Industry]	50
215	Peter Coveney (UCL) gave a talk on "Rapid, Accurate and Reliable Ligand-protein Binding Free Energy Prediction From Molecular Dynamics Simulation" at the OpenEye Conference, 10-12 March 2020.	[Scientific Community (higher education, Research)], [Industry]	60
216	Peter Coveney gave a talk on "Supercomputing, COVID-19 and the Transformation of	[Scientific Community (higher education, Research)], [Industry]	200



	Medicine" at ISC2020, 22 June 2020	Research]], [Industry]	
217	Peter Coveney (UCL) gave a talk on "Computational chemistry to analyse drug-protein interaction for COVID-19" at VPH2020, 24 August 2020	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
218	Peter Coveney (UCL) gave a talk on "Verified and validated concurrent multiscale modelling enabled by optimised high-performance computing" at WCCM-ECCOMAS 2020, 11-15 January 2021	[Scientific Community (higher education, Research)], [Industry]	50
219	Marco Viceconti (UNIBO) co-chaired and gave a talk on "Verification, validation, uncertainty quantification and applicability: a theoretical framing" at the IEEE BHI - BSN 2021 workshop, 27 July 2021 https://www.bhi-bsn-2021.org/wp-content/uploads/2021/07/IEEE-BHI-workshop-credibility-IST-v5.pdf	[Scientific Community (higher education, Research)], [Industry]	20
220	Mark Parsons (EPCC) made CompBioMed promotional material available on EPCC booth at Supercomputing 2019, Denver, Colorado, USA, on 17-22 November 2019 https://sc19.supercomputing.org/	[Scientific Community (higher education, Research)], [Industry], [Policy makers], [Medias], [Customers], [Other]	1,000
221	Brian Wylie from the POP CoE gave a presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020	[Scientific Community (higher education, Research)], [Industry]	100
222	The POP CoE ran a half day tutorial on "Practical Hybrid Parallel Application Performance Engineering" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020	[Scientific Community (higher education, Research)], [Industry]	100
223	Brian Wylie from the POP CoE disseminated a printable cube showing a Score-P summary measurement of HemeLB application execution on 32 JUWELS/V100 compute nodes with 129 MPI processes and 128 GPUs, at Supercomputing 2020, on 9-19 November 2020 https://fz-juelich.sciebo.de/s/damsq3zJROQRVgu	[Scientific Community (higher education, Research)], [Industry]	100
224	POP, FocusCoE, and CompBioMed held a booth at BioFIT 2019 in Marseille on 10-11 December 2019	[Scientific Community (higher education, Research)], [Industry]	50
225	Andy Grant (Atos) gave a talk on "HPC - Evolution and advances" at "Global CIO Forum - Advances in High Performance Computing Tackling the world's largest problems" on 25 August 2021 https://globalcioforum.com/unitevirtualsummit/advances-in-high-performance-computing/	[Industry]	65
226	Natalia Jimenez (Atos) gave a CompBioMed talk at the Atos BDS Foundation on 9-11 March 2021	[Industry]	30
227	Natalia Jimenez (Atos) gave a talk on "Advanced Computing Technologies Boosting Sciences Breakthroughs" at Cambridge New Therapeutics Forum, on 4 March 2021 https://www.ats.cam.ac.uk/events/cambridge-new-therapeutics-forum-camnf-march-meeting	[Scientific Community (higher education, Research)], [Industry]	30
228	Natalia Jimenez (Atos) gave a talk on "Present, past and future of the bioinformatics in Spain" at Bioinformatics Granada on 11 May 2021		30
229	Natalia Jimenez (Atos) gave a talk on "HPC, AI and Quantum Life Sciences CoE" at Defra event (workshop with customer) on 28 June 2021	[Industry], [Customers]	10
230	Natalia Jimenez (Atos) gave a talk on "Transforming the Future of Health and Life Sciences" at Atos Innovation week on 1 July 2021	[Industry]	20
231	Andy Grant (Atos) gave a CompBioMed talk at Atos Innovation week on 1 July 2021	[Industry]	20
232	Jon McCullough (UCL) gave a talk on "Towards virtual human-scale simulation of blood flow with HemeLB" at LRZ Results Workshop 2021, 10 June 2021	[Scientific Community (higher education, Research)], [Industry]	30
233	Jon McCullough (UCL) gave a talk on "Performance of HemeLB on Archer2 - Experience from the early-user program" at UKCOMES Winter Symposium, on 15 December 2020	[Scientific Community (higher education, Research)], [Industry]	30
234	Marco Verdicchio (SURF) gave a talk on "Developing HPC services for the biomedical community" at HiPEAC 2021, on 20 January 2021 https://www.hipeac.net/2021/budapest/#/	[Scientific Community (higher education, Research)], [Industry]	30
235	Marco Verdicchio (SURF) gave a round table discussion on "REPRODUCIBILITY - PARALLEL SESSION" at "Reliability and reproducibility in computational science" at the Alan Turing Institute on 24 January 2020 https://www.turing.ac.uk/events/reliability-and-reproducibility-computational-science	[Scientific Community (higher education, Research)], [Industry]	50
236	Vicente Grau (Oxford) gave a CompBioMed talk at Miccai - STACOM workshop on 1 September 2020	[Scientific Community (higher education, Research)]	150
237	Marco Viceconti (UNIBO) gave a CompBioMed talk at the EC stakeholder workshop 'Human Digital Twin', on 6 November 2020 https://www.oactive.eu/human-digital-twin-ec-workshop/	[Scientific Community (higher education, Research)], [Industry], [Policy makers]	40
238	Marco Viceconti (UNIBO) gave a talk on "Adoption of In Silico Trials: barriers and future perspectives" at InSilc Workshop: In Silico Clinical Trials Concepts and Adoption, at 5 March 2021 https://insilc.eu/insilc-workshop/	[Scientific Community (higher education, Research)], [Clinicians]	40
239	Marco Viceconti (UNIBO) gave a talk on "Medicine In Silico: the heart of the future Italian Digital Health Hub" at La Medicina in Silico in Italia: uno sguardo prospettico, on 29 April 2021 https://indico.chem.polimi.it/event/32/	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	100
240	Gianni De Fabritiis (UPF) gave an invited talk on "Neural network potentials for molecular simulations" at WE-Heraeus-Seminar on "Advanced Physical and Computational Techniques to Investigate Protein Dynamics" on 26-28 April 2021 https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2021/advanced-physical-and-computational-techniques-to-investigate-protein-dynamics/	[Scientific Community (higher education, Research)] [Industry]	40
241	Peter Coveney (UCL) gave a talk on "The Use of Supercomputers for High Fidelity, Actionable Predictions" at a keynote presentation at SURFsara Super Day, EYE Amsterdam, 17 December 2019	[Scientific Community (higher education, Research)], [Industry]	40
242	Peter Coveney (UCL) gave a talk on "Reproducibility, computability and the scientific method" at the workshop on "Reliability and reproducibility in computational science" workshop at The Alan Turing Institute, London, UK, 24 January 2020	[Scientific Community (higher education, Research)], [Industry]	60
243	Peter Coveney (UCL) gave a talk on "Supercomputing, Covid-19 and the Transformation of	[Scientific Community (higher education, Research)], [Industry]	40

	Medicine" at the CECAM event "The importance of being H.P.C. Earnest", 2 July 2020	Research]], [Industry]	
244	Peter Coveney (UCL) "Applications and Challenges for Systems Engineering on the Road to the Exascale" at the EXCALBUR Workshop III: Towards Exascale Simulation of Integrated Engineering Systems, 21-22 January 2021	[Scientific Community (higher education, Research)], [Industry]	30
245	Peter Coveney (UCL) gave a talk on "The role of simulation-based science in decision-making for healthcare, government and industry" at UvA's Institute for Advanced Study (IAS), 26 February 2021	[Scientific Community (higher education, Research)]	20
246	Peter Coveney (UCL) gave a talk on "The Fluid Dynamics of Blood Flow at the Exascale with HemeLB" at the "Next-Generation CFD: Cutting-Edge Applications, Advanced Modelling and Machine Learning" seminar showcase, 23 March 2021	[Industry]	30
247	Peter Coveney (UCL) gave a talk on "Visualization of human-scale blood flow simulation using Intel OSPRay Studio on SuperMUC-NG" at the EXCALBUR Workshop V: Data Visualisation and Data Flows, 16-17 June 2021	[Scientific Community (higher education, Research)], [Industry]	30
248	Andrea Townsend-Nicholson (UCL) gave a talk at EuroCC Greece Chapter meeting: Introducing CompBioMed for HPC for the Greek Health & Life Sciences Sector, on 17 June 2021	[Scientific Community (higher education, Research)]	50
249	CompBioMed participated in the FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 5 November 2020	[Scientific Community (higher education, Research)], [Industry]	25
250	CompBioMed participated in the second FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 21 January 2021	[Scientific Community (higher education, Research)], [Industry]	25
251	Andrea Townsend-Nicholson gave a talk on "Virtual Human - The body double that could improve your health" at Soapbox Science on 10 September 2020 http://soapboxscience.org/soapbox-science-2020-london/	[General Public]	200
252	Jazmin Aguado-Sierra (BSC) gave a seminar on "Towards supercomputer-based in-silico drug-induced cardiac arrhythmic risk stratification using 3D biventricular heart populations" at Cardiotoxicity interest group meeting in 2021 https://cipaproject.org/	[Policy Makers]	20
253	David Oks (BSC) gave a talk on "Talk and Hands-on Workshop: Fluid-Structure Interaction methods for biomechanics" at PATC: Short course on HPC-based Computational Bio-Medicine on 11-13 February 2020 https://www.bsc.es/education/training/patc-courses/patc-short-course-hpc-based-computational-bio-medicine-0	[Scientific Community (higher education, Research)]	30
254	David Oks (BSC) gave a talk on "Talk and Hands-on Workshop: Fluid-Structure Interaction methods for biomechanics" at PATC: Short course on HPC-based Computational Bio-Medicine, 16-19 February 2021 https://www.bsc.es/education/training/patc-courses/online-patc-short-course-hpc-based-computational-bio-medicine	[Scientific Community (higher education, Research)]	30
255	Blanca Rodriguez (Oxford) gave a webinar on "Enabling Precision Medicine through the Digital Twin and In Silico Trials" at Avicenna Alliance, Virtual, in February 2021	[Industry]	30
256	Blanca Rodriguez (Oxford) gave a seminar on "Enabling Precision Medicine through the Digital Twin and In Silico Trials" at Department of Biomedical Engineering, University of Ohio, Virtual, on 20 November 2020	[Scientific Community (higher education, Research)]	30
257	Daniele Tartarini (USFD) gave a talk on "pFIRE: parallel framework for image registration" at Insigneo Winter Symposium, on 8 December 2020	[Scientific Community (higher education, Research)], [Clinicians]	50
258	Jon McCullough (UCL) gave a webinar on "CompBioMed CoE - Addressing Biomedical Challenges with High Performance Computing" at POP Centre of Excellence on 15 May 2020 https://pop-coe.eu/blog/15th-pop-user-webinar-addressing-biomedical-challenges-with-high-performance-computing	[Scientific Community (higher education, Research)], [Industry]	30
259	Jon McCullough (UCL) gave a talk on "Visualization of human-scale blood flow simulation using Intel OSPRay Studio on SuperMUC-NG" at ISC21 - Intel Innovation Showcase on 23 June 2021 https://hpcevents.intel.com/partners/innovation-showcase/lrz-ucl	[Scientific Community (higher education, Research)], [Industry]	50
260	Marco Viceconti (UNIBO) discussed CompBioMed in the talk "ISW project and the regulatory landscape that are emerging in Europe, and that we need to overcome" at the invited talk at the Sixth Insist All-hands meeting on 27 May 2021 https://www.insist-h2020.eu/index.php/latest-news/meetings/past-insist-meetings	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	40
261	Marco Viceconti (UNIBO) gave an invited talk on "How to provide healthcare to a world of 10 billions" at the Bilateral Italy-South Africa Meeting "Civilian and Defence Applications of Artificial Intelligence, Big Data and High Performance Computing" organised by the Italian Embassy in Pretoria, on 3 June 2021 https://bigdata.eventi.co.za/videos/	[Scientific Community (higher education, Research)], [Industry], [Medical Students], [Clinicians], [Civil Society], [General Public], [Policy makers], [Medias], [Investors], [Customers], [Other]	100
262	Gianni De Fabritiis (UPF) gave an Invited talk on "From symbolic to neural network potentials in molecular simulations" at the University of Basel, on 11 March 2020	[Scientific Community (higher education, Research)]	30
263	Gianni De Fabritiis (UPF) gave an Invited talk on "Simulations and AI from proteins to bots" at IIT, on 7 October 2020	[Scientific Community (higher education, Research)]	30
264	Xinshan Li (USFD) gave an invited talk on "Suggestions from bioengineering for obstetric and gynecologic modelling" at the International perspective meeting at the Clara Angela Foundation in November 2019	[Scientific Community (higher education, Research)], [Clinician]	50
265	Peter Coveney (UCL) gave a talk on "Supercomputing, COVID-19 and the Transformation of Medicine" featuring CompBioMed coronavirus and other research at the CECAM event "The importance of being H.P.C. Earnest" on 2 July 2020	[Scientific Community (higher education, Research)]	50
266	Roger Highfield (Science Museum) presented the Virtual Humans film during an ET Works webinar on "Tomorrow's Technology Today" on 13 November 2020	[Scientific Community (higher education, Research)], [Industry], [General Public]	50
267	Peter Coveney (UCL) gave a presentation on "The Fluid Dynamics of Blood Flow at the Exascale with HemeLB" at the "Next-Generation CFD: Cutting-Edge Applications, Advanced Modelling and Machine Learning" seminar showcase on 23 March 2021	[Industry]	50
268	Peter Coveney (UCL) gave a presentation on "The role of simulation-based science in decision-making for healthcare, government and industry" for UvA's Institute for Advanced Study (IAS) on 26 February 2021	[Scientific Community (higher education, Research)]	50
269	Peter Coveney (UCL) gave a talk on "Reproducibility in computational science" at an invited talk at the National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA, 15	[Scientific Community (higher education, Research)]	30

	November 2019		
270	Peter Coveney (UCL) gave a talk on "Supercomputers and the Future of Medicine" Science Museum Patron Dinner, 8 July 2020	[General Public]	40
271	Vicente Grau (Oxford) gave a presentation to potential industry partners on CompBioMed in May 2021	[Industry]	10

10.8 Other

No.	Description of Activity	Audience(s) (see above table)	No. of People
272	Andrea Townsend-Nicholson (UCL) gave an Invited Lecture on "Virtual Humans, Supercomputers and Health" at UCL Minds Lunch Hour Lecture on 29 April 2021	[General Public]	100
273	Antonino Amedeo La Mattina (UNIBO) disseminated CompBioMed at the Web Marketing Festival Award Ceremony of "Big Data and Artificial Intelligence WMF-IFAB National Award – 1 st Edition" in Rimini, Italy, on 15 July 2021 https://www.ifabfoundation.org/event-directory/big-data-and-artificial-intelligence-wmf-ifab-national-award-1-edition/	[Industry], [Civil Society], [General Public], [Investors]	100
274	Xinshan Li (USFD) gave an invited seminar on "Multiscale modelling to predict strain in the femoral neck during level walking" at the Mathematical Institute seminar series, University of Oxford, on June 2020	[Scientific Community (higher education, Research)]	30
275	UCL CompBioMed coronavirus research featured in the UCL email circulated to all UCL staff and students "Daily coronavirus (Covid-19) update: issue 25", on 16 April 2020	[Scientific Community (higher education, Research)]	55,000
276	UCL CompBioMed coronavirus research featured in the UCL email circulated to all UCL staff "Alumni News Coffee Connect, Supercomputers and Crystal Balls", on 23 April 2020	[Scientific Community (higher education, Research)]	13,000
277	The WHO published a Nature Computational Science paper on "Quantifying the uncertainty of CovidSim" that discusses primarily the CompBioMed CovidSim UQ paper, on 22 February 2021 https://www.nature.com/articles/s43588-021-00031-0	[Scientific Community (higher education, Research)], [Industry]	1,529
278	Brian Wylie from the POP CoE published his presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020 https://fz-juelich.sciebo.de/s/damsq3zJROQRVgu	[Scientific Community (higher education, Research)], [Industry]	100
279	FocusCoE disseminated CompBioMed services through their WP3 industry surveying activities	[Industry]	100
280	CompBioMed features in the best practices booklet produced by FocusCoE WP3	[Industry]	100
281	CompBioMed featured in the FocusCoE News Flash (an email sent to the CoE mailing list) to the CoEs, featuring their involvement at HiPEAC 2021, on 11 May 2021	[Scientific Community (higher education, Research)], [Industry]	50

10.9 Dissemination Activities Related to the Virtual Humans Film

No.	Description of Activity	Audience(s)	No. of People
1	Futura Sante posted an article titled "In video: your digital avatar will serve as a medical guinea pig" featuring CompBioMed research, the Virtual Humans film, and the Euronews video, on 29 August 2020, https://www.futura-sciences.com/sante/actualites/medecine-video-votre-avatar-numerique-servira-cobaye-medical-82637/	[General Public] [Medias]	1,400,000
2	Playtech.ro posted an article titled "Oamenii de știință vor să îți creeze un geamă virtual, iar motivul e cât se poate de îmbucurător" featuring CompBioMed research, and the Virtual Humans Film, on 26 August 2020	[General Public] [Medias]	1,000,000
3	Yahoo! Actualités posted an article titled "In video: meeting with the digital avatar, virtual double of your body" leading to the Futura Sante article, on 26 August 2020 https://fr.news.yahoo.com/vid%C3%A9o-rencontre-l-avatar-num%C3%A9rique-103000487.html?guccounter=1&guce_referrer=aHR0cHM6Ly93d3cuZ29vZ2x1LmNvbS8&guce_referrer_sig=AQAAAN6cw55oN4gKBUSVuOk7vxXfqHppD4azwq7X01t6wXXKie4l-h0cFtmEWdpUUrQXCTjpnq1VBuqW7LMx04q61YPBD9p3UgtNVJWYz2r-n5FcInou1m8nalJQeFTzq4C0ORSotuxx1AdxOeUq-NHl2hG4HDz9JwGFwJAMq2W4W	[General Public] [Medias]	2,000,000
4	Nacional Neovisni News Magazin posted an article titled "Koncept virtualnog pacijenta i dalje koristan zdravstvenim radnicima" covering CompBioMed research, on 25 August 2020 https://www.nacional.hr/koncept-virtualnog-pacijenta-ce-dalje-biti-koristan-zdravstvenim-radnicima/	[General Public]	80,000
5	iPro Up posted an article titled "Biomedicina: así funcionan los "gemelos humanos virtuales" que prometen salvar miles de vidas en los próximos años" featuring CompBioMed research and the Virtual Humans film,	[General Public]	80,000
6	Ziarul de Iasi posted an article titled "Oamenii de știință vor să îți creeze un geamă virtual. Ai accepta?" linking to the playtech.ro article featuring CompBioMed research and the Virtual Humans film, on 26 August 2020	[General Public]	150,000
7	WIRED IT (Italy) published an article titled "Il gemello Virtuale" on CompBioMed's virtual human work, on 16 March 2021. Wired IT, Vol 96, Spring 2021 Health Edition, ISSN 2035-7397	[Scientific Community (higher education, Research)], [Industry], [Medias], [General Public]	6,300,000
8	Il Sole 24ORE's (Italy) associated magazine "Platinum Aziende & Protagonisti" published an article on	[General Public], [Medias]	382,112

	"High performance computing and machine learning to defeat the pandemic" concerning CompBioMed coronavirus research, on 19 July 2021		
9	PCMag UK posted an article on "Welcome to the Virtual Humans Factory" featuring CompBioMed research, on 8 April 2021 https://uk.pcmag.com/health-fitness/132648/welcome-to-the-virtual-humans-factory	[General Public]	200,000
10	EPCC posted an article titled "Creating Virtual Humans" about CompBioMed2 and CBMC21 in the EPCC News Publication, in Summer 2021 https://issuu.com/epccedinburgh/docs/epcc_news_89_web	[Scientific Community (higher education, Research)], [Industry]	845
11	Peter Coveney and Andrea Townsend-Nicholson (UCL) appeared on the EuroNews Futuris Programme, on a piece about "Virtual Humans to map the future of major surgery", on 10 September 2020, the piece ran multiple times throughout the day		7,000,000
12	The Euronews Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 24 August 2020 https://www.youtube.com/watch?v=1gUI1N_YwC4	[General Public], [Medias]	615
13	The Euronews Next Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 24 August 2020 https://youtu.be/yeCcHuQeEPU	[General Public], [Medias]	1,512
14	The Digital EU Youtube Channel posted the Euronews TV segment with Peter Coveney (UCL) and the Virtual Humans film, on 31 August 2020 https://youtu.be/8DrE3dD-ywQ	[General Public], [Medias]	97
15	LRZ posted a news item on linkedin featuring CompBioMed and the Euronews piece, on 26 August 2020 https://www.linkedin.com/posts/leibniz-supercomputing-centre_virtual-humans-to-map-the-future-of-major-activity-6704676553021771776-t4-K/	[Scientific Community (higher education, Research)], [Industry]	1,170
16	ET Works (@etworksit) tweeted about a Roger Highfield (Science Museum) webinar on "Tomorrow's Technology Today" in which he presented the Virtual Humans, on 12 November 2020	[Scientific Community (higher education, Research)], [Industry], [General Public]	250
17	SURF posted an article on "Working towards virtual humans in the CompBioMed project" on the SURF website https://www.surf.nl/en/working-towards-virtual-humans-in-the-combiomed-project	[General Public]	100
18	iatranshumanisme.com posted an article titled "Virtual humans: the future of surgical procedures" featuring CompBioMed research and the Virtual Humans film on 28 August 2020 https://iatranshumanisme.com/2020/08/28/humains-virtuels-le-futur-des-interventions-chirurgicales/	[Scientific Community (higher education, Research)], [Industry], [General Public]	100
19	Patient Numérique posted an article titled "La médecine personnalisée passe-t-elle par les "jumeaux numériques"?" featuring CompBioMed research and the Virtual Humans film, on 31 August 2020 https://www.patientnumerique.com/actus/actualites/2020/08/la-medecine-personnalisee-passe-t-elle-par-les-jumeaux-numeriques/	[General Public]	200
20	Daily Factline posted an article title "Virtual Humans Assist In Mapping The Future Of Major Surgery" featuring CompBioMed research, on 7 September 2020 https://dailyfactline.com/virtual-humans-assist-in-mapping-the-future-of-major-surgery/	[General Public]	200
21	ECH Alliance posted an article titled "Virtual humans to map the future of major surgery" featuring CompBioMed research and the Virtual Humans Film, on 3 September 2020	[General Public]	200
22	EPCC posted an article "CompBioMed: creating virtual humans" on the EPCC website, on 22 Jul 2021 https://www.epcc.ed.ac.uk/blog/2021/07/combiomed-creating-virtual-humans	[Scientific Community (higher education, Research)], [Industry]	100
23	CompBioMed's news and twitter feeds appear on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/combiomed-2/	[Scientific Community (higher education, Research)], [Industry]	100
24	CompBioMed Conference 2021 (CBMC21) was held on 15-17 September 2021 https://cbmc21.vfairs.com/ and www.combiomed-conference.org	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	185
25	Gabor Zavodszky (UVA) gave invited talk on "Current scaling limits of a large-scale cellular blood flow simulation" at CMBBE2021 on 7-9 September 2021	[Scientific Community (higher education, Research)]	40
26	Jon McCullough (UCL) gave a talk on "3D Blood Flow for the Virtual Human with HemeLB: Steps Towards the Exascale" at EuroHPC Summit Week 2021 on 25 March 2021	[Scientific Community (higher education, Research)], [Industry]	50
27	Jon McCullough (UCL) gave a talk on "Visualization of human-scale blood flow simulation using Intel OSPRay Studio on SuperMUC-NG" at ISC21 - Intel Dev Summit at 23 June 2021	[Scientific Community (higher education, Research)], [Industry]	100
28	Jon McCullough (UCL) gave a talk on "Taking blood flow simulation towards the exascale with HemeLB" at CMBBE21 at 9 September 2021	[Scientific Community (higher education, Research)], [Industry]	75
29	Gabor Zavodszky (UVA) gave a talk showing the Virtual Humans film at "Celebration of the past, the present and the future", an invitational conference for European Medical Associations in Amsterdam, Netherlands on 6-7 November 2019	[Clinicians]	25
30	Emily Lumley (UCL) hosted a CompBioMed booth at the ESBiomech 2021 conference on 11-14 July 2021	[Scientific Community (higher education, Research)], [Industry], [Clinicians]	50
31	Peter Coveney (UCL) gave a talk on "Reproducibility in computational science" at an invited talk at Supercomputing Conference 2019 (SC19), Gaithersburg, MD, USA, 17 November 2019	[Scientific Community (higher education, Research)], [Industry]	50
32	POP, FocusCoE, and CompBioMed held a booth at BioFIT 2019 in Marseille on 10-11 December 2019	[Scientific Community (higher education, Research)], [Industry]	50
33	Jon McCullough (UCL) gave a talk on "Towards virtual human-scale simulation of blood flow with HemeLB" at LRZ Results Workshop 2021, 10 June 2021	[Scientific Community (higher education, Research)], [Industry]	30
34	Marco Verdicchio (SURF) gave a talk on "Developing HPC services for the biomedical community" at HiPEAC 2021, on 20 January 2021 https://www.hipeac.net/2021/budapest/#/	[Scientific Community (higher education, Research)], [Industry]	30
35	Roger Highfield (Science Museum) presented the Virtual Humans film during an ET Works webinar on "Tomorrow's Technology Today" on 13 November 2020	[Scientific Community (higher education, Research)], [Industry], [General Public]	50
36	Andrea Townsend-Nicholson (UCL) gave an Invited Lecture on "Virtual Humans, Supercomputers and Health" at UCL Minds Lunch Hour Lecture on 29 April 2021	[General Public]	100
37	POP, FocusCoE, and CompBioMed held a booth at BioFIT 2019 in Marseille on 10-11 December 2019	[Scientific Community (higher education, Research)], [Industry]	50
38	CompBioMed's news and twitter feeds appear on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/combiomed-2/	[Scientific Community (higher education, Research)], [Industry]	100

10.10 Collaborative Dissemination Activities with EC Funded Projects

No.	Description of Activity	Audience(s) (see above table)	No. of People
1	Andrea Townsend-Nicholson (UCL) gave a talk at EuroCC Greece Chapter meeting: Introducing CompBioMed for HPC for the Greek Health & Life Sciences Sector, on 17 June 2021	[Scientific Community (higher education, Research)]	50
2	CompBioMed worked with POP AND E-CAM on the presentation "Reaching HemeLB and SCeMa Codes for Exascale with POP and E-CAM Centres of Excellence" at PASC21, on 7 July 2021 https://pasc21.pasc-conference.org/program/schedule/presentation/?id=msa142&sess=142	[Scientific Community (higher education, Research)], [Industry]	50
3	E-CAM's work with HemeLB of CompBioMed featured in FocusCoE newsletter #9, in March 2021 https://www.hpccoe.eu/?mailpoet_router&endpoint=view_in_browser&action=view&data=WzcsImE4OTM3ZDdIMDNjMjlsMCwLdAsMV0	[Scientific Community (higher education, Research)], [Industry]	100
4	E-CAM posted an article on "February Module of the Month: ALL library implementation in HemeLB, a CoE collaboration" on 26 February 2021, https://www.e-cam2020.eu/all-library-implementation-in-hemelb-a-coe-collaboration/	[Scientific Community (higher education, Research)], [Industry]	100
5	HemeLB featured in FocusCoE Newsletter #5 in July 2020, https://www.hpccoe.eu/?mailpoet_router&endpoint=view_in_browser&action=view&data=WzMsmZlODE2NWFiMTVMiMTAsImI2YjYxZiIsMyYwWwXQ	[Scientific Community (higher education, Research)], [Industry]	100
6	Brian Wylie from the POP CoE gave a presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020	[Scientific Community (higher education, Research)], [Industry]	100
7	Brian Wylie from the POP CoE published his presentation on "Exascale Potholes for HPC: Execution Performance and Variability Analysis of the Flagship Application Code HemeLB" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020 https://fz-juelich.sciebo.de/s/damsq3zJROQRVgu	[Scientific Community (higher education, Research)], [Industry]	100
8	The POP CoE ran a half day tutorial on "Practical Hybrid Parallel Application Performance Engineering" involving HemeLB in collaboration with CompBioMed, at Supercomputing 2020, on 9-19 November 2020	[Scientific Community (higher education, Research)], [Industry]	100
9	Brian Wylie from the POP CoE disseminated a printable cube showing a Score-P summary measurement of HemeLB application execution on 32 JUWELS/V100 compute nodes with 129 MPI processes and 128 GPUs, at Supercomputing 2020, on 9-19 November 2020 https://fz-juelich.sciebo.de/s/damsq3zJROQRVgu	[Scientific Community (higher education, Research)], [Industry]	100
10	CompBioMed listed several CompBioMed services on the EOSC-hub platform, in November 2020	[Scientific Community (higher education, Research)], [Industry]	100
11	Innovation Radar listed CompBioMed software on their platform - Alya, HemeLB, HemoCell, OpenBF, Palabos-Vertebroplasty simulator, Palabos - Flow Diverter Simulator, BAC, HTMD, Playmolecule, Virtual Assay, CT2S, Insigneo Bone Tissue Suit https://www.innoradar.eu/innovation/38359	[Industry]	100
12	Wouter Edeling (CWI) of the VECMA project posted a video seminar of the CompBioMed CovidSim UQ work on Youtube, on 10 June 2021 https://www.youtube.com/watch?v=HzNeByTh74E	[Scientific Community (higher education, Research)], [Industry], [General Public]	12
13	FocusCoE disseminated CompBioMed success stories through their WP3 activities including CompBioMed's work with Janssen Pharmaceutica, which also appears on the hpccoe.eu website https://www.hpccoe.eu/success-stories/	[Industry]	100
14	FocusCoE disseminated CompBioMed services through their WP3 industry surveying activities	[Industry]	100
15	POP, FocusCoE, and CompBioMed held a booth at BioFIT 2019 in Marseille on 10-11 December 2019	[Scientific Community (higher education, Research)], [Industry]	50
16	CompBioMed features in the best practices booklet produced by FocusCoE WP3	[Industry]	100
17	CompBioMed coronavirus research appeared on the FocusCoE hpccoe.eu page "How EU projects work on supercomputing applications to help contain the corona virus pandemic" https://www.hpccoe.eu/2020/12/07/how-eu-projects-work-on-supercomputing-applications-to-help-contain-the-corona-virus-pandemic/	[Scientific Community (higher education, Research)], [Industry]	100
18	CompBioMed's news and twitter feeds appear on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/compbiomed-2/	[Scientific Community (higher education, Research)], [Industry]	100
19	CompBioMed's services are listed on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/technological-offerings-of-the-eu-hpc-coes-3/	[Scientific Community (higher education, Research)], [Industry]	100
20	Three of CompBioMed's use cases appear on the FocusCoE hpccoe.eu website https://www.hpccoe.eu/use-cases/	[Scientific Community (higher education, Research)], [Industry]	100
21	CompBioMed's training events have appeared on the FocusCoE hpccoe.eu training registry https://www.hpccoe.eu/coe-training-calendar/	[Scientific Community (higher education, Research)], [Industry]	100
22	CompBioMed collaborated with FocusCoE, BioExcel and PerMedCoE during a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference on 4 May 2021	[Scientific Community (higher education, Research)], [Industry]	50
23	A video of CompBioMed's collaboration with FocusCoE, BioExcel and PerMedCoE was posted on the HiPEAC Youtube channel. It was a thematic session on "Industrial Challenges and Innovation Opportunities of CoEs in Medical/Bio/Pharma" at the HiPEAC conference 2021. The video was posted on 7 May 2021 https://www.youtube.com/watch?v=CNa2j7HAXmU	[Scientific Community (higher education, Research)], [Industry]	90
24	CompBioMed featured in the FocusCoE News Flash (an email sent to the CoE mailing list) to the CoEs, featuring their involvement at HiPEAC 2021, on 11 May 2021	[Scientific Community (higher education, Research)], [Industry]	50
25	CompBioMed featured in the ETP4HPC Handbook of European HPC Projects, 31 August 2021 https://www.etp4hpc.eu/pujades/files/European%20HPC%20Handbook%202021%20final.pdf	[Scientific Community (higher education, Research)], [Industry]	100
26	CompBioMed participated in the FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 5 November 2020	[Scientific Community (higher education, Research)], [Industry]	25
27	CompBioMed participated in the second FocusCoE Sustainability Workshop organised by FocusCoE WP4, on 21 January 2021	[Scientific Community (higher education, Research)], [Industry]	25
28	CompBioMed co-organised a workshop with FocusCoE, EXCELLERAT, EoCoE, CHEESE, HIDALGO,	[Scientific Community (higher	50

BioExcel, at the HiPEAC conference 2021 on "The HPC CoE services and applications" on 20 January 2021 https://www.hpccoe.eu/events/1972/	education, Research]], [Industry]	
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10.11 Capture of products and services

Invention/Idea	What is it?	Product, Method or Service	CompBioMed Activity	Which Partner(s) own it?	Possible Route to Exploitation	Any Protections Needs?	Current Exploitation Plan	Help Needed from Innovation
COMBIOMED1								
Serpens	Multiphysics HPC simulation suite produced by BSC, focused on biomedical research for the cardiovascular system. Alya is the simulation engine of Serpens.	Product, software as a service, deployed in the cloud or on-site HPC cluster.	Work Package or cross project	BSC	Commercial offering	Current copyrighting and non-disclosure in place (Spain)	Creation of ELEM.BIO, a dedicated software company started up from BSC	Likely in future
Sheffield cardiac arrhythmia model (S-CAM)	Finite difference code for cardiac electrophysiology	Product	Work Package or cross project	USFD	1) Free for research 2) Commercial offering		Research by agreement	No
HPC for Medics Course	Course slides, handout, Qiime scripts and input files	Service	Work Package or cross project	UCL and UEDIN (EPCC)	Commercial offering		Partner expansion	No
HPC for BioScientists Course	Course slides, handout, Qiime scripts and input files	Service	Work Package or cross project	UCL and UEDIN (EPCC)	Commercial offering		Partner expansion	No
OpenBF	1D Blood Flow solver	Product	Work Package or cross project	USFD	1) Free for research 2) Commercial offering		Open access	Dissemination
Insigneo Bone Tissue Suite	Range of related software tools for analysing bone medical data	Product series	Work Package or cross project	USFD	Free for research		Open access	Dissemination
pFire	Parallel image registration code for local machine and HPC use	Product	Work Package or cross project	USFD	1) Free for research 2) Commercial offering		Open access	Dissemination
HTBAC	High performance bio-simulation framework for running molecular dynamics simulations locally or on supercomputers.	Product series	Work Package or cross project	UCL	1) Free for research 2) Commercial offering		Exploitation company Ensemble MD formed to offer services using HTBAC	No
PolNet	PolNet is a software tool for the computer simulation of blood flow in realistic microvascular networks imaged with a wide variety of microscopy and clinical imaging techniques	Product	Work Package or cross project	UEDIN	1) Free for research 2) Commercial offering		Open access	No
The Hoff	The HemeLB offload system is a simple REST API that allows clients to run jobs on remote HPC resources via HTTP requests.	Service, allowing non-HPC specialists to easily run HPC jobs	Work Package or cross project	UEDIN	Free for research		Open access	No
AngioSupport	Angiosupport comprises of a python implementation of 1D flow simulation models embedded in a workflow environment.	Product	Work Package or cross project	LifeTec Group	Commercial offering		Investigating licencing models	Possibly
Virtual Assay	Software for simulation of drug effects on populations of human ventricular models	Product	Work Package or cross project	University of Oxford	1) Free for research 2) Commercial offering		Open access	Possibly
CT2S	Online service form predicting bone strength from CT scans	Service	Work Package or cross project	USFD	Commercial offering		Online service	No

Invention/Idea	What is it?	Product, Method or Service	CompBioMed Activity	Which Partner(s) own it?	Possible Route to Exploitation	Any Protections Needs?	Current Exploitation Plan	Help Needed from Innovation
COMPBIOMED2								
DICE/ CompBioMed data transfer infrastructure	Workflow for intensive data transfer across HPC centre. Developed and implemented within FAIR principles	Service, Support HPC simulations	Work Package or cross project. External collaboration with DICE project.	SURF	This will depend on the tools and infrastructure used. I would imagine a commercial offering where external not federated user would have to pay to use the tools.		Online service	No
CompBioMed automated benchmark environment	framework for automatic testing of codes: code execution, analysis, postprocessing (generation of a static webpage for documentation of results)	Product / Service	WP4	LRZ	1) Free for research (Product) 2) Commercial offering (Service)		Open access	Possibly
Scalability Support	Scalability Services offered to clients from both inside and outside of CBM2. Support for users and authors to parallelise applications and port them to CBM2 HPC platforms.	Service	T2.4, T4.3	UEDIN, SARA, UNIBO	Commercial offering	T&Cs (under development), Data Privacy Policy (published), Data Security Policy (published), Adequacy Agreement to cover data movement in and out of the EU (under development)	Open access	Possibly
LEXIS/CompBioMed data transfer infrastructure	Workflow for intensive data transfer across HPC centre. Developed and implemented within FAIR principles	Service for Data Staging	Work Package 3, Task 3.3 or cross project. External collaboration with LEXIS project.	LRZ, SURF	This will depend on the tools and infrastructure used. I would imagine a commercial offering where external not federated user would have to pay to use the tools.		Online service	No
CompBioMed support for open data publishing	Providing guidance on publishing data openly using tools of the EUDAT CDI such as B2SHARE	Service	Work Package 3, Task 3.4	LRZ, SURF	Has to be determined		Online service	No
HPC for Medics Course (Online)	Course slides, handout, Qiime scripts and input files	Service	T6.2	UCL, USFD	Commercial offering		Online service	No
Medics on HPC Summer School Modules	Course slides, handout, scripts and input files	Service	T6.2	UCL, SURF, LRZ, USFD (and others as new content added)	Commercial offering		Online service	No