D7.4 Third Dissemination Report

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1 Executive summary

The ComPat consortium strongly believes that Science, R&D, and innovation is strengthened with a comprehensive dissemination plan and carefully considered knowledge exploitation activities. Thus, dissemination and exploitation play an important role in the ComPat project, based on collaborative efforts between the project partners.

This document, D7.4 Third Dissemination Report, reviews the events and dissemination results of ComPat for months 18 to 36 of the project (1 April 2017 to 30 September 2018), and provides statistics and discussion of the full 36 months of the project.

In summary, there was a substantial amount of dissemination activity in all 36 months of ComPat, the key highlights include:

- The publication or submission of 33 scientific papers
- Participation in 68 major conferences and workshops
- Delivery of 106 presentations at various events
- The organisation of 13 workshops/conferences

2 Report

2.1 Dissemination Materials and Channels

This section describes the various activities via ComPat's dissemination channels and materials throughout months 18-36 of the project. The ComPat name and logo, as well as reference to the funding source, has been used in all dissemination materials, be it in the form of leaflets, posters etc. Versions of slides and reports, along with a poster and leaflet that can be used as a template, were used by all contributors and are described below. These actions have helped to increase the brand recognition of the ComPat project.

2.1.1 Scientific Papers

In the months 18-36 of the project, 23 peer-reviewed, open-access scientific publications have been published, accepted for publication, or submitted to a journal. Over the whole project, 33 papers have been published, these are listed below:

1. O. Luk, O. Hoenen, A. Bottino, B. Scott, D. Coster, "ComPat Framework for Multiscale Simulations Applied to Fusion Plasmas", Computer Physics Communications, Submitted (2018)
2. O. Luk, O. Hoenen, A. Bottino, B. Scott, D. Coster, "Optimization of Multiscale fusion Plasma Simulations within the ComPat Framework", EPS Proceedings, P1.1102 (2018), ISBN: 979-10-96389-08-7
3. S. Alowayyed, G. Zavodszky, V. Azizi, and A. G. Hoekstra, "Load balancing of parallel cell-based blood flow simulations", Journal of Computational Science, 24, 1-7, DOI: 10.1016/j.jocs.2017.11.008

4. S. Alowayyed, T. Piontek, J. L. Suter, O. Hoenen, D. Groen, O. Luk, B. Bosak, P. Kopta, K. Kurowski, O. Perks, K. Brabazon, V. Jancauskas, D. Coster, P.V. Coveney, A.G. Hoekstra, "Patterns for High Performance Multiscale Computing", Future Generation Computer Systems, 91, 335-346 (2018), DOI: 10.1016/j.future.2018.08.045.
5. B. Chopard, J. Falcone, P. Kunzli, L. Veen, A. Hoekstra, "Multiscale modeling: recent progress and open questions", Multiscale and Multidisciplinary Modeling, Experiments and Design, 1, 57–68 (2018), DOI: 10.1007/s41939-017-0006-4
6. S. Alowayyed, V. Azizi, G. Zavodszky and A. G. Hoekstra, "Load Balancing Massively Parallel Cell-based Blood Flow Simulations", Computer Physics Communications, Submitted (2018)
7. V. Jancauskas, T. Piontek, P. Kopta, B. Bosak, "Predicting Queue Wait Time Probabilities for Multi-Scale Computing", Philosophical Transactions of the Royal Society, submitted (2018)
8. M. S. Fujii, J. Bédorf, J. Baba, S. P. Zwart, "The dynamics of stellar discs in live dark-matter haloes", Monthly Notices of the Royal Astronomical Society, 477, 1451–1471, DOI: 10.1093/mnras/sty711
9. S. P. Zwart, S. Torres, I. Pelupessy , J. Bédorf, M. X. Cai, "The origin of interstellar asteroidal objects like 1I/2017 U1 `Oumuamua", Monthly Notices of the Royal Astronomical Society, 479, L17-L22, DOI: 10.1093/mnrasl/sly088
10. D. Groen, R. A. Richardson, R. Coy, U. D. Schiller, H. Chandrashekar, F. Robertson, P. V. Coveney, "Validation of patient-specific cerebral blood flow simulation using transcranial Doppler measurements", Frontiers in Physiology, 9, 721 (2018), DOI: 10.3389/fphys.2018.00721
11. D. Groen, "Development of a multiscale simulation approach for forced migration", ICCS 2018, Springer Lecture Notes in Computer Science (LNCS), Accepted (2018)
12. N. T. Chan, D. Suleimenova, D. Bell, D. Groen, "Modelling Refugees Escaping Violent Events: A Feasibility Study From An Input Data Perspective", Proceedings of the Operational Research Society Simulation Workshop 2018, In Press (2018)
13. A. Nikishova, L. Veen, P. Zun, A. G. Hoekstra, "Uncertainty Quantification of a Multiscale Model for In-Stent Restenosis", Cardiovascular Engineering and Technology, 1-14 (2018), DOI: 10.1007/s13239-018-00372-4
14. S. Portegies Zwart and S. McMillan. Textbook: "Astrophysical Recipes: the Art of AMUSE" AAS IOP Astronomy (2018).
15. S. Succi, P. V. Coveney, "Big Data: the End of the Scientific Method?" Phil Trans R Soc (Series A) (in press) arxiv.org/abs/1807.09515
16. J. Suter, P. V. Coveney, "Chemically Specific Multiscale Modelling of the Shear-Induced Exfoliation of Clay-Polymer Nanocomposites", ACS Omega, 3(6), 6439-6445 (2018), DOI: 10.1021/acsomega.8b00542
17. M. O. Bernabeu, M. L. Jones, R. W. Nash, A. Pezzarossa, P. V. Coveney, H. Gerhardt, and C. A. Franco, "PolNet: A Tool to Quantify Network-Level Cell Polarity and Blood Flow in Vascular Remodeling", Biophysical Journal, 114 (9), 2052-2058 (2018) DOI: 10.1016/j.bpj.2018.03.032
18. A. Bhati, S. Wan, Y. Hu, B. Sherborne, P. V. Coveney, "Uncertainty Quantification in Alchemical Free Energy Methods", Journal of Chemical Theory and Computation, 14 (6), 2867–2880 (2018), DOI: 10.1021/acs.jctc.7b01143
19. R. C. Sinclair, J. L. Suter, P. V. Coveney, "Graphene-graphene interactions: friction, superlubricity and exfoliation", Advanced Materials, 30 (2018) 17057091, DOI: 10.1002/adma.201705791
20. G. Zavodszky, B. Rooij, V. Azizi, S. Alowayyed, A. Hoekstra, "Hemocell: a high-performance microscopic cellular library", Procedia Computer Science, 108, 159-165 (2017), DOI: 10.1016/j.procs.2017.05.084

21. M. X. Cai, M. B. N. Kouwenhoven, S. Portegies Zwart, R. Spurzem, “Stability of multiplanetary systems in star clusters”, Monthly Notices of the Royal Astronomical Society, 470, 4337-4353 (2017), DOI: 10.1093/mnras/stx1464
22. S. Alowayyed, D. Groen, P. V. Coveney, A. G. Hoekstra, “Multiscale Computing in the Exascale Era”, Journal of Computational Science, 22, 15-25, DOI: 10.1016/j.jocs.2017.07.004
23. R. C. Eccleston, S. Wan, N. Dalchau, P. V. Coveney, “The role of multiscale protein dynamics in antigen presentation and T lymphocyte recognition”, Frontiers in Immunology, Available Online (2017), DOI: 10.3389/fimmu.2017.00797
24. P. S. Zun, T. Anikina, A. Svitenkov, A. G. Hoekstra, “A Comparison of Fully-Coupled 3D In-Stent Restenosis Simulations to In-vivo Data” Frontiers in Physiology, 8, 1-12 (2017), DOI:10.3389/fphys.2017.00284
25. D. Groen and S. Zwart, “From Thread to Transcontinental Computer: Disturbing Lessons in Distributed Supercomputing”, IEEE 11th International Conference one-Science (e-Science) 2015, 15557226 (2015), DOI: 10.1109/eScience.2015.81
26. S. Schmieschek , L. Shamardin, S. Frijters, T. Krueger, U. D. Schiller, J. Harting, and P. V. Coveney, “LB3D: A Parallel Implementation of the Lattice-Boltzmann Method for Simulation of Interacting Amphiphilic Fluids”, Computer Physics Communications, 217, 149–161 (2017), DOI: 10.1016/j.cpc.2017.03.013
27. S. Wan, A. Bhati, S. Skerratt, K. Omoto, V. Shanmugasundaram, S. Bagal, P. V. Coveney, “Evaluation and Characterization of Trk Kinase Inhibitors for the Treatment of Pain: Reliable Binding Affinity Predictions from Theory and Computation”, Journal of Chemical Information and Modelling, 57 (4), 897–909 (2017), DOI: 10.1021/acs.jcim.6b00780
28. S. Wan, A. P. Bhati, S. J. Zasada, I. Wall, D. Green, P. Bamborough, and P. V. Coveney, “Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: a Computational Study”, J. Chem. Theory Comput., 13 (2), 784–795 (2017), DOI: 10.1021/acs.jctc.6b00794
29. A. Bhati, S. Wan, D. Wright, P. V. Coveney, “Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration”, Journal of Chemical Theory and Computation, 13 (1), 210–222 (2017), DOI: 10.1021/acs.jctc.6b00979
30. A. G. Hoekstra, S. Alowayyed, E. Lorenz, N. Melnikova, L. Mountrakis, B. van Rooij, A. Svitenkov, G. Závodszky, P. Zun, “Towards the virtual artery: a multiscale model for vascular physiology at the physics–chemistry–biology interface”, Philosophical Transactions of the Royal Society A, 374 (2016), DOI: 10.1098/rsta.2016.0146
31. D. Groen, A. Bhati, J. Suter, J. Hetherington, S. Zasada, P. V. Coveney, “FabSim: facilitating computational research through automation on large-scale and distributed e-infrastructures”, Computer Physics Communications, 207, 375–385 (2016), DOI: 10.1016/j.cpc.2016.05.020
32. S. J. Zasada and P. V. Coveney, “A Distributed Multi-agent Market Place for HPC Compute Cycle Resource Trading”, CoRR (2015), arXiv:1512.04343
33. J. Suter, D. Groen, and P. V. Coveney, “Mechanism of exfoliation and prediction of materials properties of clay-polymer nanocomposites from multiscale modeling”, Nano Lett., 15, 8108–8113 (2015), DOI: 10.1021/acs.nanolett.5b03547

Figure 1: JCTC cover for a ComPat paper

A few highlights among the publications are shown in this section.

The Journal of Chemical Theory and Computation awarded the cover of their April 2017 issue to the ComPat paper "Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration". The cover image is shown in Figure 1.

The paper "On the calculation of equilibrium thermodynamic properties from molecular dynamics" was published in Physical Chemistry Chemical Physics and was awarded the cover image, which can be seen in Figure 2.

Figure 2: PCCP cover for a ComPat paper

One major publication piece will not be completed by the official end of the project, but it will take place shortly following the project end. We are deep into the process of publishing a special themed issue of Phil Trans Roy Soc A, called "Multiscale Modelling, Simulation & Computing: from the Desktop to the Exascale". The guest editors are Peter Coveney, Simon Portegies Zwart, and Alfons Hoekstra. Currently, the expected date of publication is the start of 2019 and among the ComPat papers there is the inclusion of a paper by the H2020 project ESiWACE as part of our outreach activity to other projects.

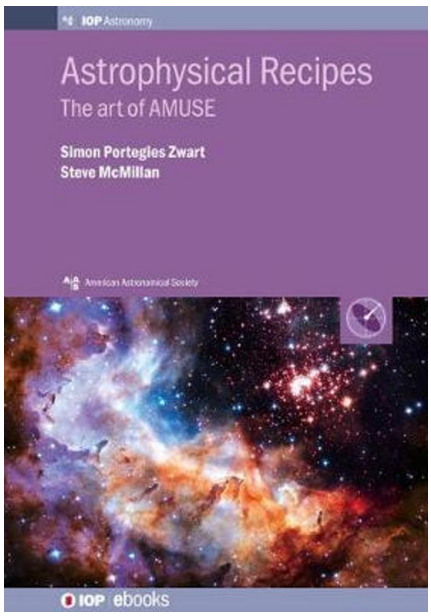

Figure 3: Cover of ComPat textbook

For the Advanced Materials paper on "Graphene-graphene interactions: friction, superlubricity and exfoliation", we worked with the journal to create a video abstract to post around our dissemination channels and on the Advanced Materials YouTube channel. The video is described further in Section 2.1.2.

Simon Portegies, Leiden University, published a textbook: S. Portegies Zwart, and S. McMillan. "Astrophysical Recipes: the Art of AMUSE" AAS IOP Astronomy (2018). The textbook outlines the fundamentals for computational astrophysics, focusing on the use of the Astronomical Multipurpose Software Environment (AMUSE), a general-purpose simulation environment in astrophysics written in Python, enabling the growth of multi-physics and multi-scale application software in a hierarchical fashion, testing each intermediate step as the complexity of the software continues to increase. All examples in the book are associated with codes that run on a simple laptop or workstation. All figures are

reproducible with a simple script, and all scripts are available online to be downloaded and run accordingly. The cover of this textbook is shown in Figure 3.

In addition to the publications described above, there were two PhD theses prepared during the course of ComPat by members of the consortium:

- S. Alowayyed, “Patterns for multiscale computing,” PhD thesis, Universiteit van Amsterdam, 2018.
- T. Piontek, PhD thesis on "Management methods of multi-scale applications and run-time environments in high-performance computing systems regarding energy efficiency", Poznan University of Technology, Due to be reviewed in 2019

2.1.1.1 Interdisciplinary nature of research papers

The interdisciplinary nature of the research undertaken in the ComPat project has been emphasised on our website (http://www.compat-project.eu/about-2/), in our leaflets and posters, in our talks, and below we show some instances described in our research papers:

- S. Alowayyed, D. Groen, P. V. Coveney, A. G. Hoekstra, “Multiscale Computing in the Exascale Era”, Journal of Computational Science, 22, 15-25, DOI: 10.1016/j.jocs.2017.07.004
  "Indeed, multiscale phenomena are everywhere around us [1], [2], [3], [4], [5], [6], [7]. If we study the origin and evolution of the universe [8] or properties of materials [9], [10], [11], [12], [13], if we try to understand health and disease [3], [14], [15], [16], [17], [18], [19], [20], [21] or develop fusion as a potential energy source of the future [22]."

- D. Groen, A. Bhati, J. Suter, J. Hetherington, S. Zasada, P. V. Coveney, “FabSim: facilitating computational research through automation on large-scale and distributed e-infrastructures”, Computer Physics Communications, 207, 375–385 (2016), DOI: 10.1016/j.cpc.2016.05.020
  "... we present exemplar FabSim use cases in three scientific domains where FabSim has so far been applied. These include simulations of cerebrovascular bloodflow, multiscale simulations of clay-polymer nanocomposites, and ensemble molecular dynamics simulations used to calculate ligand–protein binding affinities."

- B. Chopard, J. Falcone, P. Kunzli, L. Veen, A. Hoekstra, “Multiscale modeling: recent progress and open questions”, Model. Exp. and Des., 1, 57–68 (2018), DOI: 10.1007/s41939-017-0006-4
  "Many important scientific problems are inherently multi scale. This is, for instance, the case in models in material science or environmental science."

2.1.1.2 Non-Peer Reviewed Publications

ComPat featured in a number of non-peer reviewed publications, these are listed in Annex 1: Non-Peer Reviewed Publications. This included a handbook and popular magazines.

2.1.2 Video Content

In the second 18 months of the project, we created video content to populate our YouTube channel (https://www.youtube.com/channel/UCNX_tqv1w2NzdKemQhaGydw), display on our website, on our Twitter account, and leverage for use elsewhere.

We filmed interviews with ComPat consortium members describing various aspects of the project, spliced with interesting animations and images. The videos were produced with professional quality and they served to explain aspects of ComPat to stakeholders. The full set of videos are listed in Annex 2: Video Content. One of the videos, "The ComPat Project", was entered into the europa.eu showcase to include it in the "EU-funded R&I projects" YouTube playlist. Three screenshots from these videos are shown in Figure 4.

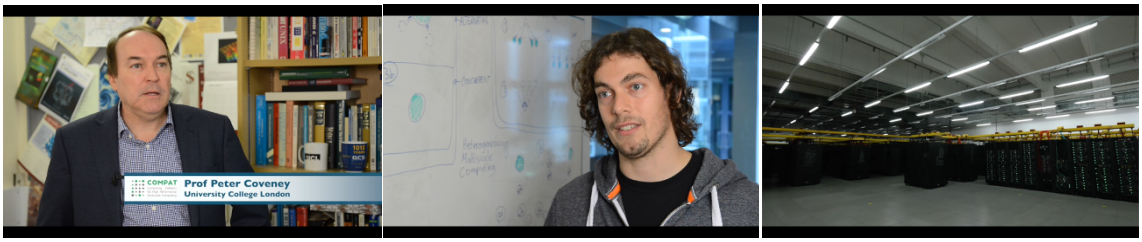

Figure 4: Screenshots from the ComPat video interviews

As part of the video production, animations were created to describe the three ComPat multiscale computing patterns. These were animations created using elements of the ComPat logo, with a voice over recorded to describe the patterns. The resulting video was included in the video interviews described above. Additionally, GIFs were created of the computing pattern animations and included on the ComPat website to give it a visually arresting edge to visitors. The GIFs have also been included in talk slides as a visual aid in describing the computing patterns. Three screenshots of the animations are shown in Figure 5.

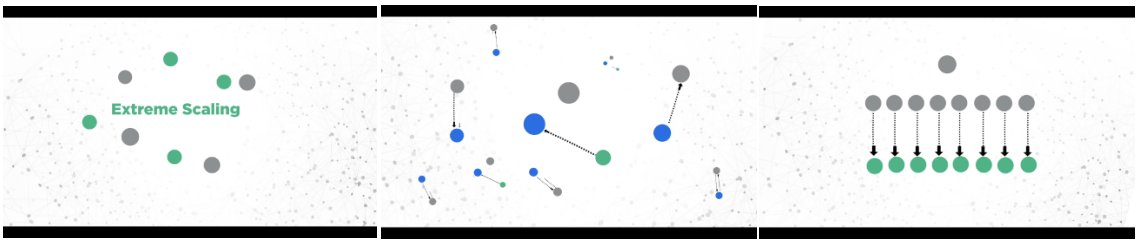

Figure 5: Screenshots from the ComPat multiscale computing pattern animations

An abstract video was created as part of the media campaign for the following paper:

- R. C. Sinclair, J. L. Suter, P. V. Coveney, "Graphene-graphene interactions: friction, superlubricity and exfoliation", Advanced Materials, 30 (2018) 17057091, DOI: 10.1002/adma.201705791

We worked with the Advanced Materials journal to produce a video containing video interviews and computer-generated animations describing the graphene-graphene interactions in the paper. The video can be viewed at the Advanced Materials YouTube channel at the following URL: https://www.youtube.com/watch?v=mujuvO9vUJI. Three screenshots of the video can be viewed in Figure 6.

Figure 6: Screenshots from the Advanced Materials ComPat Graphene video

2.1.3 Websites

ComPat content has appeared on various websites in the second 18 months of the project. This includes the Science Museum Blog publishing an article on UCL's graphene research, titled "Supercomputer Peels Away Graphene's Sticky Secrets"[1], and a WIRED article on "How weather forecasts could help develop 'designer' drugs personalised to your illness"[2], featuring Peter Coveney (UCL) and ComPat's JCTC paper on "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study". Further instances are listed in Annex 3: Websites.

On the project website (http://www.compat-project.eu/) there are 26 pages and 60 news stories. There have been 13,341 page views (shown in Figure 7) and 6790 unique users.

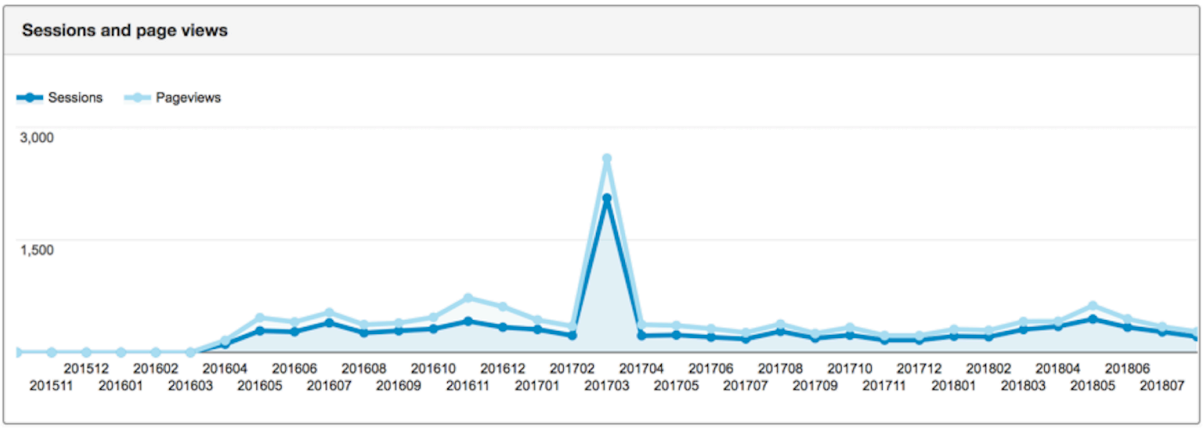

Figure 7: Project website page views and sessions since the project start, tracking of figures began in April 2016. It is unclear why there is a major peak of visitors during March 2017.

In the second 18 months of the project, the website was enhanced by integrating the computing pattern GIFs and video interviews into the pages to improve the visual impact and interactivity on the 'Home' and 'About' pages. The major features of the website also include a software resources page that lists ComPat software/tools repositories, the Experimental Execution Environment (EEE) Wiki, the ComPat intranet to store project documents, a feed of the ComPat twitter account, a news and events page, a list of ComPat publications and public access to public ComPat deliverables, and a description of the consortium partners and people. A screenshot of the ComPat website homepage is shown in Figure 13 in Annex 3: Websites.

[1] *https://blog.sciencemuseum.org.uk/supercomputer-peels-away-graphenes-sticky-secrets/*
[2] *https://www.wired.co.uk/article/personalised-drugs-simulations*

The ComPat website is hosted by CBK Sci Con, who are committed to keeping the website online for the foreseeable future.

2.1.4 Social Media

The ComPat Twitter account (@compatproject) has gathered 33,782 impressions over the course of the project. The account has posted 187 tweets, 253 followers, and 28 likes. The Twitter impressions per month are listed in Figure 8. The ComPat YouTube page has 625 views and 9 videos.

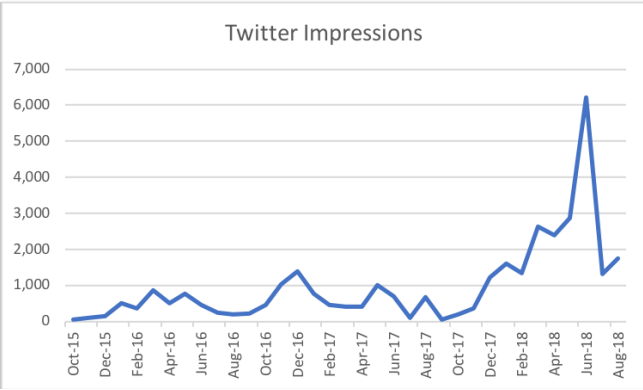

Figure 8: ComPat Twitter Impressions

Our experience with LinkedIn (as discussed in previous dissemination reports) and Reddit (where the ComPat Graphene-Graphene video was posted), and our observations of other H2020 projects using Facebook and Instagram allowed us to conclude that those platforms yield low amounts of interactions with the uploaded content, relative to the investment of time required. On the other hand, in our experience Twitter and YouTube have proven to be effective tools, with the potential to reach over 6,000 people in a month, and act as useful platforms to host content such as videos and links, and they allow targeting of most of our major stakeholders including Academia, Industry, General Public, Media, and Customers. Both of these platforms have therefore justified an investment of time.

Further details of social media activity in the second 18 months of the project are listed in Annex 4: Social Media.

2.1.5 Leaflets

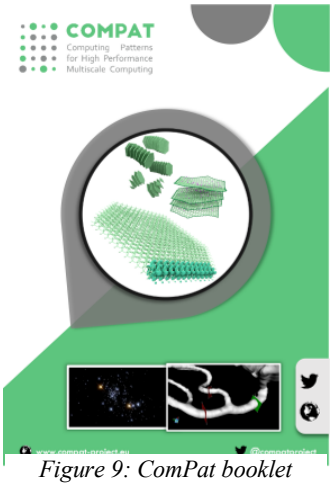

Figure 9: ComPat booklet

In addition to the ComPat posters and leaflet produced in the first 18 months of the project, in the second 18 months we produced a 16-page booklet describing the ComPat project and two of the ComPat applications. The cover of the booklet is shown in Figure 9.

The booklet was printed and delivered to all consortium partners for distribution to stakeholders at various events. Events included the 5th International Conference on Protective Structures 2018 in Poznan, the European HPC Summit Week 2018 in Ljubljana, and the International Supercomputing Conferences in 2017 and 2018 in Frankfurt.

2.1.6 Outreach

In this section, we report on the activity towards specific outreach targets.

2.1.6.1 Outreach to external applications

It was planned that, for the second phase of the project, ComPat would reach out to other applications outside the consortium. The majority of our dissemination efforts would in some way act as outreach to external applications, including our Lorentz Center Workshop in Leiden, the ComPat Industry Event in Daresbury, and the ComPat webinar.

Given the progress made in developing ComPat software and tools over the project, it was not possible to have a concerted effort in adapting multiple external applications into using ComPat tools, and exploring the challenges they would present. However, we were able to use the STFC-based application called ChemShell as a test case.

ChemShell was used to benchmark the energy metrics on the Hartree supercomputers run through the QCG middleware. With ChemShell installed on Hartree Neale, trial benchmarks assessed by Arm MAP were successfully performed. The QCG account and certificate were also configured for performing ChemShell calculations.

A charge fitting module in ChemShell has been successfully implemented and code development for refining force field parameters is nearing completion, as requested by the ComPat group at UCL. The UCL group require optimised force field description and accurate charges for carrying out high-throughput screening for finding promising drug candidates. The outstanding HPC features of ChemShell will assure these types of computations are performed in a high-throughput manner.

2.1.6.2 Outreach with other projects

We took various actions during the course of the project in order to liaise with other projects and inform them about ComPat's tools and ideas. These outreach items are listed in Annex 5: Outreach to Other Projects. Below we describe our interactions with some projects in more detail:

TSERO – the Total Software Energy Reporting and Optimization project, which brings together monitoring of HPC systems and compiling programs for energy efficiency in order to provide an end-to-end system to significantly reduce the energy used by such systems. STFC conducted a major cross over effort with TSERO, working with them for energy collection work and then looking at how to interpret energy and performance data in conjunction with each other. The results of this went into tooling for ComPat.

ESiWACE – a Centre of Excellence in Simulation of Weather and Climate in Europe, aims to substantially improve efficiency and productivity of numerical weather and climate simulation on high-performance computing platforms by supporting the end-to-end workflow of global Earth system modelling in HPC environment. With this project, we discussed the similarities of multiscale modelling from ComPat and workflow orchestration from within ESiWACE, specifically around their Cylk workflow engine. We also worked with one of the ESIWACE partners on how performance data could be collected and aggregated, then running some machine learning and analytics against it. Following that, we then looked at the visualisation side of data collection with the EsiWACE team members.

Furthermore, ESiWACE will contribute to the ComPat special issue in Phil Trans Roy Soc A due to be released at the start of 2019, as described in Section 2.1.1. Furthermore, Philipp Neumann from ESiWACE gave a talk at the ComPat Lorentz Center workshop on "From Convergence of Weather and Climate Simulations to a Coupling Software for Massively Parallel Molecular-Continuum Flows".

SAGE – Percipient Storage for Exascale Data Centric Computing, aims at building a next generation storage system suitable for Exascale supercomputers and applications that generate, consume and process immense volumes of data. With SAGE we were focused on running applications and performing deeper analysis. We coordinated with the SAGE team to look at how performance data should be exported and visualised. Specifically, we worked on how to 'join' performance data from different runs. We developed a set of open source analysis scripts[3], which let a researcher query multiple performance profiles to look at components such as MPI scaling.

NEXTGenIO – Next Generation I/O for the Exascale, addresses a key challenge not only for Exascale, but also for HPC and data intensive computing in general: the challenge of I/O performance. With NEXTGenIO, we looked at workflows and how to profile them and visualise the results. We liaised with the NEXTGenIO team about how best to collect all the data and what it means to profile a workflow.

OpenMultiMed – Open Multiscale Systems Medicine is a European Commission funded e-COST Action, the aim of which is to evaluate a transdisciplinary framework for multiscale systems medicine, consisting of novel concepts, methodologies and technologies. Three ComPat consortium members were involved in OpenMultiMed, which readily allowed the exchange of ideas between the projects. We gave a talk about ComPat and OpenMultiMed during the ICCS 2016 conference in San Diego and during an OpenMultiMed Winter School in Erlangen. ComPat consortium members also contributed to an OpenMultiMed survey on multiscale computing.

CompBioMed – a Centre of Excellence in Computational Biomedicine, is focused on the on the use and development of computational methods for biomedical applications. ComPat and CompBioMed share a number of consortium members, which allowed the two projects to coordinate their dissemination efforts at numerous events, on social media, and ensured substantial usage of ComPat tools, software, and ideas in CompBioMed applications.

VECMA – Verified Exascale Computing for Multiscale Applications, aims to enable a diverse set of multiscale, multiphysics applications to run on current multi-petascale computers and emerging exascale environments with high fidelity such that their output is "actionable". This new project involves the majority of the ComPat consortium and continues many of the ideas formed in the ComPat project, including the use of its tools and software in a major way.

HiDALGO - HPC and Big Data Technologies for Global Systems, is a Horizon 2020 Centre of Excellence project that is slated to begin in 2019. The proposal refers to several works from ComPat and will rely on some of the tools from ComPat including mainly FabSim and MUSCLE.

2.2 Events

[3] *https://github.com/arm-hpc/allinea_json_analysis*

In this section, we describe the events that the ComPat consortium organised and participated in.

2.2.1 Events Organised

Each event that we organised in the second 18 months of the project is listed in Annex 6: Events Organised, with key highlights described in more details below.

2.2.1.1 Lorentz Center Workshop

Figure 10: Poster for the ComPat Lorentz Center Workshop

A major event that we organised in the second 18 months of the project was the Lorentz Center workshop in Leiden on "Multiscale Computing: From the desktop to the Exascale" on 16-20 April 2018. The goal of this workshop was to bring together a group of computational scientists and scientists from several different scientific disciplines to further explore generic methods, algorithms, specification and modelling languages, and software environments for multiscale computing. By building upon the current understanding of multiscale modelling the focus of the workshop was mainly on multiscale computing on state-of-the-art computing resources, with focus on high end HPC/Cloud ecosystems.

A main scientific output of the workshop will be a special issue in the Philosophical Transactions of the Royal Society A, on "Multiscale Modelling, Simulation & Computing: from the Desktop to the Exascale", expected to be published in the beginning of 2019. This special issue will feature a position paper summarising the main the conclusions of the workshop, as well as a collection of ten research papers dedicated to the theme of the workshop and written by participants of the workshop.

A main theme within the workshop was to identify generic algorithms and techniques for multiscale computing, and we agreed that the vision of multiscale computing patterns is very useful for a large range of multiscale models, independent of specific application domains. We also realised that such patterns would be more broadly applicable than only in a multiscale computing setting, and that such patterns should be applicable in any scenario where coupled components need to be executed on HPC environments, certainly when either the number of components or their coupling is dynamic, or both. This triggered deeper discussion on how generic software environments for multiscale computing could be developed, and how to make such environment useful in the context of HPC. Discussions were based on existing systems such as the MMSF/Muscle or AMUSE, but also by considering such environments with the needs from different communities (e.g. from weather and climate, biomedicine, materials, fusion).

The workshop featured plenary lectures on specific topics, working sessions in smaller groups with rapporteurs making notes in a google doc shared among all participants. The working sessions were planned in detail (topics for discussion, intended outcomes), nominating participants to take part in specific sessions to foster contacts and cross-disciplinary discussions. Two months before the workshop the organizers distributed relevant papers to participants and asked them to study this material, and to form their opinion on specific issues identified by the organisers. We also asked all participants to bring one (or more) posters of their current (and if relevant, past work) and put these on display. We organised

a few speed sessions where participants had 5 minutes to present their poster in order to draw attention to their work and to trigger discussions. These speed sessions were always just before a scheduled break, so that discussions could immediately start. Overall, we were satisfied with this format, although the speed sessions and poster presentations were not very crowded, meaning that most participants unfortunately did not bring a poster. This would probably work better in a larger setting, for example in the large Lorentz Center room Oort, and less so in in the smaller Lorentz Center Snellius room.

2.2.1.2 Workshop: High Performance Computing for Your Business

Figure 11: Picture of the workshop in progress

On 6 June 2018, ComPat organised a workshop on "High Performance Computing for Your Business" at Sci-Tech Daresbury, UK. The event was hosted by the Hartree Centre to engage with industry about the use of High Performance Computing (HPC) within business. At the event, we described the ComPat approach and gave an overview of Multiscale Modelling. The event was pitched at a level where companies who currently using Cloud based computing would be able to understand the steps needed to embrace HPC.

The venue of the event was the main conference room at Sci-Tech Daresbury which is located within a UK Enterprise zone that is the home to over 100 Small to Medium Enterprises within high technology industries from the Chemicals Industry to High Value Manufacturing. The British Government had the first cabinet meeting outside of London under Teresa May's leadership at the site in 2017. Invites were sent across the site and via the wider networks within the North West (and wider Northern Powerhouse) region of the UK which Hartree is located within.

Before the event the Hartree Centre conducted a focus study to assist in determining the focus of the workshop. The focus group was conducted as a staged process with an initial survey being sent, this was followed up with a smaller group meeting of responders over lunch to explore in more detail the responses. 33 people completed the survey and the face-to-face session involved 6 of the responders. Feedback from the group highlighted that the workshop is likely to attract two communities of users. The first being parties using Cloud based compute with an interest but little knowledge of HPC and the other set of HPC users who have varying degrees of understanding in relation to Multiscale Modelling. This feedback was split into 6 core objectives that were set for planning the workshop, which are listed below:

1. Give a clear introduction to High Performance Computing at the start of the workshop. Unless a company uses HPC it is unlikely that they will have much knowledge of different HPC architectures and methods of provision even if HPC would be of direct benefit to their business.
2. Give real world examples. Move the discussion onto real world uses of HPC within familiar domains to the attendees i.e. automotive.
3. Link to facilities on site and call for action to use HPC. Describe how a company can use HPC via the Hartree Centre.
4. Explain why Multiscale Modelling is needed. Give examples and motivation for ComPat
5. Define Multiscale Modelling. Make the ComPat approach clear giving examples and benefits.

6. Link to wider ComPat community and call for action to work with the project's technology. Describe how a company can start to use ComPat technology.

Thus, the workshop was planned to address both communities of industry new to HPC and experienced users.

The session started with a networking event where scientists from ComPat could mingle and chat to attendees from business. The event was attended by 27 people from a range of industries and large corporations including IBM and Atos. The event concluded with further networking and the ability for participants to discuss elements of the presentations on an individual basis with the speakers.

Following the workshop, the Hartree Centre has engaged with three of the attendees around possible use of HPC within business. In addition to this, the workshop provided a link into the ComPat project within the Scientific Computing Department of STFC. This group is now looking to compare approaches it has around Multiscale Modelling with that of the ComPat project. This work will be written up as a paper.

2.2.1.3 Multiscale Modelling and Simulation Workshops 2017 and 2018

Following the 2016 Multiscale Modelling and Simulation Workshop discussed in D7.2, ComPat consortium members Derek Groen (UBRUN) and Alfons Hoekstra (UvA) then organised the 2017 and 2018 editions in the second 18 months of the project. Each edition was held as part of the International Conference of Computational Science (ICCS), which is a yearly conference alternating between Europe, Asia and the USA.

The workshops aim to provide a forum for multiscale application modellers, framework developers and experts from the distributed infrastructure communities to identify and discuss challenges in, and possible solutions for, modelling and simulating multiscale systems, as well as their execution on advanced computational resources and their validation against experimental data.

The 2017 edition of the workshop took place in Zurich, Switzerland on 11-14 June 2017, resulting in a paper in Procedia Computer Science (DOI: 10.1016/j.procs.2017.05.275). The 2018 edition took place in Wuxi, China on 11-13 June 2018, and will also result in an open-access Procedia Computer Science paper. Selected papers will be invited for inclusion in a special issue of the Journal of Computational Science.

2.2.1.4 HPC Summit Week 2018 Session

At the HPC Summit Week in Ljubljana, Slovenia on 31 May 2018, representatives of the ComPat consortium held a dedicated 4.5-hour session on "Computing Patterns for High Performance Multiscale Computing". In the session, we presented the various aspects around the development of multiscale computing algorithms capable of producing high-fidelity scientific results and scalable to exascale computing systems. Attendees were taken through the lifecycle of a multiscale application, from definition to optimisation to execution. The session finished with 3 demonstrations, the first was a multiscale fusion demo from MPG, the second was the binding affinity calculator from UCL, and the third was an HMC demonstration from UCL.

Figure 12: Pictures of the talks during the ComPat session

Overall, around 10-15 people attended the session, 51 people signed up to attend. We felt that, while the HPC Summit Week itself serves as a great networking event, the effort put into the dedicated session did not yield an attendance level that made it worthwhile.

2.2.1.5 ComPat Webinar

We had originally planned to hold a ComPat Training session on "Multiscale Modelling & Simulation on HPC" alongside PASC18 in Basel, Switzerland. The intention was to hold a 3-hour session in which attendees would be taught to use one of our applications and couple it in a multiscale manner. Following that, attendees would run that multiscale application on a supercomputer using ComPat tools and services. We would describe the principles, concepts, tools, and codes along the way. By the end of the session, we would have shown attendees how to run a multiscale application on HPC. We carried out a major and thorough advertising campaign to inform potential attendees, including directly notifying every relevant postgraduate department and research group in every Swiss university. However, the registration numbers were so slim that we had to cancel the event.

In place of the in-person training session, we have opted to hold a 1.5-hour online webinar, with the session's content adjusted to be suit the webinar platform. In order to make the webinar impactful and representative of the achievements in the ComPat project, we are aiming to include pieces of software that have just been finalised, therefore the webinar itself will be held after the project's end, funded by other sources after the ComPat end date. The webinar will be recorded and the complete video will be uploaded to the ComPat YouTube channel to act as a resource thereafter. We anticipate that the webinar will take place on Tuesday 30 October 2018.

The target audience for the webinar is computational researchers and PhD students; we will advertise the event on our project website, Twitter account, to a list of contacts of those who expressed interest in the cancelled PASC18 event, through the dissemination channels of related projects, the institutions of those in the consortium, and by harnessing the consortium members' personal dissemination networks such as relevant mailing lists and contacts. For the PASC18 training event, we largely appealed only to those who were already intending to attend the wider PASC18 conference, and although we carried out a major advertising campaign that targeted all Swiss Universities, the end result was registered participation that was too low to proceed. Since the webinar will not require a commitment of travel or a major commitment of time, and can be accessed by people from around the globe, we anticipate an improved level of participation.

2.2.2 Participation in Events

In the second 18 months of the project, the ComPat consortium participated in many conferences, workshops, and other events. The full listing is given in Annex 7: Participation in Events. In the second 18 months of the project, the consortium organised 5 booths (7 in 36 months), 4 posters (8 in 36 months), and 70 talks (106 in 36 months). These took place across many events, including 45 major conferences or workshops (68 in 36 months), which are listed below:

- International Supercomputing Conference 2017, Frankfurt, Germany
- International Supercomputing Conference 2018, Frankfurt, Germany
- European HPC Summit Week 2017, Barcelona, Spain
- European HPC Summit Week 2018, Ljubljana, Slovenia
- International Conference on Computational Science 2017, Zurich, Switzerland
- International Conference on Computational Science 2018, Wuxi, China
- Supercomputing 2017, Denver, USA
- 11th Parallel tools workshop, Dresden, Germany
- High Performance and Embedded Architecture and Compilation, GoingArm Workshop, Manchester, UK
- Argonne Simulation.Data.Learning Workshop, Chicago, USA
- TERATEC Forum 2018, Paris, France
- Arm Research Summit 2017, Cambridge, UK
- 12th International Conference on Parallel Processing and Applied Mathematics (PPAM) Conference in Lublin, Poland
- 5th International Conference on Protective Structures in Poznan, Poland
- Supercomputing Frontiers Europe 2018, Warsaw, Poland
- The European Association for Predictive, Preventive & Personalised Medicine (EPMA) World Congress 2017, Malta
- International Conference on Numerical Simulation of Plasmas, Leuven, Belgium
- The Institute of Electrical and Electronics Engineers (IEEE) eScience 2018, Amsterdam, Netherlands
- IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid) 2018, Washington DC, USA
- Think Science Conference, Dubai, UAE
- 253rd American Chemical Society (ACS) National Meeting, San Francisco, California
- 2017 Materials Research Society (MRS) Spring Meeting, Phoenix, Arizona
- Cambridge Ophthalmological Symposium, Cambridge, UK
- Middle East Molecular Biology Sources (MEMBS) Congress 2017, Abu Dhabi, UAE
- Data Intensive Studies Center (DISC) Fall Symposium in Massachusetts, USA
- New York Scientific Data Summit (NYSDS) Data-Driven Discovery in Science and Industry, New York, US
- Sixth Palestinian Conference on Modern Trends in Mathematics and Physics, Palestine
- NVIDIA's GPU Technology Conference 2018, San Jose, USA
- Konferencję Użytkowników Komputerów Dużej Mocy (KUKDM) 2018, Zakopane, Poland
- Austrian High Performance Computing (AHPC) 2018, Linz, Austria
- Big Data made in Germany, Berlin, Germany
- Cloud & High Performance Computing in Biomedicine, London, UK

- Sixth National Conference on Cloud Computing and Commerce, Dublin, Ireland
- Supercomputing in Scientific and Industrial Problems (2017/SSIP), Stuttgart, Germany
- Computational and Mathematical Biomedical Engineering (CMBE) 2017, Pittburgh, USA
- Multiscale Computing: From the Desktop to the Exascale, Leiden, Netherlands
- 10th International Workshop on Science Gateways in Edinburgh, UK
- New Perspectives in Scheduling Theory Conference, Aussois, France
- HPC for your business, Daresbury, UK
- European Physical Society (EPS) 2018, Prague, Czech Republic
- 9th International Workshop on Science Gateways, Poznan, Poland
- CompBioMed/Vheart Workshop, Amsterdam, Netherlands
- International Space Science Institute (ISSI) 2018, Bern, Switzerland
- AMUSE workshop 2018, Leiden, Netherlands
- Virtual Institute High-Productivity Supercomputing, Tuning Workshop 2017, Southampton, UK

2.2.3 Impact on HPC

In the second half of the project, we made a concerted effort to increase our impact on high performance computing. In terms of publications, we increased the number of publications and the majority of these were in journals with relevance to HPC, listed below:

- Future Generation Computer Systems
- Journal of Computational Science
- Multiscale and Multidisciplinary Modeling, Experiments and Design
- Computer Physics Communications
- Journal of Chemical Theory and Computation
- Journal of Chemical Information and Modelling
- Procedia Computer Science
- IEEE 11th International Conference one-Science (e-Science) 2015
- Proceedings of the Operational Research Society Simulation Workshop 2018
- Springer Lecture Notes in Computer Science (LNCS)

In terms of event participation, as shown in Section 2.2.2, almost all of the 45 major events in the second half of the project had direct HPC relevance, with 16 of them being focused on HPC.

2.3 Measuring Impact

There are three key performance indicators (KPIs) that are relevant to the dissemination work package in the project:

- The number of publications – at least 20 by month 36
- The number of presentations given – at least 50 by month 36
- The number of multiscale computational pattern ARM visualisation demonstrations presented at workshops or tradeshows – 10 by month 36

For the first two KPIs, the dissemination reports D7.2, D7.3, and D7.4 provide the statistics and give the following:

- 33 publications produced over the project
- 106 presentations given over the project

As for the number of multiscale computational pattern ARM visualisation demonstrations presented at workshops or tradeshows, the goal was to give demonstrations at 10 events by month 36 of the project, and ARM have managed to give 12 demos over the course of the project, these are as follows:

- VI-HPS – Tuning workshop 2017 Southampton[4]
- ISC 17 – Booth Demos
- HPCSW 17 – Workshop presentation (CompBioMed Workshop)
- ICCS 17 – Workshop presentation
- SC 17 – Booth Demos
- 11th Parallel tools workshop[5,6]
- HIPEAC – Workshop presentation (GoingArm workshop)
- Argonne Simulation.Data.Learning workshop[7]
- HPCSW18 – Workshop demo (ComPat workshop)
- TERATEC 18 – Booth Demo
- ISC 18 – Booth Demos
- GoingArm presentation at 2017 Arm Research Summit

As for other statistics demonstrating project impact, the number of talks, posters, and booths, as well as the number of major events participated in was shown in Section 2.2.2. Website and social media statistics were shown in Sections 2.1.3 and 2.1.4. Finally, the right-most column in each of the tables in the appendices of this document gives the estimated audience sizes for each piece of dissemination activity. This adds up to a total audience size in the hundreds of thousands (the sum total comes to 735,951, although each figure is a rough estimate in most cases).

With all of the relevant KPIs exceeded, substantially so in the case of publications and presentations given, and with other available statistics showing a very wide audience being reached, we conclude that the project impact is significant.

2.4 After the Project

The work and materials developed in the ComPat project will live on past the project end date. One set of work that will remain available after the end of the project are the software/tools repositories that are listed on the website[8], which will be kept available in the repositories for the foreseeable future. Also listed on the project website is the ComPat Experimental Execution Environment Wiki[9]: we will keep this online for 1 year after the project in order to determine user interest, if there is notable user interest

[4] *https://www.vi-hps.org/upload/material/tw24/Allinea.pdf*
[5] *http://tools.zih.tu-dresden.de/2017/*
[6] *https://tools.zih.tu-dresden.de/2017/abstracts/Lebeau_Allinea_Custom_Metrics.pdf*
[7] *https://www.alcf.anl.gov/workshops/simulation-data-learning-workshop*
[8] *http://www.compat-project.eu/software-resources/*
[9] *http://compat-eee-wiki.drg.lrz.de/dokuwiki/doku.php*

then we will extend the Wiki's duration for a longer period. Naturally, the project publications[10] will act as a resource to future researchers. The videos on our YouTube channel will also continue to be available[11].

In terms of tangible activities that will occur after the project end, the ComPat Webinar mentioned in Section 2.2.1.5 will be broadcast in the month following the project end, and then the videos of the webinar broadcast will be placed permanently on the project YouTube page.

The ComPat themed Special Issue of Phil Trans Roy Soc A mentioned in Section 2.2.1.1 will be released at the start of 2019 and remain available thereafter.

The VECMA project[12], as mentioned in Section 2.1.6.2, will continue and build upon the legacy of ComPat in a major way.

3 Conclusions

There was a substantial amount of high impact activity during the ComPat project. The actions of the ComPat consortium met and exceeded the plans laid out in the ComPat dissemination action plan and the ComPat description of work.

We came across some challenges, for instance in our initially intended plans for a training school alongside the PASC conference which did not take place due to low registration numbers. We compensated for those struggles by organising a Webinar in place of the PASC training school, and by organising additional events that were not initially planned (such as 2 extra multiscale workshops at ICCS events and the ComPat Industry event). Meanwhile, we met and, in some cases, far exceeded our key performance indicators, reaching a collective audience in the hundreds of thousands along the way.

The ComPat consortium targeted many events and dissemination channels of various scales and with a wide variety of themes, covering numerous domains aligned with ComPat's aims, from exascale computing to biomedical science, from Twitter to television, and from students to Professors. ComPat reached many stakeholders across the globe.

Through the dissemination of ComPat research findings and open-source software to academia and industry alike, we have contributed to the strength and leadership of the EU in HPC technologies, also having an impact on the emerging HPC markets. Through the building of networks in our scientific community and the encouragement of collaboration activities, in addition to our training agenda, we have accelerated European excellence in computing and algorithms in a multi-disciplinary fashion.

[10] *http://www.compat-project.eu/publications/*
[11] *https://www.youtube.com/channel/UCNX_tqv1w2NzdKemQhaGydw*
[12] *http://www.vecma.eu/*

4 Annexes

4.1 Annex 1: Non-Peer Reviewed Publications

Details	Date From	Date To	Audience(s) (see above table)	No. of People
The ComPat project featured in the 2017 European HPC Handbook. It was distributed at the Supercomputing 2017 ETP4HPC Birds-of-a-Feather Session in Denver, USA	14/11/17	14/11/17	[Scientific Community (higher education, Research)], [Industry]	100
Derek Groen (Brunel) and ComPat featured in the online article "European HPC Summit Week and PRACEdays 2018: Slaying Dragons and SHAPEing Futures One SME at a Time" on HPCWire. https://t.co/ztBCZgJSeP	20/06/18	20/06/18	[Scientific Community (higher education, Research)] [Industry]	1000s
An article, "GCS: Delivering 10 Years of Integrated HPC Excellence for Germany", featuring ComPat's giant workflow project on SuperMUC was published in InSiDE Spring 2017 edition, led by Peter Coveney (UCL). http://inside.hlrs.de/#gcs-delivering-10-years-of-integrated-hpc-excellence-for-germany	01/05/17	01/05/17	[Scientific Community (higher education, Research)], [Industry]	400
Simon Portegies Zwart, Leiden University, featured in a magazine article in KIJK called "Superzware zwarte gaten beïnvloeden stervorming". https://www.kijkmagazine.nl/space/zwarte-gaten-stervorming/	03/01/18	03/01/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	2000
Simon Portegies Zwart, Leiden University, featured in a magazine article in Science News called "We still don't know where the first interstellar asteroid came from". https://www.sciencenews.org/article/we-still-dont-know-where-first-interstellar-asteroid-came	01/12/17	01/12/17	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	2000
Simon Portegies Zwart, Leiden University, featured in a magazine article in engineersonline called "Universiteit Leiden bouwt supercomputer". https://www.engineersonline.nl/nieuws/id30070-universiteit-leiden-bouwt-supercomputer.html	25/06/18	25/06/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	500
Simon Portegies Zwart, Leiden University, featured in a magazine article in allesoversterrenkunde called "Melkwegstelsel wemelt van de kosmische zwerfkeien". http://www.allesoversterrenkunde.nl/!/!/actueel/artikelen/_detail/gli/melkwegstelsel-wemelt-van-de-kosmische-zwerfkeien/	18/11/17	18/11/17	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	1000
Simon Portegies Zwart, Leiden University, featured in a magazine article in Sky & Telescope called "Sibling Rivalry Caused Eta Carinae's Historic Explosion". http://www.allesoversterrenkunde.nl/!/!/actueel/artikelen/_detail/gli/melkwegstelsel-wemelt-van-de-kosmische-zwerfkeien/	09/08/18	09/08/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	2000
Simon Portegies, Leiden University, published a textbook: S. Portegies Zwart, and S. McMillan.	01/06/18	01/06/18	[Scientific Community (higher education, Research)], [Industry]	200

"Astrophysical Recipes: the Art of AMUSE." AAS IOP Astronomy (2018).				

4.2 Annex 2: Video Content

Details	Date From	Date To	Audience(s) (see above table)	No. of People
Advanced Materials published a video abstract of the ComPat paper on graphene-graphene interactions carried out by Robert Sinclair, James Suter and Peter Coveney. The video was based on the paper "Graphene–Graphene Interactions: Friction, Superlubricity, and Exfoliation"	13/02/18	13/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	624
Created the film "The ComPat Project" and hosted it on the ComPat Youtube page. https://youtu.be/w6lnhAIxsh4	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	299
Entered the film "The ComPat Project" into the showcase "Calling all EU-funded R&I projects" to be included in the "EU-funded R&I projects" YouTube playlist.	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	299
Created the film "Multiscale Computing Patterns" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=eY9JKMaBYCs	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	41
Created the film "Multiscale Materials" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=5GQL1kkVVsk&t=1s	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	93
Created the film "Energy Efficiency in High-Performance Computing" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=LhKjRHyfryg	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	16
Created the film "Multiscale Fusion" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=slPRoBHRkP0	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	40
Created the film "Multiscale Computational Biomedicine" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=pv8eHX7c_eI	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	26
Created the film "Multiscale Astrophysics" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=xwen3j0meEE	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	16
Created the film "The Vision of the ComPat Project" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=H4mFrX2g9og	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	83
Created the film "Overview of the ComPat Project" and hosted it on the ComPat Youtube page. https://www.youtube.com/watch?v=7dW-fiidsBo	05/02/18	05/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	5

4.3 Annex 3: Websites

Details	Date From	Date To	Audience(s) (see above table)	No. of People
Posted a news item on the UCL CCS website about the ComPat paper on "Graphene–Graphene Interactions: Friction, Superlubricity, and Exfoliation". http://ccs.chem.ucl.ac.uk/	01/04/17	01/04/17	[Scientific Community (higher education, Research)]	100
The Advanced Materials video featuring ComPat graphene research was posted on videominecraft.ru. http://videominecraft.ru/watch/mujuvO9vUJI/graphenegraphene-interactions-friction-superlubricity-and-exfoliation.html	01/04/17	01/04/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	627
Onnie Luk, MPG, posted a news item on IPP's Numerical Methods for Plasma Physics division website about the HPC Summit Week ComPat Session. https://www.ipp.mpg.de/ippcms/eng/for/bereiche/numerik	25/04/18	25/04/18	[Scientific Community (higher education, Research)], [Industry]	100
An article was posted on hpc-ch.org that featured ComPat. https://www.hpc-ch.org/pasc18-public-lecture-and-compat-workshop/	09/03/18	09/03/18	[Scientific Community (higher education, Research)], [Industry]	50
The Science Museum Blog published an article on UCL's graphene research, titled "Supercomputer Peels Away Graphene's Sticky Secrets". https://blog.sciencemuseum.org.uk/supercomputer-peels-away-graphenes-sticky-secrets/	13/02/18	13/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	5000
Roger Highfield has published a WIRED article on "How weather forecasts could help develop 'designer' drugs personalised to your illness", featuring Peter Coveney (UCL) and ComPat's JCTC paper on "Rapid and Reliable Binding Affinity Prediction of Bromodomain Inhibitors: A Computational Study". https://www.wired.co.uk/article/personalised-drugs-simulations	29/04/17	29/04/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	2000
32 news stories were posted on the ComPat website during this period. http://www.compat-project.eu/news-and-events/	01/03/17	30/09/18	[Scientific Community (higher education, Research)], [Industry]	150
Simon Portegies Zwart, Leiden University, featured in an online article on the Leiden University website called "Simon Portegies Zwart in de Volkskrant over nieuw Jupitermaantje". https://www.universiteitleiden.nl/nieuws/2018/07/simon-protegies-zwart-in-de-volkskrant-over-nieuw-jupitermaantje	19/07/18	19/07/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	500
Simon Portegies Zwart, Leiden University, featured in an online article on the NWO website called "Chaos ontrafeld – astronomen rekenen chaotisch systeem nauwkeuriger door dan ooit". https://www.nwo.nl/actueel/nieuws/2018/02/chaos-ontrafeld-%E2%80%93-astronomen-rekenen-chaotisch-systeem-nauwkeuriger-door-dan-ooit.html	13/02/18	13/02/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000

Simon Portegies Zwart, Leiden University, featured in an online article on the de Veolkskrant website called "Nieuw ontdekt Jupitermaantje beweegt als botsautootje tegen de stroom in". https://www.volkskrant.nl/wetenschap/nieuw-ontdekt-jupitermaantje-beweegt-als-botsautootje-tegen-de-stroom-in~b7ba14fd/	17/07/18	17/07/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the Trouw website called "Wetenschappers zijn er nog steeds niet uit: hebben we acht of negen planeten in ons zonnestelsel?". https://www.trouw.nl/home/wetenschappers-zijn-er-nog-steeds-niet-uit-hebben-we-acht-of-negen-planeten-in-ons-zonnestelsel-~a70de7aa/	19/06/18	19/06/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the nrc website called "Zoeken naar aliens kan nooit kwaad". https://www.nrc.nl/nieuws/2017/12/19/zoeken-naar-aliens-kan-nooit-kwaad-a1585533	19/12/17	19/12/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the nrc website called "Een rots van buiten het zonnestelsel". https://www.nrc.nl/nieuws/2017/11/21/een-rots-van-buiten-het-zonnestelsel-14125832-a1581878	21/11/17	21/11/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the tweakers website called "Supercomputer vindt oplossingen voor eeuwenoud 'driehemellichamenprobleem'". https://tweakers.net/nieuws/130093/supercomputer-vindt-oplossingen-voor-eeuwenoud-driehemellichamenprobleem.html	27/09/17	27/09/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the KENNISLINK website called "Eerste middelgrote zwarte gat gevonden". https://www.nemokennislink.nl/publicaties/eerste-middelgrote-zwarte-gat-gevonden/	06/09/17	06/09/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	1000
Simon Portegies Zwart, Leiden University, featured in an online article on the New Scientist website called "Nederlanders maken supercomputer die in een bakfiets past". https://newscientist.nl/nieuws/nederlanders-maken-supercomputer-bakfiets-past/	14/04/17	14/04/17	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	5000

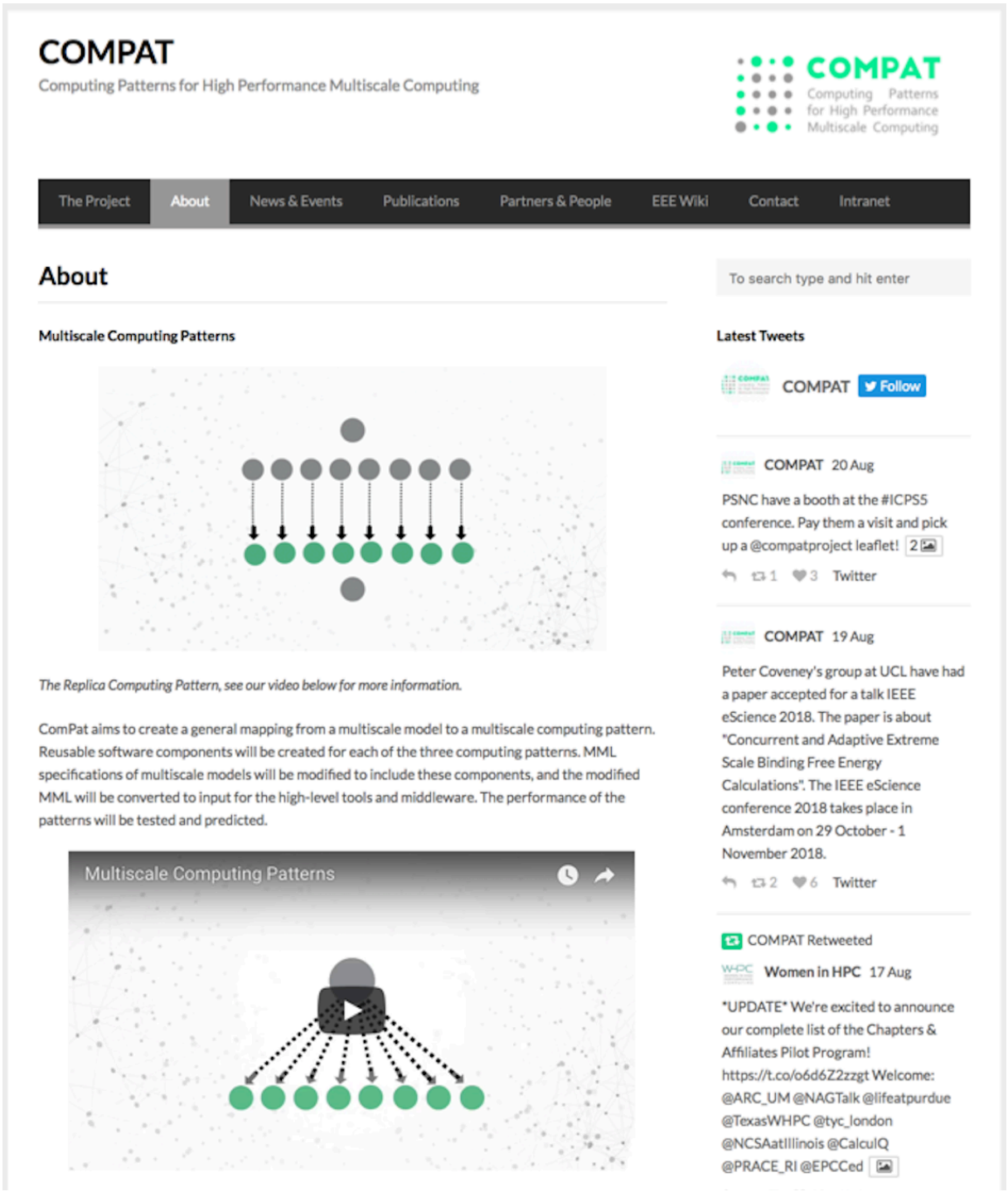

Figure 13: Homepage of the ComPat website

4.4 Annex 4: Social Media

Details	Date From	Date To	Audience(s) (see above table)	No. of People
The @sciencemuseum twitter account posted a tweet about the article they had written concerning the ComPat paper "Graphene–Graphene Interactions: Friction, Superlubricity, and	13/02/17	13/02/17	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	659,000

Exfoliation". https://twitter.com/sciencemuseum/status/963396710939680768				
The @PASC_conference twitter account posts a tweet about ComPat's PASC18 involvement. https://twitter.com/PASC_Conference/status/972206262447431680	09/03/18	09/03/18	[Scientific Community (higher education, Research)], [Industry]	220
The @compat_project twitter account made 97 Tweets in this reporting period. https://twitter.com/compatproject	01/03/17	30/09/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	24,153
The Advanced Materials video featuring ComPat graphene research was posted on the graphene subreddit on reddit.com. https://www.reddit.com/r/graphene/comments/83musr/graphenegraphene_interactions_friction/	01/03/18	01/03/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	60
The Advanced Materials video featuring ComPat graphene research was posted on qq.com. https://v.qq.com/x/page/w0609zkktpo.html	19/03/18	19/03/18	[Scientific Community (higher education, Research)], [Industry], [General Public], [Medias]	1000
UCL posted a news item in the UCL Chemistry Newsletter about the ComPat paper on "Graphene–Graphene Interactions: Friction, Superlubricity, and Exfoliation".	19/03/17	19/03/17	[Scientific Community (higher education, Research)]	200
Jodie Haigh posted the Advanced Materials video on LinkedIn featuring ComPat research on graphene. https://tinyurl.com/y89m63rw	19/03/18	19/03/18	[Scientific Community (higher education, Research)], [Industry]	242

4.5 Annex 5: Outreach to Other Projects

Details	Date From	Date To	Audience(s) (see above table)	No. of People
On behalf of the CompBioMed project, SURFsara attended the ComPat 2017 October AHM in Leiden	17/10/17	18/10/17	[Scientific Community (higher education, Research)], [Industry]	30
ComPat members participated in the COST OpenMultiMed Survey on Multiscale Computing in Biomedicine.	12/12/17	12/12/17	[Scientific Community (higher education, Research)]	10
Oliver Perks, ARM, conducted application visualisation with the Sage project.	01/06/18	01/07/18	[Scientific Community (higher education, Research)], [Industry]	5
Oliver Perks, ARM, conducted workflow modelling with ESiWACE.	01/01/18	30/09/18	[Scientific Community (higher education, Research)], [Industry]	5
Oliver Perks, ARM, worked with TSERO on energy and performance collection work.	01/01/18	30/09/18	[Scientific Community (higher education, Research)], [Industry]	5
Oliver Perks, ARM, worked with nextgenio on workflows and visualisation.	01/01/18	30/09/18	[Scientific Community (higher education, Research)], [Industry]	5
ComPat heavily collaborated with the CompBioMed project, aided by certain partners and personnel being present in both projects.	01/10/16	30/09/18	[Scientific Community (higher education, Research)], [Industry]	75

ComPat was mentioned and addressed during talks at various CompBioMed events.				
The legacy of ComPat is being continued in a major way in the VECMA project, many of the ComPat partners are involved in VECMA, the applications research, project aims, and software/tools in VECMA have a lot in common with ComPat.	15/06/18	30/09/18	[Scientific Community (higher education, Research)], [Industry]	40
Participation in events such as the HPC Summit allowed us to speak to (via talks, posters, and discussions) with many H2020 projects	01/10/15	30/09/18	[Scientific Community (higher education, Research)], [Industry]	200
ESiWACE are contributing a paper to the ComPat Special Issue with Phil Trans Roy Soc A	30/09/18	01/02/19	[Scientific Community (higher education, Research)], [Industry]	5
Philipp Neumann (ESiWACE) gave a talk at the Lorentz Center workshop on “From Convergence of Weather and Climate Simulations to a Coupling Software for Massively Parallel Molecular-Continuum Flows”.	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	1
Derek Groen, Brunel, gave a talk about OpenMultiMed during the ICCS 2016 conference in San Diego.	06/06/16	08/06/16	[Scientific Community (higher education, Research)]	40
Derek Groen, Brunel, presented ComPat material during an OpenMultiMed Winter School in Erlangen	01/02/18	01/02/18	[Scientific Community (higher education, Research)]	20

4.6 Annex 6: Events Organised

Details	Date From	Date To	Audience(s) (see above table)	No. of People
Simon Portegies Zwart, Leiden University, organised the conference MODEST-18: Dense Stellar Systems In The Era Of Gaia, Ligo & Lisa	25/06/18	29/06/18	[Scientific Community (higher education, Research)], [Industry]	120
Derek Groen (Brunel) and Alfons Hoekstra (UvA) organised the 14th Multiscale Modelling and Simulation Workshop (MMS) workshop at ICCS2017 in Zurich, Switzerland	13/06/17	13/06/17	[Scientific Community (higher education, Research)]	20
Derek Groen (Brunel) and Alfons Hoekstra (UvA) organised the 15th Multiscale Modelling and Simulation Workshop (MMS) workshop at ICCS2018 in Wuxi, China	12/06/18	12/06/18	[Scientific Community (higher education, Research)]	20
Tom Kirkham, STFC, organised the workshop "HPC for your business" at the Hartree Center, Sci-Tech, Daresbury, UK. It was aimed at industry participants	06/06/18	06/06/18	[Industry]	20
Organised the Lorentz Center Workshop on "Multiscale Computing: From the Desktop to the Exascale" in Leiden, Netherlands	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	30

Hugh Martin, CBK, organised a dedicated session on multiscale computing patterns at the HPC Summit Week in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)]	15
Simon Portegies Zwart, Leiden University, organised the AMUSE Workshop: MODEST 18a at the Faculty of Science Leiden University, Leiden, Netherlands	03/04/18	06/04/18	[Scientific Community (higher education, Research)]	8

4.7 Annex 7: Participation in Events

Details	Date From	Date To	Audience(s) (see above table)	No. of People
LRZ held a booth at Supercomputing 2017, showcasing hardware from their 100% warm-water cooled CoolMUC-3 KNL-based system, a scientific VR demo and talk about their LRZ Application Labs.	13/11/17	17/11/17	[Scientific Community (higher education, Research)], [Industry]	500
ComPat were sponsors of the PASC18 event, the ComPat logo featured on the sponsors page. https://pasc18.pasc-conference.org/about/sponsors/	09/07/05	09/07/05	[Scientific Community (higher education, Research)], [Industry]	500
Oliver Perks gave a talk on ComPat at the HPC Summit 2017 in Barcelona on "Performance Profiling of Multiscale Models and Simulations within large scale HPC Environments". The twitter account @AllineaSoftware tweeted about the talk	15/05/17	19/05/17	[Scientific Community (higher education, Research)], [Industry]	100
Krzysztof Kurowski, PSNC, hosted a booth at the PPAM Conference in Lublin, Poland. Here they demonstrated the ComPat Execution Environment. https://ppam.pl/	10/09/17	13/09/17	[Scientific Community (higher education, Research)]	200
Tomasz Piontek, PSNC, gave a presentation on "ComPat Execution Environment" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Olly Perks, ARM, gave a presentation on "The ComPat Project" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Derek Groen, Brunel, gave a presentation on "Applications that require multiscale computing" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Derek Groen, Brunel, gave a presentation on "Theoretical description of patterns" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Robin Richardson, UCL, gave a presentation on "The Description of the lifecycle of a multiscale application" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Onnie Luk, MPG, gave a presentation on "Optimisation in the lifecycle of a multiscale	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15

application" at the European HPC Summit Week 2018 in Ljubljana, Slovenia				
Tomasz Piontek, PSNC, gave a presentation on "Execution in the lifecycle of a multiscale application" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Olly Perks, ARM, gave a presentation on "Energy Efficiency in the lifecycle of a multiscale application" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Maxime Vassaux, UCL, gave a presentation on "General application information" at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Onnie Luk, MPG, gave a demonstration of multiscale fusion at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Robin Richardson, UCL, gave a demonstration of the binding affinity calculator at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Maxime Vassaux, UCL, gave a demonstration of HMC at the European HPC Summit Week 2018 in Ljubljana, Slovenia	31/05/18	31/05/18	[Scientific Community (higher education, Research)], [Industry]	15
Tomasz Piontek, PSNC, hosted a booth at the 5th International Conference on Protective Structures in Poznan, Poland. http://icps5.put.edu.pl/	19/08/18	23/08/18	[Scientific Community (higher education, Research)]	150
Tomasz Piontek, PSNC, gave a presentation on "Multiscale urban air quality numerical modelling, simulation and advanced visualisation" at the Supercomputing Frontiers Europe 2018 conference in Warsaw, Poland. https://supercomputingfrontiers.eu/2018/	12/03/18	14/03/18	[Scientific Community (higher education, Research)]	200
Krzysztof Kurowski, PSNC, gave a ComPat talk at the ETP4HPC session during the HPC Summit Week 2017	15/05/17	19/05/17	[Scientific Community (higher education, Research)]	200
Derek Groen, Brunel, presented a range of ComPat work at the OpenMultiMed-CompBioMed Joint Session at the EPMA World Congress in September 2017. The talk was titled "Multiscale computing and human brain blood flow simulation"	14/09/17	17/09/17	[Scientific Community (higher education, Research)]	30
Onnie Luk, MPG, presented a poster at the ICNSP (International Conference on Numerical Simulation of Plasmas) in Leuven, Belgium in September 2017. The poster title was “ComPat Framework for Multiscale Simulations Applied to Fusion Plasmas”.	18/09/17	20/09/17	[Scientific Community (higher education, Research)], [Industry]	100
ARM held a booth at ISC17 in Frankfurt. ComPat pens and leaflets were distributed.	18/06/17	22/06/17	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, had a paper and talk accepted at IEEE eScience 2018 conference in Amsterdam, Netherlands. The paper was on "Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations".	29/10/18	01/10/18	[Scientific Community (higher education, Research)], [Industry]	500
Peter Coveney, UCL, had a poster on "Enabling Trade-offs Between Accuracy and Computational	01/05/18	04/05/18	[Scientific Community (higher education, Research)], [Industry]	50

Cost: Executing Adaptive Algorithms to Reduce Time to Clinical Insight" at IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid) 2018 held in Washington DC				
Peter Coveney, UCL, presented a video on graphene materials and a video on computational biomedicine at the Think Science conference at the World Trade Center in Dubai.	16/04/18	16/04/18	[Scientific Community (higher education, Research)], [Industry]	5000
Peter Coveney, UCL, gave a talk on “Rapid, Accurate & Reliable Binding Affinity Calculations for Drug Discovery” at the “High Performance Computing in Life Sciences” session at ISC 2017	20/06/17	20/06/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, is to give a talk on "High performance and/or cloud computing for free energy prediction using molecular dynamics simulations?" at the 253rd ACS National Meeting in San Francisco, California	02/04/17	06/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, is to give a talk on "Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration" at the 253rd ACS National Meeting in San Francisco, California	02/04/17	06/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, is to give a talk on "Computer-based design of advanced materials: Chemically specific multiscale modelling of polymer-clay nanocomposites" at the 253rd ACS National Meeting in San Francisco, California	02/04/17	06/04/17	[Scientific Community (higher education, Research)], [Industry]	200
A ComPat paper on “High-throughput Binding Affinity Calculations at Extreme Scales”, co-authored by the teams from CCS/UCL and the RADICAL laboratory at Rutgers, was presented at the “Computational Approaches for Cancer Workshop” at ACM/IEEE International Conference on Supercomputing (SC’17). SC’17 was held in Denver in November 2017.	13/11/17	17/11/17	[Scientific Community (higher education, Research)], [Industry]	200
Robbie Sinclair, UCL, won first prize in the Computer-Based Modeling and Experiment for the Design of Soft Materials Symposium Student Presentation Contest held at the 2017 MRS Spring Meeting in Phoenix, Arizona. His paper “New Insights into Graphene Exfoliation with Molecular Dynamics” represented the first public exposure of a scientific development in the understanding of graphene properties which is of central importance to understanding its formation, synthesis and role in nanocomposites.	17/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	500
Peter Coveney, UCL, gave a talk on "Gels, Biopolymers and Active Matter" at the Materials Research Society Spring 2017 Meeting in Phoenix, Arizona, USA	18/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, gave a talk on "Polymer-Based Composites and Nanocomposites" at the	18/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	200

Materials Research Society Spring 2017 Meeting in Phoenix, Arizona, USA				
Peter Coveney, UCL, gave a talk on "Properties and Processing of Clay-Polymer Nanocomposites Modelled Using a Multiscale Approach" at the Materials Research Society Spring 2017 Meeting in Phoenix, Arizona, USA	18/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, gave a talk on "New Insights into Graphene Exfoliation with Molecular Dynamics" at the Materials Research Society Spring 2017 Meeting in Phoenix, Arizona, USA	18/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, was the founding organiser of the Symposium entitled “Computer-Based Modelling and Experiment for the Design of Soft Materials” at the Materials Research Society Spring 2017 Meeting in Phoenix, Arizona, USA	18/04/17	21/04/17	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, gave an Invited talk on Computational Biomedicine at the Cambridge Ophthalmological Symposium in Cambridge, UK	06/09/17	08/09/17	[Scientific Community (higher education, Research)]	50
Peter Coveney, UCL, gave an Invited Talk on "Rapid, Accurate and Reliable Binding Affinity Calculations for Drug Discovery & Precision Medicine" at the MEMBS Congress in 2017 in Abu Dhabi, UAE	02/11/17	02/11/17	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, gave an invited talk on "The Virtual Human: In Silico Methods for Personalised Medicine" at the MEMBS Congress in 2017 in Abu Dhabi, UAE	04/11/17	04/11/17	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, gave an invited talk on "The Virtual Human: In Silico Methods for Personalized Medicine" at the Data Intensive Studies Center (DISC) Fall Symposium in Massachusetts, USA	08/11/17	08/11/17	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, gave an invited talk on "The Virtual Human: In Silico Methods for Personalised Medicine" at the HITS Colloquium in Heidelberg, Germany	20/11/17	20/11/17	[Scientific Community (higher education, Research)]	30
Peter Coveney, UCL, gave a talk on "Big Theory for Big Data" at the 2017 New York Scientific Data Summit (NYSDS) Data-Driven Discovery in Science and Industry in New York, US	06/08/17	09/08/17	[Scientific Community (higher education, Research)]	100
Peter Coveney, UCL, gave a talk on "Floating Point Representations of the Generalized Bernoulli Map: Loss of Structure Through Computation" at the Sixth Palestinian Conference on Modern Trends in Mathematics and Physics in Palestine.	05/08/17	08/08/17	[Scientific Community (higher education, Research)]	200
Peter Coveney, UCL, chaired a Mathematics session at the Sixth Palestinian Conference on Modern Trends in Mathematics and Physics in Palestine.	05/08/17	08/08/17	[Scientific Community (higher education, Research)]	100
Jeroen Bedorf, Leiden University, gave a talk on "Conquering the Titan Supercomputer: A Star-by-Star Simulation of the Milky Way Galaxy" at GTC 2018 in San Jose, USA	26/03/18	29/03/18	[Scientific Community (higher education, Research)],[General Public], [Medias], [Industry]	500

Jeroen Bedorf, Leiden University, gave a talk on "Astrophysical Multiscale Modeling with AMUSE" at ICCS 2017 in Zurich Switzerland	12/06/17	14/06/17	[Scientific Community (higher education, Research)]	400
Dieter Kranzlmüller, LRZ, gave a talk on "Towards Smart Scaling with SuperMUC-NG" at KUKDM 2018 in Zakopane, Poland	07/03/18	07/03/18	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller, LRZ, gave a talk on "General Purpose High Performance Computing as Competitive Advantage for Scientists" at AHPC18 in Linz, Austria	19/02/18	19/02/18	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller, LRZ, gave a talk on "The new SuperMUC petascale system and applications" at HCMUT in Ho Chi Minh City, Vietnam	16/08/17	16/08/17	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller, LRZ, gave a talk on "The Leibniz Supercomputing Centre in the Landscape of High Performance Computing" at Big Data made in Germany in Berlin, Germany	29/06/17	29/06/17	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller, LRZ, gave a talk on :Der Höchstleistungsrechner SuperMUC als Werkzeug der Wissenschaft" at the Universität Salzburg in Salzburg, Austria	08/06/17	08/06/17	[Scientific Community (higher education, Research)]	25
Dieter Kranzlmüller, LRZ, gave a talk on "Wissenschaftliche Entdeckungen mit Hilfe des Leibniz-Rechenzentrums" at TUM Emeriti of Excellence in Munich, Germany	31/05/17	31/05/17	[Scientific Community (higher education, Research)]	100
Dieter Kranzlmüller, LRZ, gave a talk "On Exascaling Experience while Dealing with Large Applications" at Mathematics for Exascale and Digital Science Workshop at the HPC Summit, Barcelona, Spain	17/05/17	17/05/17	[Scientific Community (higher education, Research)], [Industry]	200
Dieter Kranzlmüller, LRZ, gave a talk on "General Purpose Supercomputing on SuperMUC" at CompBioMed - Cloud & High Performance Computing in Biomedicine, London, UK	27/04/17	27/04/17	[Scientific Community (higher education, Research)], [Industry]	90
Dieter Kranzlmüller, LRZ, gave a talk on "Is Heterogeneity A Solution To The HPC Dilemma?" at NC4 - The Sixth National Conference on Cloud Computing and Commerce, Dublin, Ireland	11/04/17	11/04/17	[Scientific Community (higher education, Research)], [Industry]	100
Dieter Kranzlmüller, LRZ, gave a talk on "Partnership Initiative Computational Science - Using HPC efficiently" at the German-Russian Conference: Supercomputing in Scientific and Industrial Problems (2017/SSIP), Stuttgart, Deutschland	27/03/17	27/03/17	[Scientific Community (higher education, Research)], [Industry]	100
Alfons Hoekstra, UvA, gave an invited lecture on "Multiscale computing on distributed resources and on HPC" at KUKDM, Zakopane, Poland	01/03/17	01/03/17	[Scientific Community (higher education, Research)], [Industry]	50
Alfons Hoekstra, UvA, gave an invited lecture on "The Virtual Artery, a Multiscale Model for Vascular Physiology" at CMBE17, Pittburgh, USA	01/04/17	01/04/17	[Scientific Community (higher education, Research)], [Industry]	100
ComPat work was included in ARM Forge product at ISC - customer discussions about these new features	01/06/18	01/06/18	[Industry], [Customer]	20

LRZ participated at ISC 2018 and had ComPat flyers on display	24/06/18	28/06/18	[Industry], [Scientific Community]	50
Ulf Schiller gave a talk on "Computational modeling of transport and soft materials" at Brunel University, UK	15/03/17	15/03/17	[Scientific Community (higher education, Research)]	20
Tomasz Piontek gave a Live demonstration of Pattern software at the Lorentz Center Workshop on Multiscale Computing: From the Desktop to the Exascale. The workshop was in Leiden, the Netherlands.	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	30
Krzysztof Kurowski participated in a panel discussion on the ComPat Execution Environment at IWSC 2018 - 10th International Workshop on Science Gateways in Edinburgh, UK	13/06/18	15/06/18	[Scientific Community (higher education, Research)]	50
Krzysztof Kurowski participated in a panel discussion on "New scheduling challenges in distributed HPC environments - ComPat use cases" at the New Perspectives in Scheduling Theory Conference in Aussois, France	03/03/18	06/03/18	[Scientific Community (higher education, Research)]	60
Derek Groen gave an invited talk on "Making ITER burn, multiscale modelling for fusion" at the Lorentz Center Workshop on Multiscale Computing: From the Desktop to the Exascale. The workshop was in Leiden, the Netherlands.	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	30
Tomasz Piontek gave a ComPat talk in the workshop "HPC for your business" at the Hartree Center, Sci-Tech, Daresbury, UK	06/06/18	06/06/18	[Industry]	20
Onnie Luk, MPG, gave a presentation on "ComPat Framework for Multiscale Simulations Applied to Fusion at the IPP Theory Seminar in Berlin, Germany	20/11/17	24/11/17	[Scientific Community (higher education, Research)]	80
Onnie Luk, MPG, presented a poster on "ComPat Framework for Multiscale Simulations Applied to Fusion Plasmas" at the Lorentz Centre Workshop "Multiscale Computing, From the desktop to the Exascale" in Leiden, Netherlands	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	25
Olivier Hoenen, MPG, gave a live demonstration on "Fusion Extreme Scaling Application Demo" at the Lorentz Centre Workshop "Multiscale Computing, From the desktop to the Exascale" in Leiden, Netherlands	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	25
Onnie Luk, MPG, presented a poster on "Multiscale Fusion Plasma Simulations of Varied Tokamak Scenarios within the ComPat Framework" at EPS 2018 in Prague, Czech Republic	02/07/18	06/07/18	[Scientific Community (higher education, Research)]	600
David Coster gave a presentation on "Bridging the Gap: Solving the Transport Equations with Fluxes from Turbulence Fusion Contribution to the EU H2020 Project ComPat at IPP-Garching in Garching, Germany	06/09/16	06/09/16	[Scientific Community (higher education, Research)]	30
Maxime Vassaux, UCL, gave a keynote presentation on "Heterogeneous Multiscale Modelling for polymer nanocomposites" at the Lorentz Center workshop on Multiscale	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	40

Computing: From the Desktop to the Exascale in Leiden, The Netherlands				
Oliver Perks, ARM, gave a talk at the ComPat STFC Industry event in Warrington, UK	01/06/18	01/06/18	[Scientific Community (higher education, Research)], [Industry]	20
Peter Coveney, UCL, gave a talk on “Practical challenges for biomedical modeling using HPC” at the Second HPC Applications in Precision Medicine Workshop at ISC18 in Frankfurt	28/06/18	28/06/18	[Scientific Community (higher education, Research)], [Industry]	50
Peter Coveney, UCL, gave a talk on "Accurate and Precise Binding Affinity Calculations for Drug Development and Precision Medicine" at the Second HPC Applications in Precision Medicine Workshop at ISC18 in Frankfurt	28/06/18	28/06/18	[Scientific Community (higher education, Research)], [Industry]	50
Peter Coveney, UCL, gave a talk on "Exploiting International e-Infrastructures for Large Scale Computational Science" at the 9th International Workshop on Science Gateways in Poznan, Poland.	19/06/18	21/06/18	[Scientific Community (higher education, Research)], [Industry]	100
Peter Coveney, UCL, was the winner of the 11th IEEE International Scalable Computing Challenge (SCALE 2018) at the IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing (CCGrid) 2018 held in Washington DC for work executing and managing large and complex campaigns of ligand binding simulations	01/05/18	04/05/18	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney, UCL, gave a talk on "Biomedical high performance computing within and outside clouds" at the OpenMultiMed/CompBioMed joint session at the EPMA World Congress 2017, University of Malta in Malta	14/09/17	17/09/17	[Scientific Community (higher education, Research)], [Industry]	30
Peter Coveney, UCL, gave a talk on "Multiscale modelling and simulation of 2d nanomaterials: from quantum to continuum level" at the "Clay Minerals Group Research in Progress meeting" at UCL, London	19/09/17	19/09/17	[Scientific Community (higher education, Research)]	20
Robin Richardson, UCL, gave a talk on "Multiscale Modelling for Cerebral Blood Flow" at the Lorentz Center Workshop on Multiscale Modelling in Leiden, Netherlands.	16/04/18	18/04/18	[Scientific Community (higher education, Research)]	20-30
Robin Richardson, UCL, gave a talk on "Exascaling of codes in CompBioMed" at the CompBioMed/Vheart Workshop in Amsterdam, Netherlands			[Scientific Community (higher education, Research)]	15
Jeroen Bedorf, Leiden University, gave a talk on "Multiscale Computing in Astrophysics" at the Lorentz Center Workshop on Multiscale Computing: From the desktop to the Exascale in Leiden, Netherlands	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	30
Derek Groen, Brunel, gave a talk on "Development of a multiscale simulation approach for forced migration" at the 15th MMS workshop in ICCS2018 in Wuxi, China	12/06/18	12/06/18	[Scientific Community (higher education, Research)]	20
Simon Portegies Zwart, Leiden University, gave a talk on "Simulating black holes in star clusters" at ISSI in Bern, Switzerland	09/07/18	11/07/18	[Scientific Community (higher education, Research)], [Industry]	100

Simon Portegies Zwart, Leiden University, gave a talk on "Snellius" at the Lorentz Center Workshop on Multiscale Modelling in Leiden, Netherlands.	16/04/18	20/04/18	[Scientific Community (higher education, Research)]	30
Simon Portegies Zwart, Leiden University, gave a talk on "Multiscale Computing" at the AMUSE workshop in Leiden, Netherlands.	03/04/18	06/04/18	[Scientific Community (higher education, Research)]	8
Simon Portegies Zwart, Leiden University, gave a talk on "Multiscale Computing" at the AMUSE workshop in Leiden, Netherlands.	08/01/18	11/01/18	[Scientific Community (higher education, Research)]	10
Derek Groen, Brunel, conducted training on automating simulations via Brunel PhD lectures in London, UK	05/06/18	05/06/18	[Scientific Community (higher education, Research)]	15
Robin Richardson, UCL, gave a lecture and demo on "Simple magnetic drug targeting simulations with HemeLB" at an MPI training course	04/09/18	04/09/18	[Scientific Community (higher education, Research)]	30
Derek Groen, Brunel, gave an invited seminar at the Academic seminar series at UvA in Amsterdam, Netherlands	19/01/18	19/01/18	[Scientific Community (higher education, Research)]	50
Derek Groen, Brunel, gave an invited seminar at the Seminar series in Tsinghua University in Beijing, China	16/08/17	16/08/17	[Scientific Community (higher education, Research)]	25
Simon Portegies Zwart, Leiden University, gave a talk on "The collision between the Andromeda and Milky Way galaxies" at TU Delft Institute for Computational Science and Engineering, Netherlands	01/06/18	01/06/18	[Scientific Community (higher education, Research)]	50
Simon Portegies Zwart, Leiden University, gave a business presentation at an HPC-day for HP in Barneveld, the Netherlands	12/06/18	12/06/18	[Industry], [Customers]	3000
Simon Portegies Zwart, Leiden University, gave a talk on "Multiscale Computing" at a Colloquium in Geneva, Switzerland	04/06/18	06/06/18	[Scientific Community (higher education, Research)]	20
Simon Portegies Zwart, Leiden University, gave a talk on "Multiscale Computing" at a Colloquium in Bologna, Italy	22/06/18	24/06/18	[Scientific Community (higher education, Research)]	20
Alfons Hoekstra, UvA, gave an Invited lecture on "Multiscale Modelling in Vascular (patho)physiology" at a CWI Scientific Computing Seminar	01/06/18	01/06/18	[Scientific Community (higher education, Research)]	20