



## D7.3 Second Annual Dissemination Report

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**CONTRIBUTORS**

<ul style="list-style-type: none"> <li>• Hugh Martin - Author</li> <li>• Pragna Kiri - Author</li> <li>• Sabrina Eisenreich - Internal Reviewer</li> <li>• Silvia Wissel – Internal Reviewer</li> <li>• All Partners - Provided Dissemination Activity</li> </ul>
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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 considered knowledge exploitation activities. Thus, dissemination and exploitation play an important role in the ComPat project, and they are collaborative efforts between the project partners.

This document, D7.3 Second Annual Dissemination Report, reviews the events and dissemination results of ComPat for months 12 to 18 of the project (1<sup>st</sup> October 2016 to 31<sup>st</sup> March 2017). The original due date for this deliverable was month 24 but it was moved ahead by 6 months to align with the 18-month review of the project. Documents D7.2 First Annual Dissemination Report and D7.1 Detailed Dissemination Action Plan provide a detailed description of ComPat's dissemination materials and channels. This document, D7.3, will provide a top of info from D7.2, covering months 12 to 18 in the project.

To summarize, there was a substantial amount of dissemination activity in the first 18 months of ComPat, the key highlights during this period include:

- The organisation of two conferences
- The organisation of a symposium
- The organisation of four workshops
- Participation at 23 major conferences and workshops
- The publication or submission of 10 scientific papers

The report also outlines the actions planned for the second 18 months of the project.

## 2 Report

### 2.1 Dissemination Materials and Channels

This section describes the various activities *via* ComPat's dissemination channels and materials throughout months 12-18 of the project. In general, we have aimed to make maximum use of already established partners' national, and European dissemination channels, such as E-infrastructure specialist groups, which allows us to maximise the impact-to-cost ratio of our activities in WP7.

The ComPat name and logo, as well as reference to the funding source, have been used in all dissemination materials, be it in the form of leaflets, posters, white papers *etc.* Versions of slides and reports, along with a poster and leaflet that can be used as a template, are used by all contributors and are described below. These actions help to increase the brand recognition of the ComPat project. Task 7.6 is concerned with the production of dissemination materials and runs throughout the 3 years.

#### 2.1.1 Scientific Papers

The ComPat consortium will publish numerous scientific, peer-reviewed papers, conference proceedings, and chapters in books in the course of the project. Such publications will contain the following passage:

*"This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671564."*

In the first 18 months of the project, ten peer-reviewed, open-access scientific papers have been published, accepted for publication, or submitted to a journal, the papers published or submitted in months 12-18 are listed below:

- 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., Available Online (2016), DOI: 10.1021/acs.jctc.6b00794
- 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, Available Online (2016), DOI: 10.1021/acs.jctc.6b00979
- S. Alwayyed, D. Groen, P. V. Coveney, A. G. Hoekstra, "Multiscale Computing in the Exascale Era", Preprint (2016), arXiv:1612.02467

The full list of publications are available at <http://www.compat-project.eu/publications/>.

### 2.1.2 Non-Peer Reviewed Publications

ComPat aims to explore many forms of dissemination, including non-peer reviewed publications that will often reach a broader audience. Below, such publications from months 12-18 of the project are detailed:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Alfons Hoestra included a piece on ComPat in the ETP4HPC and EXDCI newsletter "European Exascale Projects and their International Collaboration Potential"	16/11/2016	16/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	500

### 2.1.3 Websites

The ComPat project website is at URL [www.compat-project.eu](http://www.compat-project.eu). The website gives an overview on the project, its research, the consortium partners and staff as well as contact information. It also contains a News and Events page, a feed of the ComPat Twitter account, and a calendar showing ComPat events. We keep the news page updated with ComPat relevant stories, and at the 18 month mark have published 30 news stories.

In months 12-18 a link to the Experimental Execution Environment (EEE) Wiki (<http://compat-eee-wiki.drg.lrz.de/>) was added to the toolbar. The wiki contains information relevant to users and developers of the Experimental Execution Environment.

Dissemination activities in the months 12-18 of the project that were carried out on ComPat and other websites include the items described in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Saad Alowayyed wrote a story for the KACST website in Saudi Arabia	09/12/2016	09/12/2016	[General Public], [Scientific Community (higher education, Research)]	100
Simon Portegies-Zwart: Public educational website: <a href="http://gravitylab.nl/">http://gravitylab.nl/</a>	01/10/2016	01/12/2016	[General Public], [Scientific Community (higher education, Research)]	1000
LRZ: EEE wiki on compat-project.eu	10/10/2016	30/09/2018	[Scientific Community (higher education, Research)]	500
Update to LRZ website: <a href="https://www.lrz.de/forschung/projekte/forschung-hpc/compat/">https://www.lrz.de/forschung/projekte/forschung-hpc/compat/</a>	10/12/2016	30/09/2018	[General Public]	1000
LRZ - ComPat project description on the LRZ website <a href="http://www.lrz.de">www.lrz.de</a>	01/11/15	30/09/16	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	500

### 2.1.4 Social Media

ComPat has an effective social media presence. At the forefront of this is the ComPat Twitter account, which can be found at @compatproject. Task 7.3 is concerned with maintaining a social media presence and runs across months 1-36.

The ComPat Twitter account currently has 80 Tweets and 77 Followers, it has been used to raise awareness of ComPat related events, job positions, and more general posts that would be of interest to those in ComPat's domain. According to <https://analytics.twitter.com>, ComPat Tweets have earned 8857 impressions since the start of the project.

Similarly, a ComPat LinkedIn group was set up in February 2017, to raise awareness of ComPat related events, to encourage collaboration and discussions, post job positions, and more general posts that would be of interest to those in ComPat's domain, shown below:

The screenshot shows a LinkedIn group page for 'COMPAT: Computing Patterns for High Performance Multiscale Computing'. The group has 20 members. The page layout includes a header with the LinkedIn logo and navigation links, a group banner with the group name and a 'Manage' button, and a 'Start a conversation' section. The main content area features a 'Conversations' tab with a 'FEATURED' post by Pragna Kiri, Senior Consultant, CBK Sci Con. The post is titled 'Upcoming events of interest' and lists several events: '1 Feb 2017: HPC & Big Data 2017 - London', '20-24 Feb 2017: Lorentz Center Workshop "Formation of the Solar System and the Origin of Life" - Leiden', '17-21 Apr 2017: Materials Research Society (MRS) Spring Meeting & Exhibit 2017 - Phoenix', and '23-26 Apr 2017: HPC... Show more'. Below this, there is a post titled 'Multiscale Modelling and Simulation Workshop - Zürich Switzerland, 12-14 June 2017' by Pragna Kiri. The post describes a workshop at the International Conference on Computational Science, 14th Edition, and includes a photo of a building. The right sidebar contains an 'ABOUT THIS GROUP' section, a 'MEMBERS' list, and an 'Invite others' button. At the bottom, there are 'Ads You May Be Interested In' and a footer with 'About', 'Feedback', 'Privacy & Terms', and 'LinkedIn Corp. © 2017'.

**COMPAT: Computing Patterns for High Performance Multiscale Computing**  
20 members

**Start a conversation with your group**  
Enter a conversation title...

**Conversations** Jobs

**FEATURED** ... 1mo

**Pragna Kiri**  
Senior Consultant, CBK Sci Con

**Upcoming events of interest**  
1 Feb 2017: HPC & Big Data 2017 - London  
20-24 Feb 2017: Lorentz Center Workshop "Formation of the Solar System and the Origin of Life" - Leiden  
17-21 Apr 2017: Materials Research Society (MRS) Spring Meeting & Exhibit 2017 - Phoenix  
23-26 Apr 2017: HPC... Show more

**ABOUT THIS GROUP**  
We encourage group members to challenge the group with new thinking and innovation. You can create posts and ask questions about COMPAT topics that are important to you. We expect that there will be plenty of discussion on trends/directions on multi-... Show more

**MEMBERS** 20 members  
Invite others

**Ads You May Be Interested In**  
Got Consultant Experience  
100's of top employers looking for your consultancy skills. Connect now

**Pragna Kiri**  
Senior Consultant, CBK Sci Con

**Multiscale Modelling and Simulation Workshop - Zürich Switzerland, 12-14 June 2017**  
A workshop at the International Conference on Computational Science, 14th Edition, which aims to provide a forum for multiscale application modellers, framework developers and experts from the distributed infrastructure communities to identify and di... Show more

Like Comment 3

**Reply to this conversation...**

**Pragna Kiri**  
Senior Consultant, CBK Sci Con

**ISC High Performance 18-22 June 2017**  
The deadline for the call for posters for ISC 2017 is 3rd March 2017; for workshops the deadline is 15th Feb 2017.  
he 32nd conference in the ISC High Performance series will be held from June 18 - June 22, 2017. The city of Frankfurt remains the prefe... Show more

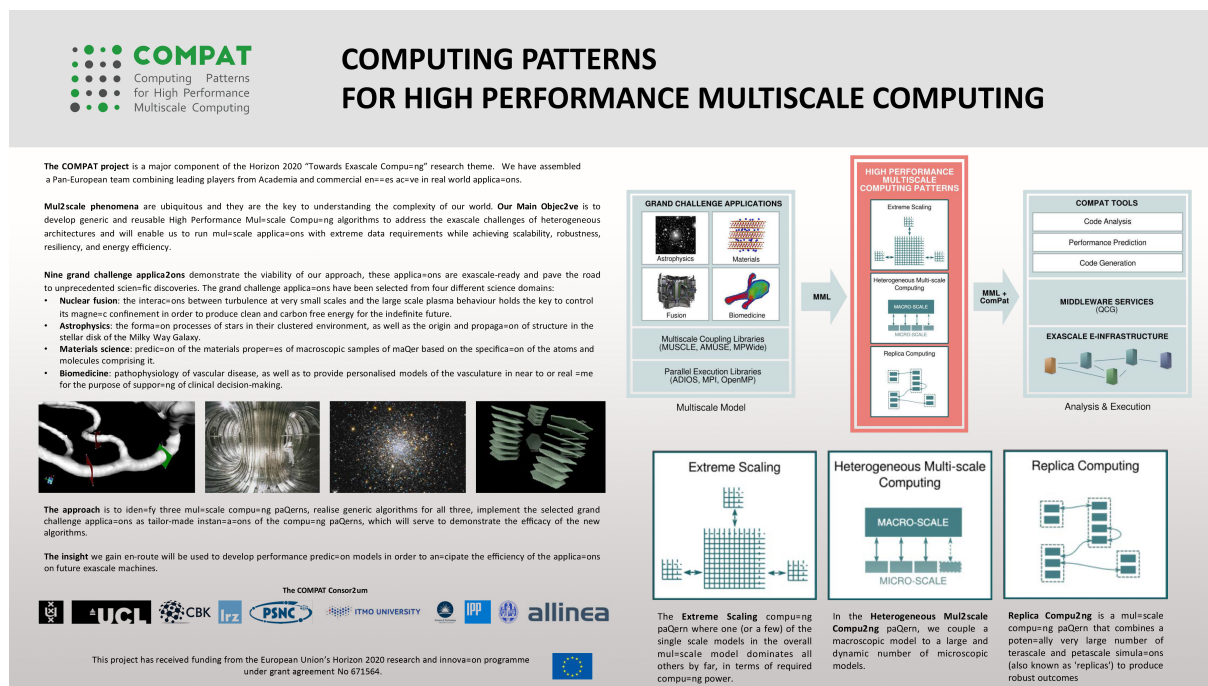
**MEMBERS** 20 members  
Invite others

**Ads You May Be Interested In**  
Got Consultant Experience  
100's of top employers looking for your consultancy skills. Connect now  
The "Entrepreneurs' MBA"  
The Diploma in Entrepreneurship at Cambridge University  
How To Hire A Grad  
The ultimate guide to what engineering Grads are looking for from you.

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### 2.1.5 Posters

ComPat presents posters at conferences and workshops to raise awareness of the project and research outcomes. In the first year of the project we produced a poster that summarises the project and its aims, which was described in D7.2. In months 12-18 of the project, partner PSNC constructed a redesigned version of this poster, which was displayed at Supercomputing 2016 in Utah, and is shown below:



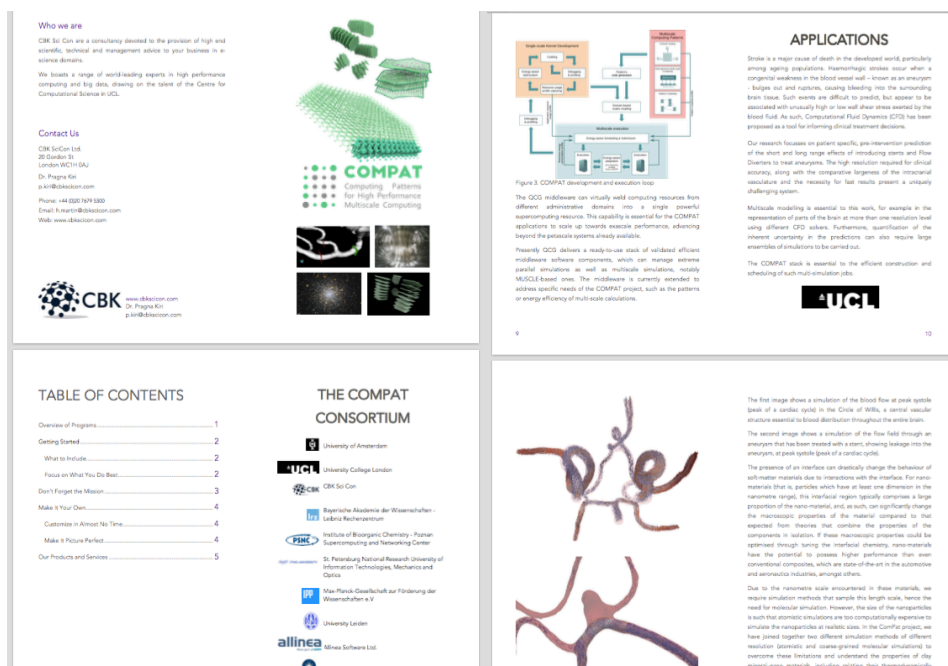
CONTACT &gt;&gt;&gt;&gt;&gt;&gt;&gt;&gt;

POZNAN SUPERCOMPUTING AND NETWORKING CENTER ([www.psnc.pl](http://www.psnc.pl))  
phone: (+48 61) 858-20-01, fax: (+48 61) 852-59-54, e-mail: [office@man.poznan.pl](mailto:office@man.poznan.pl)

Figure 1: Redesigned ComPat Poster

## 2.1.6 Leaflets

ComPat distributes leaflets to stakeholders at various events with the purpose of making them aware of the project or particular aspects of it (such as ComPat's applications). In the first year of the project, one leaflet was produced that summarises ComPat and its aims, which was described in D7.2. In addition to this leaflet, several new leaflets are currently in production. One example, currently under construction, is a booklet:





ComPat's leaflet distribution at Supercomputing 16 in Utah is outlined in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
PSNC: Distribution of ComPat materials at SC16. - PSNC booth (poster and leaflets) - EXDCI project booth (leaflets and presentation) - EXDCI BoF (poster and logo on their slide).	15/11/2016	19/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000 plus
STFC: Distribution of ComPat Materials at SC16	15/11/2016	19/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000 plus
Allinea: Distrubution of ComPat Materials at SC16	15/11/2016	19/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000 plus

### 2.1.7 Other Materials

In months 12-18 of ComPat we have produced COMPAT branded pens and USB sticks in order to distribute at various events and raise awareness of the project, these items are shown below:

<b>Pen Name:</b>	Contour Extra BP White
<b>Product Code:</b>	
<b>Type:</b>	Push Button Ballpen
<b>Refill Colour:</b>	Black

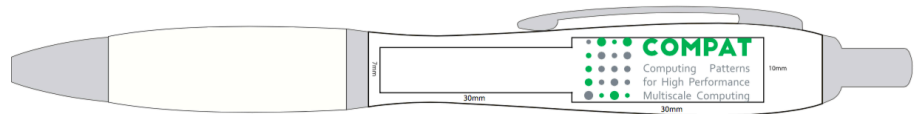


Figure 2: ComPat Pen Design

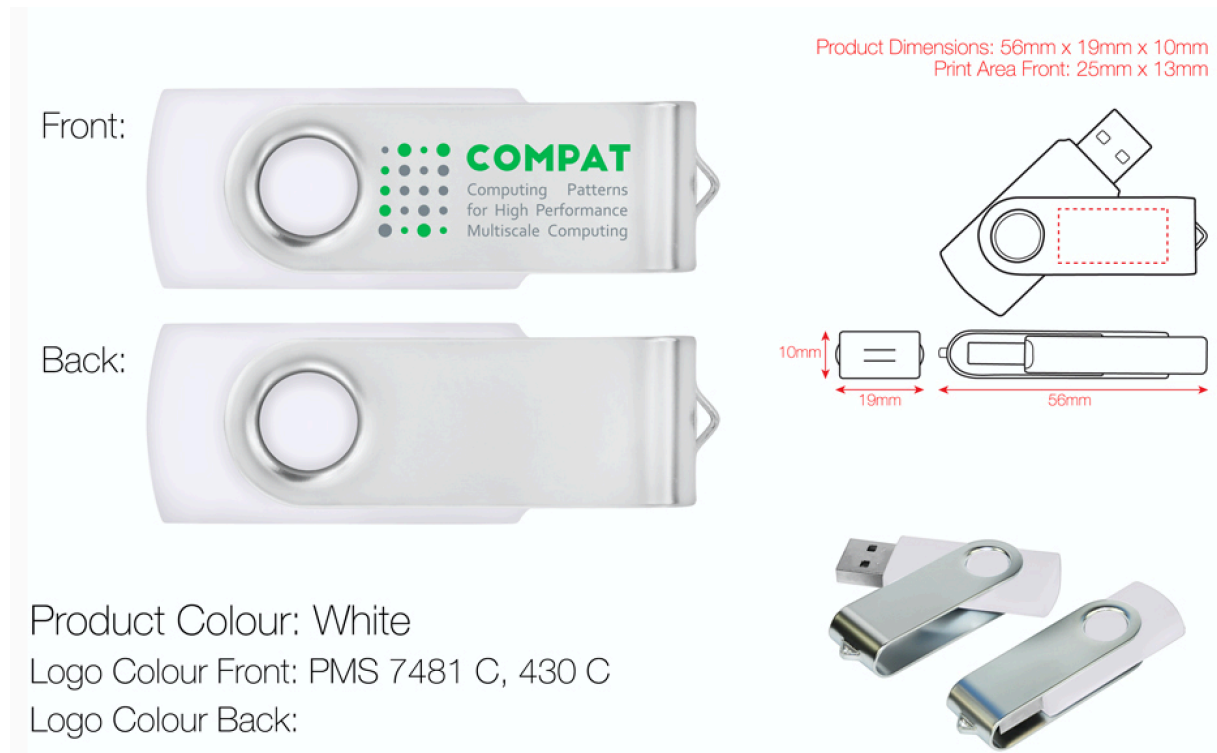


Figure 3: ComPat USB Design

## 2.1.8 Media Outreach

Media outreach activity in months 12-18 of ComPat includes UvA showing ComPat visualisations on the Dutch TV programme "Klokhuis", and ComPat's inclusion in an ETP4HPC/EXDCI newsletter.

Description	Date From	Date To	Audience(s)	Estimated Number of People
Alfons Hoestra included a piece on ComPat in the ETP4HPC and EXDCI newsletter "European Exascale Projects and their International Collaboration Potential"	16/11/2016	16/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	500
UvA showed ComPat visualisations on the Dutch TV programme "Klokhuis"	18/10/2016	18/10/2016	[General Public]	10000

## 2.1.9 Other Activities

ComPat consortium members have conducted various types of dissemination that don't fit into the categories already presented in this report. These include the forming of connections with other projects and entities, giving talks to groups and individuals at institutions, and receiving awards. Such activities from months 12-18 of the project are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Simon Portegies Zwart: Studium Generalum Maastricht	12/01/2017	12/01/2017	[General Public], [Scientific Community (higher education, Research)]	50
Simon Portegies Zwart: Colloquium Nagoya University	01/11/2016	01/11/2016	[Scientific Community (higher education, Research)]	50
Simon Portegies Zwart: Colloquium Birmingham University	30/11/2016	30/11/2016	[Scientific Community (higher education, Research)]	50
Simon Portegies Zwart: Colloquium Bad Honnef	09/12/2016	09/12/2016	[Scientific Community (higher education, Research)]	50
Derek Groen: Invited seminar @ UNIGE	24/11/2016	24/11/2016	[Scientific Community (higher education, Research)]	20
Saad Alowayyed gave telecon presentation to KACST in Saudi Arabia	24/11/2016	24/11/2016	[Scientific Community (higher education, Research)]	30
Simon Portegies Zwart: Working visit to talk about multiscale simulations Lucie Jilkova	12/12/2016	16/12/2016	[Scientific Community (higher education, Research)]	5

## 2.2 Events

ComPat aims to organize and participate in a variety of relevant events throughout the project duration, including conferences, workshops, seminars, training events and hackathons. The aim is to

organise at least two workshops and a summer school over the course of the project, which will have the objective to promote ComPat's results and success stories and to provide compelling cases to specialised audiences through involving them more actively.

Task 7.4 is concerned with the organization of a training event and two workshops, and while it was originally intended to run from months 9-36, work began on the organisation of a multiscale workshop at ICCS 2016 from the project's offset. Therefore, the task will effectively run from month 1-36. There are three milestones in this task:

- Milestone 6 - ComPat Workshop 1 (took place in month 9 at ICCS 2016)
- Milestone 11 - ComPat Training Event (now planned for the third year of project, see section 2.3)
- Milestone 17 - ComPat Workshop 2 (by month 30, targeting the Lorentz Centre)

The activity in months 12-18 of the project in this task is detailed in section 2.2.1.

Task 7.5 is concerned with the co-ordination of conference participation, running from months 1 to 36). The events attended are listed in section 0.

## 2.2.1 Events Organised

In this section, events organised by ComPat consortium members are detailed, the key events are listed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Simon Portegies Zwart: Bad Honnef meeting MODEST	07/12/2016	09/12/2016	[Scientific Community (higher education, Research)]	100
Derek Groen: SHGVA '17 @ CERN (sponsored by UN)	10/02/2017	12/02/2017	[Scientific Community (higher education, Research)], [General Public], [Civil Society]	25
Simon Portegies Zwart: Lorentz Center meeting on the evolution of the Solar system and the origin of life	20/02/2017	24/02/2017	[Scientific Community (higher education, Research)]	50
LRZ: The EEE Workshop Experimental Execution Environment Workshop	13/10/2016	13/10/2016	[Scientific Community (higher education, Research)]	10

## 2.2.2 Participation at Events

The ComPat consortium attended, participated in numerous events in months 12-18 of the project, these included:

- Supercomputing 2016, Utah
- MRS (Material Research Society) Fall Meeting 2016, Boston
- 253rd ACS (American Chemistry Society) National Meeting & Exposition, San Francisco
- 1st Conference of the European Association of Systems Medicine (EASyM), Berlin

- UKCOMES Workshop on Lattice Boltzmann Methods and Applications, London
- The Symposium on Advanced Nanomaterials for Biomedical Applications in Sheffield
- SHGVA '17 (Science Hackathon Geneva), CERN
- MODEST (Modeling and Observing Dense stellar systems), Bad Honnef
- "Evolution of the Solar system and the origin of life", Leiden

### 2.2.2.1 Participation at Conferences

In this section, the active participation of ComPat at various conferences is listed. In total, ComPat consortium members participated in 5 conferences. These are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Robin Richardson: Prize winning Poster at "1st conference of the European Association of Systems Medicine", Berlin	26/10/2016	28/10/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	500
Peter Coveney gave a talk at the MRS Fall 2016 Meeting on "Modelling Clay-Polymer Nanocomposites Using a Multiscale Approach"	30/11/2016	30/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	5000
Peter Coveney gave a talk at the 253rd ACS National Meeting in San Francisco, California, "Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration"	03/04/2017	03/04/2017	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000
Peter Coveney gave a talk at the 253rd ACS National Meeting in San Francisco, California, "Computerbased design of advanced materials: Chemically specific multiscale modelling of polymerclay nanocomposites"	03/04/2017	03/04/2017	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000
Peter Coveney gave a talk at the 253rd ACS National Meeting in San Francisco, California, "High performance and/or cloud computing for free energy prediction using molecular dynamics simulations?"	03/04/2017	03/04/2017	[Scientific Community (higher education, Research)], [Medias], [Industry]	10000
James Suter to give a talk at MRS Spring Meeting 2017	17/04/2017	21/04/2017	Science community	100
Alfons Hoekstra gave a talk at the "Birds-of-a-feather session" at Supercomputing 16 in Utah	16/11/2016	16/11/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	500

### 2.2.2.2 Participation at Workshops

In this section, the participation of ComPat at various conferences is listed. In total, ComPat consortium members participated in 6 workshops. These are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
-------------	-----------	---------	-------------	----------------------------

Allinea at VI-HPS, Tools training for Allinea tools	08/02/2017	10/02/2017	Mix of industry + academia - Tools training for Allinea tools	10
Derek Groen at UKCOMES Workshop on Lattice Boltzmann Methods and Applications"	12/12/2016	13/12/2016	[Scientific Community (higher education, Research)]	35
Derek Groen at Science Hackathon @ Univercite	25/11/2016	25/11/2016	[General Public],[Industry],[Scientific Community (higher education, Research)]	25
Robin Richardson gave a talk at "UKCOMES Workshop on Lattice Boltzmann Methods and Applications"	12/12/2016	13/12/2016	[Scientific Community (higher education, Research)], [Medias], [Industry]	200
Peter Coveney gave a talk at the 1st Annual Kennedy Institute Student Symposium, "Computational Biomedicine: The Role of Modelling and Simulation in the Life Sciences"	04/11/2016	04/11/2016	[Scientific Community (higher education, Research)], [Industry]	200
Peter Coveney gave a talk at the 'The Symposium on Advanced Nanomaterials for Biomedical Applications' in Sheffield on "Computer-based design of advanced materials: Chemically specific multiscale modelling of polymer-clay nanocomposites"	20/02/2017	21/02/2017	[Scientific Community (higher education, Research)], [Industry]	200
James Suter to give a talk at International Clay Conference workshop	17/07/2017	17/07/2017	Science Community	30

### 2.2.2.3 Participation at other events

In this section, the participation of ComPat at various events that aren't classified as conferences or workshops is detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Derek Groen: 2020 Science final meeting	12/10/2016	12/10/2016	[Scientific Community (higher education, Research)]	25
Derek Groen: 3 Minute Thesis Contest	01/02/2016	01/02/2016	[Scientific Community (higher education, Research)]	30
Derek Groen: COST Meeting Skopje (virtual attendance)	20/10/2016	21/10/2016	[Scientific Community (higher education, Research)]	25
Alfons Hoekstra gave a talk on ComPat at the CompBioMed CoE Kick Off Meeting in London	04/10/2016	04/10/2016	[Scientific Community (higher education, Research)], [Industry]	50

## 2.3 Proposed Actions for Year 2

Our proposed actions in the second 18 months of the project are described in this section, as described in the latest version of the dissemination action plan. The following tasks in the description of work will continue:

- Task 7.2: The ComPat website (M1 – M36)
- Task 7.3: Maintain a social media presence (M1 – M36)
- Task 7.4: Organise a training event and workshops (M9 – M36)
- Task 7.5: Co-ordinate conference participation (M1 – M36)
- Task 7.6: Produce dissemination materials (M1 – M36)

ComPat will have a presence at events such as:

- European HPC Summit Week 2017 in Barcelona
- ICCS2017 in Zurich
- ISC HPC 2017 in Frankfurt
- Supercomputing (SC17) in Denver

The new leaflets described in section 2.1.6 will be completed and then distributed at various events throughout the remainder of the project, along with the ComPat branded merchandise described in section 2.1.7.

Milestones for the second 18 months are as follows:

- Milestone 11 – ComPat training event (M20)
- Milestone 17 – ComPat Workshop 2 (M30)

The ComPat training event (Milestone 11) has been delayed into the third year of the project. We have realised that organising a ComPat training event in M20 of the project is too early. Our goal is to train external people in ComPat technology, and want to do so with advanced features available in the ComPat software stack. We therefore decided to move this training event to the third year of the project. In our next All Hands Meeting (M25) we will draw a final decision on the location and date of this event. We are currently considering to collocate it with the HPC Summit in 2018

In addition, the Hartree Centre will organise an industry targeted event in the third year of the project that will also act as a training event.

The second workshop to be organised by ComPat (Milestone 17) will be co-organised with the Lorentz Centre and the theme will be on High Performance Multiscale Computing Driven by Applications (also multiscale computing patterns). The workshop will have the objective of promoting ComPat's results and success stories and to provide compelling use cases to interested audiences. Relevant industrial players will be invited and the event will be collocated with relevant conferences. The deliverables for the workshop may include position papers and research papers, a piece of software written by the consortium, a white paper, and/or the core for a special issue.

Deliverables for the second 18 months are as follows:

- D7.4 Third annual Dissemination Report (M36)

### 3 Conclusions

There was a substantial amount of dissemination activity in the first 18 months of ComPat. 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, with the milestones for the period being just a small part of our overall activity. 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 high school students to Professors. ComPat thus reached a broad set of stakeholders. Through building networks within our scientific community and encouraging collaborative activities, in addition to our training

agenda, we will accelerate European excellence in mathematics and algorithms in a multi-disciplinary fashion. We believe that through effective communication of our work to standardisation bodies, we will be able to jointly develop new standards where they do not currently exist.