



## D7.2 First Dissemination Report

<b>Due Date</b>	Month 12
<b>Delivery</b>	September 30 <sup>th</sup> , 2016
<b>Lead Partner</b>	CBK Sci Con LTD
<b>Dissemination Level</b>	Public
<b>Status</b>	Final
<b>Approved</b>	Executive Board: yes
<b>Version</b>	V1.5



**DOCUMENT INFO**

<b>Date and version number</b>	<b>Author</b>	<b>Comments</b>
07.09.2016 v1.1	Hugh Martin	First Draft
15.09.2016 v1.2	Paul Best	Second Draft
20.09.2016 v1.3	Sabrina Eisenreich	First Internal Review
25.09.2016 v1.4	Alfons Hoekstra	Second Internal Review
27.09.2016 v1.5	Hugh Martin	Final Draft

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**TABLE OF CONTENTS**

1	Executive summary .....	5
2	Report .....	5
2.1	Introduction .....	5
2.2	Description of Work .....	6
2.3	Target Audiences .....	8
2.3.1	Targeting Academics .....	10
2.3.2	Targeting Industry .....	10
2.3.3	Targeting the General Public .....	11
2.3.4	Targeting Students from Secondary School to University .....	11
2.4	Dissemination Materials and Channels .....	11
2.4.1	Logo .....	12
2.4.2	Scientific Papers .....	12
2.4.3	Non-Peer Reviewed Publications .....	15
2.4.4	Websites .....	16
2.4.5	Social Media .....	19
2.4.6	Posters .....	21
2.4.7	Leaflets .....	22
2.4.8	Presentations .....	24
2.4.9	Mailing Lists .....	25
2.4.10	Media Outreach .....	26
2.4.11	Other Activities .....	26
2.5	Events .....	29
2.5.1	Events Organised .....	30
2.5.2	Participation at Events .....	34
2.6	Proposed Actions for Year 2 .....	41
3	Conclusions .....	42
4	Annexes .....	43
4.1	Life's Rocky Start on PBS .....	43
4.2	Solvay Symposium .....	43
4.3	Multiscale Workshop at ICCS 2016 .....	45
4.4	PRACEdays16 .....	46
4.5	New Scientist Article .....	46
4.6	Leidsch Dagblad Article .....	47
4.7	Sky & Telescope Magazine .....	48
4.8	NRC Article .....	49

## LIST OF TABLES AND FIGURES

Figure 1: The ComPat Project Logo.....	12
Figure 2: Image of the ComPat website. ....	17
Figure 3: Website hits versus time. ....	17
Figure 4: Image of the ComPat Twitter account. ....	20
Figure 5: ComPat project poster.....	22
Figure 6: ComPat leaflet, page 1. ....	23
Figure 7: ComPat leaflet, page 2. ....	24
Figure 8: ComPat Slide Template .....	25
Figure 9: Flyer for the Solvay Symposium. ....	32
Figure 10: Flyer for VPH2016 .....	33
Figure 11: Advert for Life's Rocky Start on PBS.....	43
Figure 12: Solvay Symposium Image 1. ....	43
Figure 13: Solvay Symposium Image 2. ....	44
Figure 14: Solvay Symposium Image 3. ....	44
Figure 15: Multiscale Workshop Image 1.....	45
Figure 16: Multiscale Workshop Image 2. ....	45
Figure 17: PRACEdays16 Image 1. ....	46
Figure 18: First 2 pages of Simon Zwart's New Scientist Article. ....	46
Figure 19: First page of Leidsch Dagblad article “Waarom Zoeken Naar Planeet Negen” .....	47
Figure 20: First 2 pages of "What Caused The Great Eruption?". ....	48
Figure 21: First page of “Het Nieuwe, Ruige Zonnestelsel” .....	49

## 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, D7.2 First Annual Dissemination Report, reviews the events and dissemination results of ComPat for the first 12 months of the project (1<sup>st</sup> October 2015 to 30<sup>th</sup> September 2016). There was a substantial amount of dissemination activity in the first year of ComPat, the key highlights during this period include:

- The organisation of a conference
- The organisation of a symposium
- The organisation of a workshop
- Participation at 14 major conferences and workshops
- The publication or submission of 7 scientific papers

The report also outlines the actions for the second year of the project, as described in the ComPat dissemination action plan.

## 2 Report

### 2.1 Introduction

Future Exascale high performance systems offer tremendous opportunities for computational science and promise to transform computation from a quantitative tool supporting theory and experimentation into a *predictive simulation science*. Fundamental technological and algorithmic challenges need to be addressed in order to realise the capabilities that fully exploit these emerging opportunities. Current approaches in high performance computing will not directly apply at the exascale to automatically deliver the envisioned step jump to scientific discoveries. ComPat will contribute significantly in this highly desirable paradigm shift, thus aiming at a strong impact on predictive simulation science that has to rely on huge multiscale simulations.

ComPat aims to significantly reduce the effort and time needed to reach exascale performance, both in case of new application development and in adapting existing applications to new, heterogeneous, extremely parallel systems. We are achieving this impact by addressing several strategic sub-goals, such as those identified by the European Technology Platform for High Performance Computing

(ETP4HPC) strategic research agenda and various standards bodies. The project aims to have an impact across the whole future HPC market (with a focus on extreme-scale systems), as well as in the theoretical foundations underpinning the emerging exascale applications and use cases.

Given this substantial impact, the stakeholders that will benefit from ComPat's work are a large and diverse set of people. These include: the scientific community, user communities, middleware developers, vendors, other industries, standardisation bodies, and related international projects. Through various dissemination actions, we are disseminating the project's outcomes to these stakeholders.

We are targeting the project stakeholders through the following channels:

- ComPat website: [www.compat-project.eu](http://www.compat-project.eu)
- ComPat Twitter account: @compatproject
- Scientific Events (conferences, workshops, seminars etc.)
- National and international press, news forums, etc.
- Scientific Journals

We are targeting the various stakeholder groups using the following dissemination materials detailed in section 2.4:

- Leaflets
- Posters
- Scientific Papers
- Non-Peer Reviewed Publications
- Website content
- Social Media Content
- Press releases

These plans are described in the ComPat dissemination action plan (deliverable 7.1).

In order to maximize the impact of ComPat and ensure its lasting effects after the project ends, the software and tools created during the project will be made available and accessible to interested parties in an open manner.

## **2.2 Description of Work**

The focus of ComPat's Work Package 7 (WP7) is to communicate the project's objectives and results, increasing the impact of ComPat in the HPC community. In the Description of Work for the project,

the key milestone objectives of WP7 include the organisation of two workshops, a Summer School, dedicated media work, participation in conferences, preparation and distribution of information material, event organization, and the establishment and nurturing of key media relations.

The dissemination targets outlined in the Description of Work for the first 12 months include:

- **Task 7.1: Production of a Dissemination Action Plan (M1 – M3)** - Writing a detailed dissemination action plan, with a clear description of tools, tasks, target audiences and deliverables.
- **Task 7.2: The ComPat website (M1 – M36)** - The website will be clear, informative, and constantly updated with news and upcoming events, to be used as a reference point for the project's on-going activities. The website will also have a section for the public training material, and a list of the scientific publications produced through the ComPat project. It will be divided in two sections: a public area and an internal area. The public area is available without signing in and is maintained by the dissemination team. The internal parts require an authorized sign-in. The website will go live in M2 of the project, and be constantly updated.
- **Task 7.3: Maintain a social media presence (M1 – M36)** - These dissemination channels are growing in importance. Our dissemination plan will take into account these channels and maintain a consistent and informative presence. Additionally, we will create suitable mailing lists, for maximum effective targeting of the ComPat community.
- **Task 7.4: Organise a training event and workshops (M9 – M36)** - ComPat will schedule a Summer School for training in Month 30. The Summer School will be an interactive forum providing training in multiscale approaches, and will target both students and external parties. ComPat will also organise a workshop as part of ICCS in 2016, which will take place roughly in month 14 of the project. The second workshop will likely be organised with the Lorentz Centre, at a later stage of the project. Workshops will have the objective to promote ComPat results and success stories and to provide compelling use cases to interested audiences. Relevant industrial players will be invited to the workshop. The workshops and training event will be collocated with relevant conferences (see task 7.5).
- **Task 7.5: Co-ordinate conference participation (M1 – M36)** - Several international conferences, like Supercomputing, International Supercomputing, and International Conference on Computational Science will be targeted. ComPat will organize partners' presence at these conferences and will consider partaking in the exhibition opportunities they offer.
- **Task 7.6: Produce dissemination materials (M1 – M36)** - During the course of the project ComPat will create White Papers as a collection of special achievements. ComPat will also disseminate, via the website and other channels, the scientific publications resulting from the

project's research. Additionally, flyers and posters will be produced and available at the workshops and conferences.

There were two WP7 deliverables for the first 12 months:

- **D7.1 Detailed Dissemination Action plan (M3)** - Writing a detailed dissemination action plan, with a clear description of tools, tasks, target audiences and deliverables.
- **D7.2 First annual Dissemination Report (M12)** - Review events and dissemination results of past year and proposes actions for the coming one, including update of dissemination action plan.

Concerning D7.1, this was produced on schedule, in month 3 of the project. The action plan is a live document that will be updated as necessary in order for it to continually act as a guide for the consortium in our dissemination plans and activities.

Additionally, there was one WP7 milestones in the first 12 months, and a second that was carried out earlier than planned so is included in this document:

- **Milestone 1 – Websites and mailing lists (M2)**
- **Milestone 6 – ComPat Workshop 1 (M14)**

Each task, deliverable, and milestone has been carried out on or before schedule, this will be detailed in the sections below.

### **2.3 Target Audiences**

Given the substantial impact of ComPat, the stakeholders that will benefit from ComPat's work are a large and diverse set of people. These include:

- The scientific community
- User communities
- Middleware developers
- Vendors
- Other industries
- Standardisation bodies
- Related international projects.

Through our dissemination actions, ComPat has communicated the project aims and its outcomes (publications, software, best practice, etc.) to these stakeholders. In the first year of ComPat, this has primarily been the communication of the project and its aims. The communication of specific results is expected to increase in the second and third years of the project.

A combination of dedicated media relations, participation in conferences, preparation and distribution of information material, and event organization is being harnessed to implement our impact objectives, the following table outlines our target audiences and the channels we are using to reach them. In the sections below, we discuss some of the target audiences in more detail.

ComPat Output	Target audience	Possible Measures/Channels
<i>Realisation of Exascale performance levels by applications developers worldwide</i>		
Demonstrated Computing Patterns	Software and hardware developers, Exascale Labs	Web site, papers, conference presentations and demonstrations
Energy consumption optimisation service (ECOS)	Applications Developers, Facilities providers and users	ComPat web site and Software partner web sites
Performance Toolkit for design of multiscale models for exascale execution	Applications software designers	Allinea products and services
Performance Prediction methodology	Application developers, S/H developers, exascale labs	Published models, embedded in open source software
Requirements for interoperability	Standardisation Bodies	White Papers, 1-on-1 meetings
<i>Influencing next generation compute architectures (co-design)</i>		
Understanding of bottlenecks on Experimental Execution Environment	Hardware companies	STFC/IBM Hartree Collaboration (see letter of support)
Benchmarks / test cases for evaluation of future systems	Hardware companies, exascale research labs	ComPat web site
<i>Influencing policies of funding organisations and service providers to create the infrastructure needed for exascale deployment and new use cases for HPC</i>		
Demonstrations, popular articles written about ComPat, White papers (project + contributions to others)	National and European bodies, HPC Centres, Media	Medial liaisons, Presence on advisory groups (list)

<i>Scientific results arising from improved fidelity of simulations in applications areas</i>		
Improved HPC algorithms for multiscale simulation	Domain scientists	Scientific literature, mature software
Coupled applications with demonstrated reliability	ComPat Partners	Existing research programmes
	Industrial users	ComPat meetings, Business development and outreach
	Academic Users	Scientific support services offered to academia
<i>Enhanced skills in next generation of researchers</i>		
ComPat Courses/Workshops	PhD students, Postdocs, and other interested parties	Exascale course run by the project
On-line Training materials	PhD students, Postdocs, and other interested parties	Project web site
<i>Public understanding of opportunities arising from exascale computing within Europe</i>		
Popular articles in on-line forums	General audience	Web site, Social media, demonstrations, competitions

### 2.3.1 Targeting Academics

Targeting academics is naturally a major focus for ComPat. Much of our event activities and dissemination channels target PhD students, postdoctoral research associates, and both junior and senior academics. Such activity also targets Industry in parallel wherever possible. The tables in sections 2.4 and 2.5 list activity in the first year of the project that has targeted academics.

### 2.3.2 Targeting Industry

The table in Section 2.3 shows the industrial audiences for ComPat's various outputs. In particular, the HPC industry is one of the most important target audiences for ComPat's contributions to improve innovation capacity. A legal advisor at the UvA (the coordinating partner) has been established to bring in expertise on the legal aspects of knowledge use, exploitation (e.g. patents) and is available to the consortium for questions of legal nature. When appropriate, an independent third party (for instance a patent office or ethicist) is consulted.

Through their extensive links with industry across many sectors STFC, PSNC, and BADW-LRZ are in a unique position to disseminating ComPat know-how as widely as possible within this audience. IBM

has committed to provide support for the project; both through complementary research from IBM and by having our team working closely with the consortium.

Industry is not only on our dissemination radar, but they have also been involved in our conferences/workshops and will be included in our training activities. Through ComPat, it is anticipated that our results will make their way into software and hardware design, thereby shaping the next generation of HPC infrastructure. This will initially impact vendors that have the strongest links to the consortium, but will eventually spread to others. We strongly believe that industry inclusion from the project's outset is enhancing our innovation ambitions.

The tables in sections 2.4 and 2.5 list activity in the first year of the project that has targeted industry.

### **2.3.3 Targeting the General Public**

We are employing several approaches to target the wider public. For example we will continue to produce content for popular science magazines such as New Scientist (see section 2.4.3 for activity in the first 12 months of the project), and participate in general public events such as the Royal Society Exhibition in London (see section 2.5.2.3 for activity in the first 12 months of the project).

### **2.3.4 Targeting Students from Secondary School to University**

All partner universities in the ComPat consortium are active in school engagement, which provides ComPat with many pre-existing school programmes to exploit. UCL for instance lists a number of engagement programmes, which include Junior Conferences, Spring and Summer Schools, Masterclasses, Summer Challenges, Taster Courses, UCL visits to schools, and school visits to UCL. For example, ComPat consortium member Jeroen Bedorf from Leiden University gave an introductory talk to high school students, as listed in section 2.4.11.

## **2.4 Dissemination Materials and Channels**

In this section, the various dissemination channels used and the materials developed by ComPat are described. In general, we have aimed to make maximum use of already established partner, national, and European dissemination channels such as E-infrastructure specialist groups, thus maximising the impact to cost ratio of our activities in WP7.

The ComPat name and logo have been used in all of our dissemination materials, be it in the form of leaflets, posters, white papers etc. Templates 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. Task 7.6 is concerned with the production of dissemination materials and runs throughout the 3 years.

### 2.4.1 Logo

The ComPat logo has been designed to be clean, clear, and recognisable, with a strong image and style. The logo is shown below:



**Figure 1: The ComPat Project Logo**

The logo is used in png and eps format in various resolutions, and also in black & white as well as colour. In full colour, the Teal shading is R;G;B 0;237;148, while the grey shading is R;G;B 154;153;154.

### 2.4.2 Scientific Papers

Throughout the project, the ComPat consortium will publish numerous scientific, peer-reviewed papers, conference proceedings, and chapters in books. 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 12 months of the project, seven peer-reviewed, open-access scientific papers have been published, accepted for publication, or submitted to a journal, these are listed below:

1. **Type:** Article in journal

**Title:** "Mechanism of exfoliation and prediction of materials properties of clay-polymer nanocomposites from multiscale modeling"

**DOI:** 10.1021/acs.nanolett.5b03547

**Authors:** J. Suter, D. Groen, and P. V. Coveney

**Journal:** Nano Lett.

**Number, Date:** 15, 2015

**Publisher:** ACS

**URL:** <http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.5b03547>

**Pages:** 8108-8113

**Peer Review:** Yes

**Open Access:** Yes, Gold, €665

2. **Type:** Article in journal

**Title:** "A Distributed Multi-Agent Market Place for HPC Compute Cycle Resource Trading"

**DOI:** arXiv:1512.04343

**Authors:** S. J. Zasada and P. V. Coveney

**Journal:** CoRR

**Number, Date:** 2015

**Publisher:** arXiv

**URL:** <https://arxiv.org/abs/1512.04343>

**Pages:** N/A

**Peer Review:** No

**Open Access:** Yes, Gold, €0

3. **Type:** Article in journal (Submitted)

**Title:** "Load Balancing of Parallel Cell-based Blood Flow Simulations"

**DOI:** N/A

**Authors:** S. Alowayyed , L. Mountrakis, E. Lorenz, A.G. Hoekstra

**Journal:** Computer Physics Communications

**Number, Date:** N/A

**Publisher:** Elsevier

**URL:** N/A

**Pages:** N/A

**Peer Review:** Yes

**Open Access:** Yes

4. **Type:** Article in journal (In Print)

**Title:** "Towards the virtual artery: a multiscale model for vascular physiology at the physics–chemistry–biology interface"

**DOI:** N/A

**Authors:** Alfons G. Hoekstra, Saad Alowayyed, Eric Lorenz<sup>1,4</sup>, Natalia Melnikova, Lampros Mountrakis, Britt van Rooij, Andrew Svitenkov, Gábor Závodszky<sup>1</sup> and Pavel Zun

**Journal:** Philosophical Transactions of the Royal Society A

**Number, Date:** 374 (2016)

**Publisher:** The Royal Society

**URL:** TBD

**Pages:** TBD

**Peer Review:** Yes

**Open Access:** Yes

5. **Type:** Article in journal

**Title:** “FabSim: Facilitating computational research through automation on large-scale and distributed e-infrastructures”

**DOI:** 10.1016/j.cpc.2016.05.020

**Authors:** Derek Groen, Agastya Bhati, James Suter, James Hetherington, Stefan J. Zasada, and Peter V. Coveney

**Journal:** Computer Physics Communications

**Number, Date:** 207 (2016)

**Publisher:** Elsevier

**URL:** <http://www.sciencedirect.com/science/article/pii/S0010465516301448>

**Pages:** 375-385

**Peer Review:** Yes

**Open Access:** Yes

6. **Type:** Article in journal

**Title:** “Bridging the gaps at the physics–chemistry–biology interface”

**DOI:** TBD

**Authors:** P. V. Coveney, J. P. Boon and S. Succi

**Journal:** Philosophical Transactions of the Royal Society A

**Number, Date:** 374 (2016)

**Publisher:** The Royal Society

**URL:** TBD

**Pages:** TBD

**Peer Review:** Yes

**Open Access:** Yes

7. **Type:** Article in journal

**Title:** “Big data need big theory too”

**DOI:** TBD

**Authors:** Peter V. Coveney, Edward R. Dougherty and Roger R. Highfield

**Journal:** Philosophical Transactions of the Royal Society A

**Number, Date:** 374 (2016)

**Publisher:** The Royal Society

**URL:** TBD

**Pages:** TBD

**Peer Review:** Yes

**Open Access:** Yes

### 2.4.3 Non-Peer Reviewed Publications

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

Description	Date From	Date To	Audience(s)	Estimated Number of People
Simon Zwart - New Scientist article	08/06/16	08/06/16	General Public, Scientific Community, Public Sector	5000
Simon Zwart - NRC (Dutch Newspaper) article “Waarom Zoeken Naar Planeet Negen”	19/08/16	19/08/16	General Public, Scientific Community, Public Sector	2000
Simon Zwart – Sky & Telescope Article – “What caused the Great Eruption?”	01/10/16	01/10/16	General Public, Scientific Community, Public Sector	1000
LRZ - SuperMUC enables major finding in personalized medicine; HPCwire: <a href="https://www.hpcwire.com/off-the-wire/supermuc-enables-major-finding-personalized-medicine/">https://www.hpcwire.com/off-the-wire/supermuc-enables-major-finding-personalized-medicine/</a>	20/06/16	20/06/16	Scientific Community, Industry	2000

LRZ - LRZ Newsletter: New H2020 projects started at LRZ	01/11/15	01/11/15	Scientific Community, Industry	500
LRZ - Supercomputer verbessert Brustkrebsbehandlung (Supercomputer improves treatment of breast cancer) eGovernmentComputing: <a href="http://www.egovernment-computing.de/supercomputer-verbessert-brustkrebsbehandlung-a-538823/">http://www.egovernment-computing.de/supercomputer-verbessert-brustkrebsbehandlung-a-538823/</a>	16/06/16	16/06/16	General Public, Scientific Community, Public Sector	1000
LRZ - Durchbruch für personalisierte Medizin dank SuperMUC (Breakthrough in personalised medicine thanks to SuperMUC) e-health: <a href="http://www.e-health-com.eu/details-news/durchbruch-fuer-personalisierte-medizin-dank-supermuc/ab60024bdef3ab9a1b16fedecbce7a39/">http://www.e-health-com.eu/details-news/durchbruch-fuer-personalisierte-medizin-dank-supermuc/ab60024bdef3ab9a1b16fedecbce7a39/</a>	15/06/16	15/06/16	General Public, Scientific Community, Public Sector	2000

#### 2.4.4 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.

Additionally, the website provides a separate intranet page, which is accessible to consortium members only and acts as a storage service for ComPat project documents such as reports, publications lists etc.

Task 7.2 is concerned with the set up and maintenance of the ComPat website and runs across months 1-36. Milestone 1 was set to take place in the second month of the project and was the final construction of the website (and mailing lists); this was created on schedule.

Below is an image of the website in its current state, this is subject to change in the future:

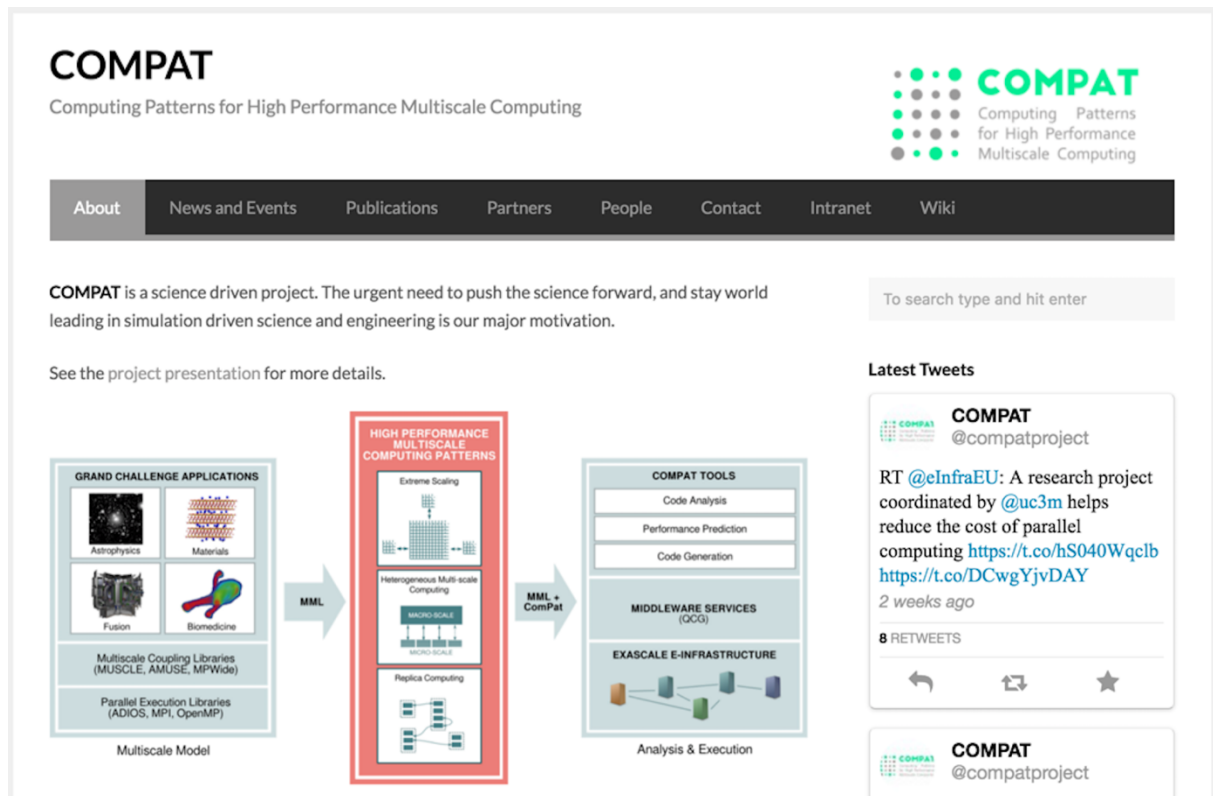


Figure 2: Image of the ComPat website.

The image below shows the website traffic since April 2016 (there is no data available prior to this point):

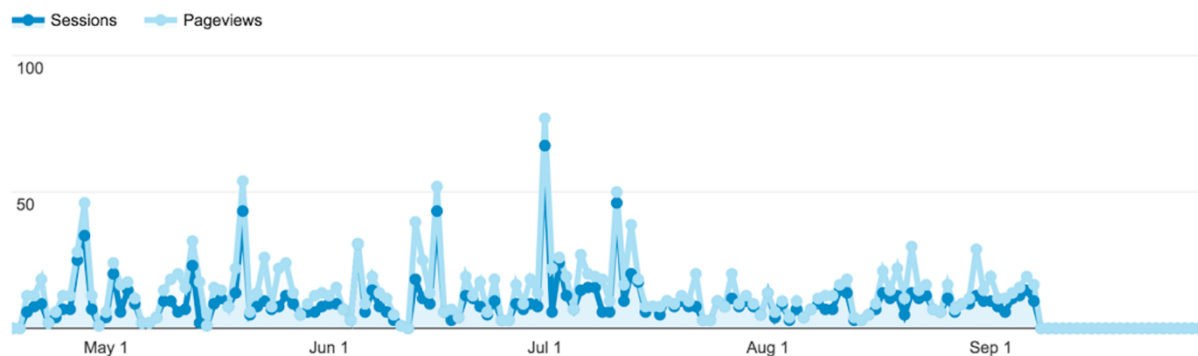


Figure 3: Website hits versus time.

The key statistics for the website are as follows:

- Sessions: 1401
- Page views: 2036
- Unique users: 1152
- Page views per session: 1.45
- News Stories: 20

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

Description	Date From	Date To	Audience(s)	Estimated Number of People
Peter Coveney - Distinguished science writer and journalist Dr Roger Highfield has written a blog post about the experience of running a Giant Workflow on Phases 1 and 2 of SuperMUC. The activity turned out to be a big success for the CCS, led by Peter Coveney.	13/06/16	13/06/16	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	2000
Hugh Martin - posted 20 news stories on compat-project.eu	07/07/05	08/07/05	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	1152
Hugh Martin - posted a news story on ccs.chem.ucl.ac.uk to introduce ComPat	01/10/15	01/10/15	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	500
PSNC - posted a news story on www.man.poznan.pl to introduce ComPat	01/10/15	01/10/15	[Scientific Community (higher education, Research)] [Industry] [Civil	500

			Society] [General Public] [Policy makers] [Medias]	
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

#### 2.4.5 Social Media

ComPat aims to have an effective social media presence. At the forefront of this is the ComPat Twitter account, which can be found at [@compatproject](https://twitter.com/compatproject). Task 7.3 is concerned with maintaining a social media presence and runs across months 1-36.

The ComPat Twitter account currently has 57 Tweets and 44 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.

An image of the Twitter account is shown below:



**Figure 4: Image of the ComPat Twitter account.**

Twitter activity in the project is summarised in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Hugh Martin - posted 57 tweets on the twitter account @compatproject	07/07/05	08/07/05	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	44
Derek Groen - Promotion of ComPat related content through Twitter (@whydoitweet)	15/10/15	18/08/16	[Scientific Community (higher education, Research)] , [General Public],[Medias]	366

#### 2.4.6 Posters

ComPat presents posters at conferences and workshops in order to raise awareness of the project and its results. All posters contain:

- The ComPat logo
- A URL to the ComPat website
- The funding line “This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 671564.”
- An image of the European flag
- Images of ComPat research
- Summaries of ComPat research and outcomes

In the first year of the project we have produced a poster that summarises the project and its aims. It was presented at PRACEdays16 in Prague, which was a part of the European HPC Summit Week. The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class high performance computing service for scientists and researchers from academia and industry in Europe. PRACEdays16 was therefore a conference platform for researchers to disseminate HPC-relevant science. A picture from the event is shown in Annex 4.4, and the poster itself is shown below:

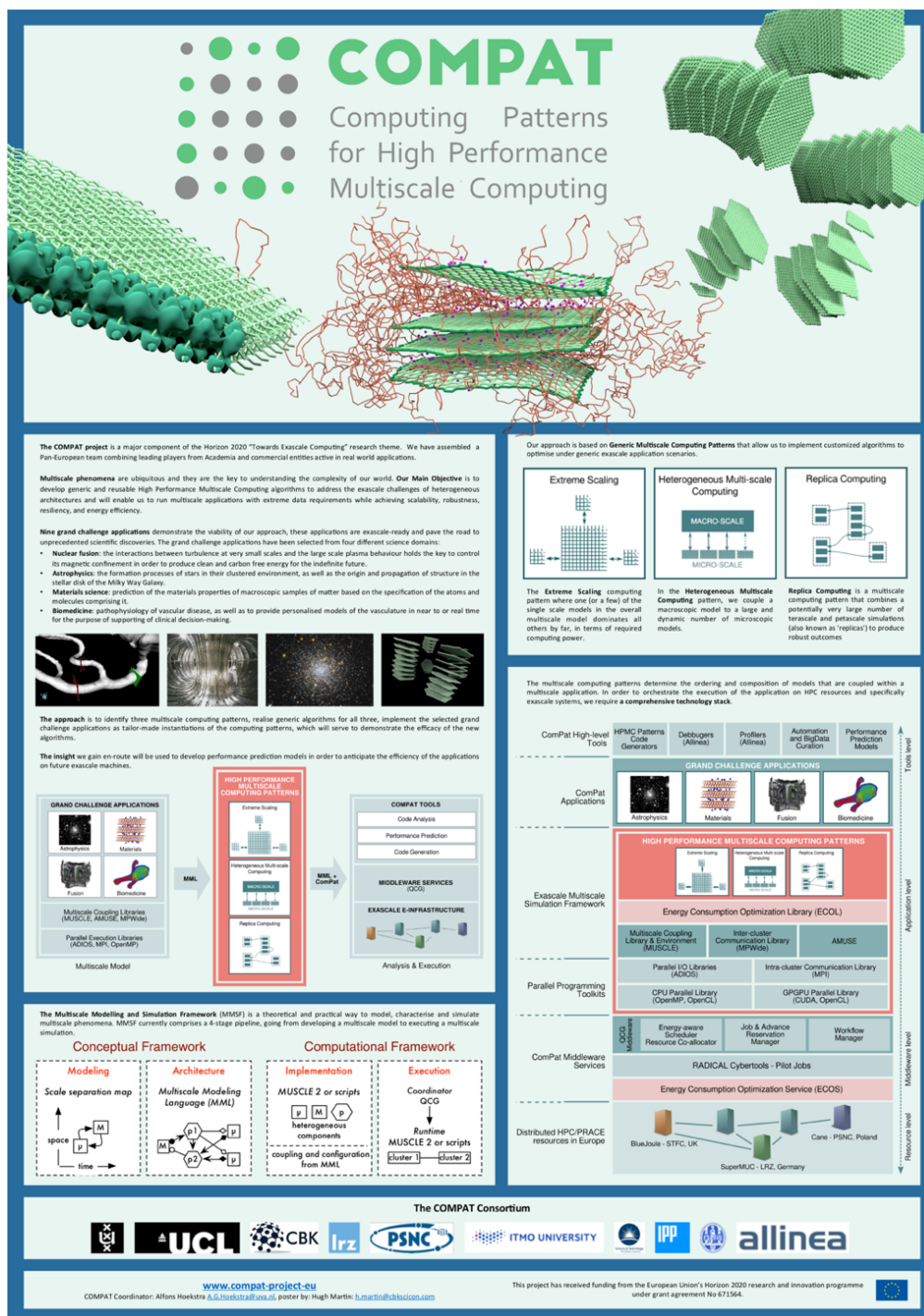


Figure 5: ComPat project poster.

### 2.4.7 Leaflets

ComPat distributes leaflets to stakeholders at various events with the purpose of making them aware of the project or particular aspects of it. In the first year of the project, one leaflet was produced that summarises ComPat and its aims, it contained the following:

- ComPat logo
- A URL to the ComPat website

- The funding line “This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 671564.”
- An image of the European flag
- A summary of the ComPat project
- Images of ComPat research

The leaflet was distributed at PRACEDays16 and is shown below:

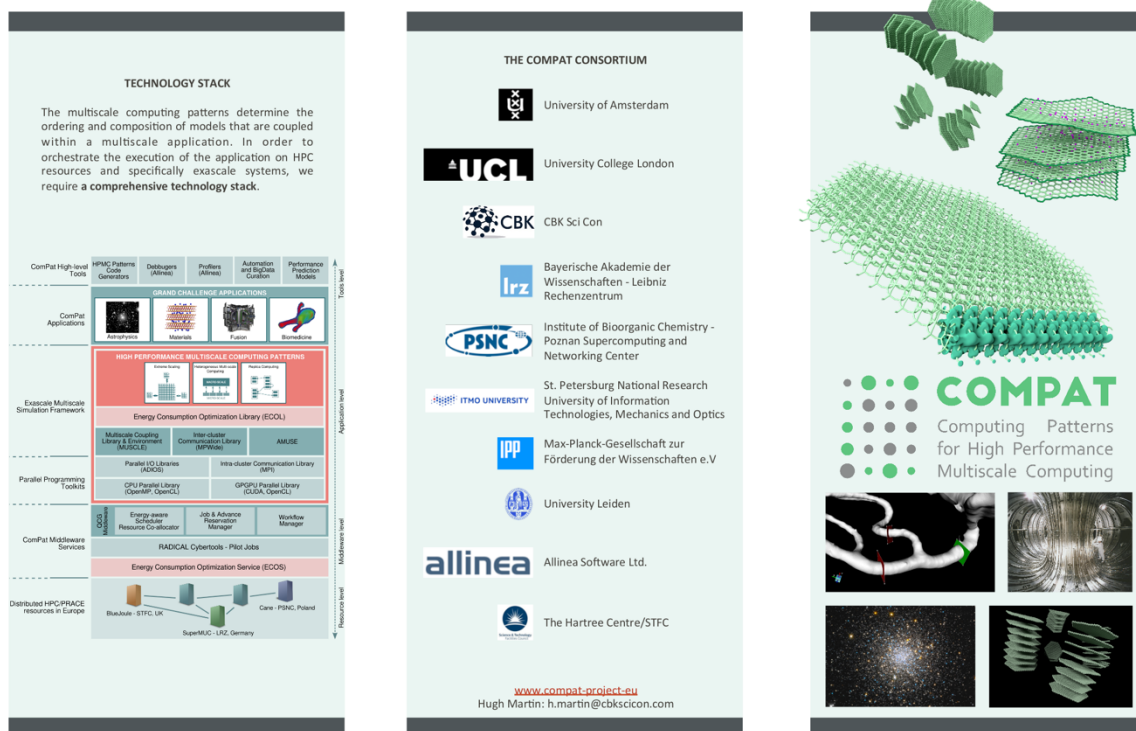


Figure 6: ComPat leaflet, page 1.

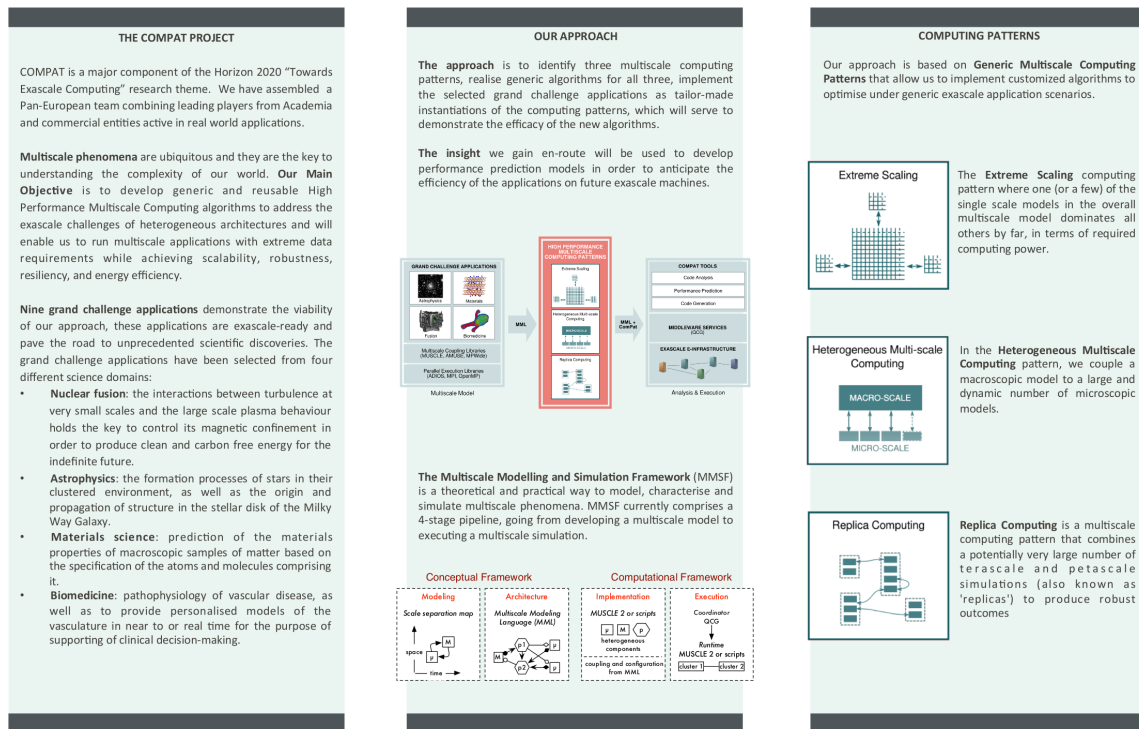


Figure 7: ComPat leaflet, page 2.

## 2.4.8 Presentations

ComPat participates in talks at conferences, workshops and seminars throughout the project. Where appropriate, the slides for such talks will contain a section or slide which summarises the ComPat project, this contains:

- ComPat logo
- A URL to the ComPat website
- The funding line "This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671564."
- An image of the European flag

In other cases, it will be appropriate to have each slide as ComPat themed. In these instances, a template is available that displays the ComPat logo on each page, and the rest of the slide aesthetic has been adjusted to match that of the logo, as shown below:



# ComPat KO Meeting

## Work Package 7 – Dissemination

5<sup>th</sup> October 2015

Hugh Martin  
CBK Sci Con

26/10/15

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



1

**Figure 8: ComPat Slide Template**

Details of the events that members of ComPat participated in during the first 12 months of the project are detailed in section 2.5.

### 2.4.9 Mailing Lists

ComPat mailing lists have been set up to aid communication within the project, these allow communication to everyone in the consortium and to everyone within a particular work package. We will add additional mailing lists as required. Milestone 1 was set to take place in the second month of the project and concerns the construction of and mailing lists (and the website), these were created on schedule. At the time of writing there are 13 mailing lists, these are for the following purposes:

- “All” – for all members of the ComPat consortium
- “WP1” – for work package 1
- “WP2” – for work package 2
- “WP3” – for work package 3
- “WP4” – for work package 4
- “WP5” – for work package 5
- “WP6” – for work package 6
- “WP7” – for work package 7
- “Support” – for hardware and software support
- “PIs” – for the principle investigators of ComPat
- “Maintenance” – for hardware maintenance staff

#### 2.4.10 Media Outreach

Media outreach activity in the first year of ComPat include a TV appearance by Peter Coveney and a set of press releases. See Annex 4.1 for the advert for the US television show "Life's Rocky Start", which aired on PBS NOVA in the USA, featuring Peter Coveney. General press releases were harnessed by ComPat consortium members for results and instances of particular significance, these are listed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Simon Zwart - Chaos in Halley's orbit, <a href="http://www.astronomie.nl/">http://www.astronomie.nl/</a>	30/05/16	30/05/16	[Scientific Community], [General Public]	500
Simon Zwart - verklaring structuur sterrenhopen, <a href="http://www.astronomie.nl/">http://www.astronomie.nl/</a>	19/01/16	19/01/16	[Scientific Community], [General Public]	500
Simon Zwart - Eta Carina explained, <a href="http://www.astronomie.nl/">http://www.astronomie.nl/</a>	25/11/15	25/11/15	[Scientific Community], [General Public]	500
LRZ - Durchbruch für personalisierte Medizin dank SuperMUC (Breakthrough in personalised medicine thanks to SuperMUC), <a href="http://www.badw.de">www.badw.de</a>	15/06/16	15/06/16	[General Public], [Media], [Policy Makers]	500
Peter Coveney featured in a US television show called "Life's Rocky Start". The 50 minute programme aired on Wednesday 13th January at 9pm EST across the USA on PBS NOVA.	13/01/16	13/01/16	[Scientific Community (higher education, Research)] [Industry] [Civil Society] [General Public] [Policy makers] [Medias]	10000

#### 2.4.11 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 the first 12 months of the project are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Peter Coveney has been made the vice chair of a working group on LifeSciences and Health for EXDCI ("European eXtreme Data & Computing Initiative"). The objectives of EXDCI are to coordinate the development and implementation of a common strategy for a European HPC Ecosystem.	08/07/05	08/07/05	[Scientific Community (higher education, Research)] [Industry] [Policy makers]	N/A
Peter Coveney (UCL) and Alfons Hoekstra (UvA) - COST Action CA15120 on Open Multiscale Systems Medicine (OpenMultiMed) started on April 5th 2016, with Peter Coveney and Alfons Hoekstra as participants. The overarching aim OpenMultiMed is to gather a critical mass of international researchers and coordinate them as a team that develops and evaluates a transdisciplinary framework for multiscale systems medicine, consisting of novel concepts, methodologies and technologies.	07/07/05	08/07/05	[Scientific Community (higher education, Research)] [Industry]	N/A
Peter Coveney gave a talk on "Data science and optimal learning for materials discovery and design" in Santa Fe, New Mexico, on 17 May 2016 at a meeting organized by Los Alamos National Laboratory	17/05/16	17/05/16	[Scientific Community (higher education, Research)]	50
Derek Groen - ARCHER Early Career Impact Award	10/11/15	10/11/15	[Scientific Community (higher education, Research)]	N/A
Olivier Hoenen - Answer to a Computing cycle project call (Marconi-EF)	07/07/16	07/07/16	[Scientific Community]	N/A

			(higher education, Research)]	
Jeroen Bedorf - Intro for high school students	14/03/16	14/03/16	[Scientific Community (higher education, Research)], ] [General Public]	30
Simon Zwart - SURF Innovation award to S. Portegies Zwart and S. Sultan	11/11/15	11/11/15	N/A	N/A
Simon Zwart - Organized World Championship Computational diplomacy	07/03/15	07/03/15	[Scientific Community (higher education, Research)]	N/A
Simon Zwart Interview - Software, sterrenhopen en supercomputers, <a href="http://www.universiteitleiden.nl">www.universiteitleiden.nl</a>	07/06/16	07/06/16	[Scientific Community (higher education, Research)]	500
PSNC - Krzysztof Kurowski presented ComPat and QCG to SurfSARA.	08/06/16	08/06/16	[Industry]	10
James Suter attended project kick-off meeting for ARCHER-RAP award (24,791.040 kAU) for a project titled "Predicting the performance properties of graphene-polymer and clay-polymer nanocomposites from multiscale modelling".	10/06/16	10/06/16	[Industry]	6
Allinea - 1. Conversation with other H2020 projects (NEXTGenIO and SAGE). Discussion of overlap with ComPat	21/06/16	21/06/16	[Scientific Community], [Industry]	4
Ulf Schiller - Two Invited Presentations at Center for Nonlinear Studies (Co-Design Lab) of Los Alamos National Laboratory	25/07/16	27/07/16	[Scientific Community (higher education, Research)]	20
Paul Best - Meeting with Head of Sky Performance Hub - use of simulation in high performance sport	15/06/16	15/06/16	[Industry]	2
Paul Best - South Australian Government	28/06/16	28/06/16	[Policy makers]	10

Annual Dinner - London - introduction			[Industry]	
Paul Best - Digital Catapult - London - introduction	04/07/16	04/07/16	[Scientific Community (higher education, Research)] [Industry]	2
Paul Best - Satellite Applications Catapult - Harwell introduction	20/07/16	20/07/16	[Scientific Community (higher education, Research)] [Industry]	3
Paul Best - Visit to Centre For Modelling & Simulation (CFMS) - located in Bristol, CFMS is the premier collaborative research centre in the UK funded by industry for industry, led by Rolls-Royce and Airbus UK) outlining project aims and potential for industry engagement	11/08/16	11/08/16	[Industry]	4 direct, many members

Several ComPat members are involved with a COST Action titled "Open Multiscale Systems Medicine", or "OpenMultiMed". COST Actions are Pan-European networking instruments that allow researchers, engineers or scholars from COST Member Countries and Cooperating State to develop jointly their ideas and new initiatives in a field or topic of common interest. "Open Multiscale Systems Medicine" aims to develop novel multiscale systems medicine concepts, methods and technologies that provide effective, efficient and economical solutions for emerging and future approaches to multiscale systems medicine. It also aims to develop a transdisciplinary multiscale systems medicine framework that integrates systems medicine, multiscale modelling, multiscale data science, and multiscale computing. ComPat will explore collaborative opportunities with with this COST Action. More information on OpenMultiMed can be found [here](#).

## 2.5 Events

ComPat aims to organize and participate in many events throughout the project duration, including conferences, workshops, seminars, training events and more. 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 results and success stories and to provide compelling use cases to interested audiences.

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 (by month 14, targeting ICCS 2016)
- Milestone 9 - ComPat Training Event (by month 20, targeting a partner institution)
- Milestone 15 - ComPat Workshop 2 (by month 30, targeting the Lorentz Centre)

The activity in the first year of the project in this task is detailed in section 2.5.1.

Task 7.5 is concerned with the co-ordination of conference participation, running from months 1 to 36). Many events have been targeted in the first year of the project, these are listed in section 2.5.2.

### 2.5.1 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
Peter Coveney - The Solvay Symposium on "Bridging the Gaps at the PCB Interface" took place on 19-21 April 2016 at the International Solvay Institutes Brussels. The Symposium was centred about the rising multi-modelling paradigm, with special focus on emergent phenomena flourishing at the PCB interface. Peter Coveney was on the Organising and Scientific Committee	19/04/16	21/04/16	[Scientific Community (higher education, Research)] [Industry]	50

Alfons Hoekstra - Overall chair of VPH2016, September 2016, <a href="http://www.vph-conference.org">www.vph-conference.org</a>	26/09/16	28/09/16	[Scientific Community (higher education, Research)] [Industry]	250
Derek Groen – 13 <sup>th</sup> Annual Multiscale Modelling and Simulation Workshop at ICCS 2016	06/06/16	08/06/16	[Scientific Community (higher education, Research)], [Civil Society]	30

#### 2.5.1.1 The 13<sup>th</sup> Annual Multiscale Modelling and Simulation Workshop

In the first year of the project, the first ComPat organised workshop took place. The workshop, titled “The 13<sup>th</sup> Annual Multiscale Modelling and Simulation Workshop”, was part of the International Conference of Computational Science (ICCS), which is a yearly conference alternating between Europe, Asia and the USA. There were 10 speakers in total at the workshop, including 2 ComPat consortium members. The ComPat talks were on the following subjects:

- “FabSim: facilitating computational research through automation on large-scale and distributed e-infrastructures”, Derek Groen, Agastya, James Suter, James Hetherington, Stefan Zasada, Peter Coveney.
- “Coupled lattice Boltzmann and link-flux simulations of electrokinetic transport in porous media”, Ulf Schiller and Peter Coveney.

The workshop was published in the ICCS 2016 conference proceedings:

- “Multiscale Modelling and Simulation, 13th International Workshop Derek Groen”, Valeria Krzhizhanovskaya, Bartosz Bosak, Timothy Scheibe, and Alfons Hoekstra, ICCS 2016. The International Conference on Computational Science, 80 (2016), Pages 1242–1243, doi: 10.1016/j.procs.2016.05.494

Pictures from the event are shown in Annex 4.3.

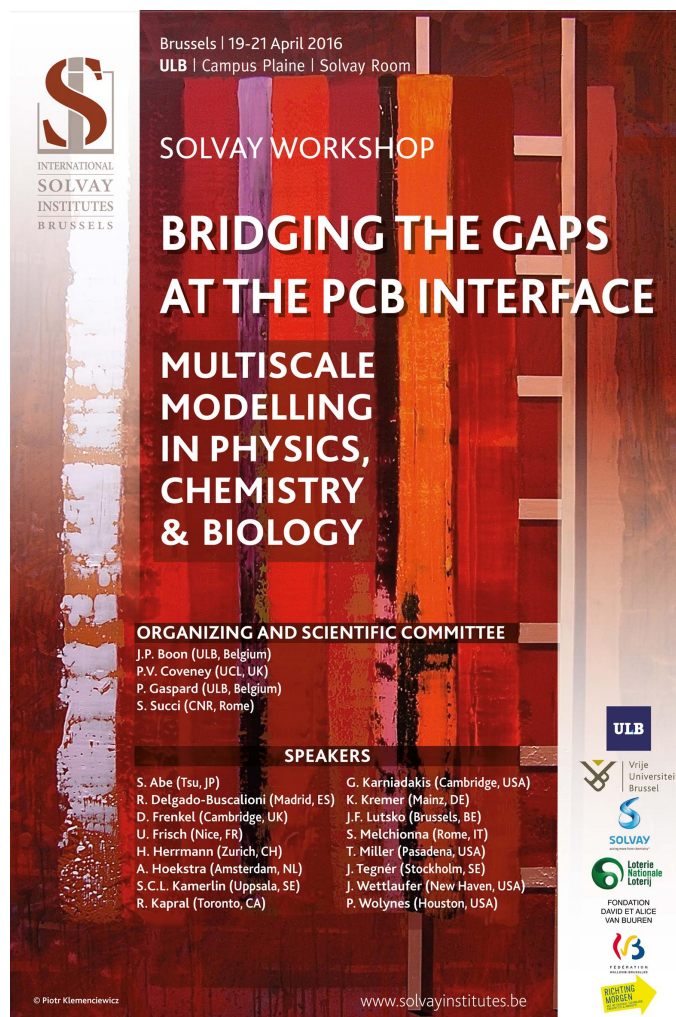
#### 2.5.1.2 Multiscale Modelling at the PCB Interface

The Solvay Institute Symposium on "Multiscale Modelling at the PCB (Physics, Chemistry, Biology) Interface" took place on 19 - 21 April 2016 in Brussels at ULB. ComPat consortium member Peter Coveney was on the organising and scientific committee for the event, and Alfons Hoekstra was a speaker.

The Symposium was centred on the rising multi-modelling paradigm, with special focus on emergent phenomena flourishing at the PCB interface, with the aim of helping to focus on the present state of the art in the field, and to foster and shape up new cooperative research efforts to advance this forefront of modern science.

The Symposium resulted in an accompanying publication under the same title as a Theme Issue of Proceedings of the Royal Society of London (Series A), this is listed in section 2.4.2.

Additionally, there was a poster session on the evening of the second day. Pictures from the event are shown in Annex 4.2 and the flyer for the event is shown below:



**Figure 9: Flyer for the Solvay Symposium.**

### 2.5.1.3 Virtual Physiological Human 2016

Alfons Hoekstra was the chair of the Scientific and Organising committee and overall chair for Virtual Physiological Human Conference 2016 (VPH2016), held in Amsterdam on 26-28 September 2016. Four members of the ComPat consortium gave talks at the event, detailed below:

- Alfons Hoekstra – “Towards the Virtual Artery, a multiscale model for vascular pathophysiology”
- Peter Coveney – “Rapid, Accurate and Reproducible Binding Affinity Calculation for Personalized Medicine and Drug Development”
- Robin Richardson – “Reducing the computational cost of clinical lattice-- Boltzmann simulations through velocity and resolution scaling”
- Stefan Zasada – “Distributed Binding Affinity Calculations for Drug Discovery and Patient Treatment”

The flyer for the event is show below:



virtual physiological human conference

Translating VPH to the Clinic

26-28 September 2016    Amsterdam, the Netherlands    [www.vph-conference.org](http://www.vph-conference.org)

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## INVITATION



The VPH conference series offers a platform to present research related to the Virtual Physiological Human and more broadly into **Computational Systems Biomedicine**, as well as applications in **clinical settings**, underpinning the move towards **predictive personalised medicine**. After the successful conference in Trondheim in 2014, VPH2016 continues to offer an exciting program of state-of-the-art science & engineering in computational (bio)medicine, ranging from foundational research to clinical applications, all contributing to this year's theme: **Translating VPH to the Clinic**.

**You are invited to participate in this event.**

**Abstract submission deadline:** May 15, 2016  
**Early Registration deadline:** July 8, 2016  
**Location:** the monumental Royal Tropical Institute, Amsterdam, The Netherlands

The Virtual Physiological Human will revolutionise the way health knowledge is produced, stored and managed as well as the way in which healthcare is currently delivered.

The Virtual Physiological Human (VPH) initiative strongly contributes to the emerging vision of **Personalised Medicine**. It will have major impacts on future healthcare, and on healthy living and in ageing. Many VPH research results are on the brink of being applied in clinical practice, with already some very spectacular examples in (pre-) clinical trial phases. In the coming years major breakthroughs are expected, opening up **huge opportunities**. Most, if not all, major medical (device) industries are involved in VPH research projects and are taking up results in their businesses. **Public-Private-Partnerships** (e.g. related to *in-silico medicine*) are currently being established, offering even more opportunities to develop new VPH-based services and products.

Each day will start with a **keynote speaker**. Next, the program offers two parallel thematic sessions, dedicated to **Personalised Medicine**, the **Digital Patient**, **Systems Medicine**, and **In-Silico Clinical Trials**. Finally, there will be four daily focused symposia running in parallel, half dedicated to VPH research at large, and the other half concentrating on **medical specialisms**, strongly linked to the theme of the conference. For all details we refer to the website of the conference, where you will also find all information on submitting contributions and registration.

[info@vph-conference.org](mailto:info@vph-conference.org)  
[www.vph-conference.org](http://www.vph-conference.org)

Figure 10: Flyer for VPH2016

## 2.5.2 Participation at Events

The ComPat consortium attended, participated in, and organised numerous events in the first year of the project, these included:

- The 252nd ACS (American Chemical Society) National Meeting, Philadelphia
- The MRS (Materials Research Society) Fall Meeting & Exhibit 2015 in Boston
- European HPC (High Performance Computing) Summit week, Prague (including the EXDCI Workshop 2016, ETP4HPC Extreme-Scale Demonstrators Workshop, and PRACEdays16)
- EASC2016 (Exascale Application & Software Conference), Stockholm
- Toward 100 Anniversary of I.P. Pavlov's Physiological Society Russian Conference with International Participation "Experimental and Computational Biomedicine", Yekaterinburg
- 15th European Conference on the Mathematics of Oil Recovery, Amsterdam
- Solvay Symposium on "Bridging the Gaps at the PCB Interface", Brussels
- ICCS (International Conference on Computational Science) 2016, San Diego (including the 13th International Workshop on Multiscale Modeling and Simulation)
- GTC (GPU Technology Conference) 2016, San Jose
- ISC (International Supercomputing Conference) 2016, Frankfurt
- BioExcel 1st Annual Meeting: "Advanced Simulations for Biomolecular Research" SIG at ECCB (European Conference on Computational Biology) 2016, The Hague
- LRZ Extreme Scaling Workshop, Garching
- Conference of the High Performance Computers' Users - towards Exascale Computing, Poznan
- VPH2016 (Virtual Physiological Human), Amsterdam

Details on the conferences and workshops that ComPat participated in are detailed below.

### 2.5.2.1 Participation at Conferences

In this section, the participation of ComPat at various conferences is listed. In total, ComPat consortium members participated in 11 conferences. These are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Peter Coveney gave a talk on “Rapid, accurate and reproducible binding affinity calculation for drug discovery: A retrospective analysis of the Pfizer Pan-Trk Program” at the 252nd ACS National Meeting, Philadelphia, PA, USA	22/08/16	22/08/16	[Scientific Community (higher education, Research)] [Industry]	300
Peter Coveney gave a talk on “Modelling clay-polymer nanocomposites using a multiscale approach” at the 252nd ACS National Meeting, Philadelphia, PA, USA	22/08/16	22/08/16	[Scientific Community (higher education, Research)] [Industry]	300
Peter Coveney gave a talk at the MRS Fall Meeting & Exhibit 2015 in Boston, United States, on December 3rd 2015. The talk was titled “Towards the Virtual Laboratory: Modelling Clay-Polymer Nanocomposites Using a Multiscale Approach”. Peter spoke about advanced multiscale simulation systems used to predict the properties of polymer-clay nanocomposites based on their molecular structures and composition, (J.L. Suter, D Groen, P.V. Coveney, Adv. Mater. 2015, 27, 966-984)	03/12/16	03/12/16	[Scientific Community (higher education, Research)] [Industry]	300
Peter Coveney attended European HPC Summit week: EXDCI Workshop 2016, Prague	09/05/16	09/05/16	[Scientific Community (higher education, Research)] [Industry]	200
Peter Coveney attended EASC2016, Stockholm	28/04/16	28/04/16	[Scientific Community (higher education, Research)] [Industry]	200

Peter Coveney – Presentation at VPH2016, Amsterdam, titled “Rapid, Accurate and Reproducible Binding Affinity Calculation for Personalized Medicine and Drug Development”	26/09/16	28/09/16	[Scientific Community (higher education, Research)] [Industry]	250
Hugh Martin - Presented a Poster, "ComPat: Computing Patterns for High Performance Multiscale Computing" at PRACEdays16 in Prague	10/05/16	12/05/16	[Scientific Community (higher education, Research)] [Industry]	100
Hugh Martin - Handed out ComPat Flyers at PRACEdays16 in Prague	10/05/16	12/05/16	[Scientific Community (higher education, Research)] [Industry]	10
Alfons Hoekstra (UvA) – Toward 100 Anniversary of I.P. Pavlov’s Physiological Society Russian Conference with International Participation “EXPERIMENTAL AND COMPUTATIONAL BIOMEDICINE”. In memory of Professor Vladimir S. Markhasin; Keynote lecture	10/04/16	12/04/16	[Scientific Community (higher education, Research)] [Industry]	250
Alfons Hoekstra (UvA) - Invited lecture 15th European Conference on the Mathematics of Oil Recovery, September 2016, Amsterdam, The Netherlands, “Fluid Flow Simulations with the Lattice Boltzmann Method - From Flow in Porous Media to Multiscale Modelling of Blood Flow	29/08/16	31/08/16	[Scientific Community (higher education, Research)] [Industry]	300
Alfons Hoekstra gave a talk titled “Towards the Virtual Artery, a multiscale model for vascular pathophysiology” at VPH2016 in Amsterdam	26/09/16	28/09/16	[Scientific Community (higher education, Research)] [Industry]	250

Robin Richardson – Presentation at VPH2016, Amsterdam, titled “Reducing the computational cost of clinical lattice-- Boltzmann simulations through velocity and resolution scaling”	26/09/16	28/09/16	[Scientific Community (higher education, Research)] [Industry]	250
Stefan Zasada – Presentation at VPH2016, Amsterdam, titled “Distributed Binding Affinity Calculations for Drug Discovery and Patient Treatment”	26/09/16	28/09/16	[Scientific Community (higher education, Research)] [Industry]	250
Derek Groen gave a talk at ICCS 2016, San Diego	06/06/16	08/06/16	[Scientific Community (higher education, Research)], [Civil Society]	30
Jeroen Bedorf - GTC 2016, San Jose, USA	04/04/16	08/04/16	[Scientific Community (higher education, Research)] ,[Industry] ,[Medias] ,[Investors]	5000
Jeroen Bedorf - ISC 2016, Frankfurt, Germany	20/06/16	23/06/16	[Scientific Community (higher education, Research)] ,[Industry] ,[Medias] ,[Investors]	2500
Agastya Bhati gave a talk on "Advances in Computational Biomedicine" at the BioExcel 1st Annual Meeting: “Advanced Simulations for Biomolecular Research” SIG at ECCB 2016 in the Netherlands	04/09/16	04/09/16	[Scientific Community (higher education, Research)] [Industry]	50

### 2.5.2.2 Participation at Workshops.

In this section, the participation of ComPat at various conferences is listed. In total, ComPat consortium members participated in 9 workshops. These are detailed in the table below:

Description	Date From	Date To	Audience(s)	Estimated Number of People
Alfons Hoekstra (UvA) - invited lecture Moscow State University, Multiscale Modelling of Blood Flow, Blood Suspensions and Vascular Disease,	08/04/16	08/04/16	[Scientific Community (higher education, Research)]	50
Alfons Hoekstra (UvA) - Invited lecture <i>Children's Center for Hematology</i> , Cell-based computational modelling of blood suspensions and platelet transport, April 8. 2016	08/04/16	08/04/16	[Scientific Community (higher education, Research)]	20
Alfons Hoekstra (UvA) - Invited lecture "Multiscale Modelling in Vascular Disease" at Solvay Symposium on "Bridging the Gaps at the PCB Interface" Multiscale Modelling in Physics, Chemistry & Biology April 19-21, 2016, Brussels, Belgium	19/04/16	20/04/16	[Scientific Community (higher education, Research)]	50
Robin Richardson - LRZ Extreme Scaling Workshop	29/02/16	04/03/16	[Scientific Community (higher education, Research)]	30
Derek Groen - Solvay Symposium	19/04/16	21/04/16	[Scientific Community (higher education, Research)]	50
Robin Richardson - Presentation at Solvay Symposium in Brussels	19/04/16	21/04/16	Scientific Community (Research)	40
Derek Groen - UKCOMES Meeting	17/12/15	17/12/15	[Scientific Community (higher education, Research)]	20

Derek Groen - UKCOMES Meeting	20/06/16	20/06/16	[Scientific Community (higher education, Research)]	20
Derek Groen - QRNF Project Meeting	04/05/16	04/05/16	[Scientific Community (higher education, Research)],[Civil Society]	15
PSNC - Participation to the workshop. ETP4HPC Extreme-Scale Demonstrators Workshop (Tomasz Piontek - presentation about the goals and progress of the ComPat project)	12/05/16	12/05/16	[Scientific Community (higher education, Research)]	70
PSNC - Participation to the workshop. Konferencja Użytkowników KDM - w kierunku obliczeń Exaskalowych (Conference of the High Performance Computers' Users - towards Exascale Computing) PSNC. Tomasz Piontek - presentation: "Usługi i narzędzia QCG dla symulacji wielkoskalowych i obliczeń z wykorzystaniem infrastruktury KDM", "QCG Services and tools for multi-scale computing and simulations using HPC infrastructure"	27/06/16	28/06/16	[Scientific Community (higher education, Research)]	100
James Suter attended The Solvay Symposium on "Bridging the Gaps at the PCB Interface" took place on 19-21 April 2016 at the International Solvay Institutes Brussels. The Symposium was centred about the rising multi-modelling paradigm, with special focus on emergent phenomena flourishing at the PCB interface.	19/04/16	21/04/16	[Scientific Community (higher education, Research)] [Industry]	50

Allinea - 1. Presentation on 'Scalable and Efficient HPC' with Allinea tools at Extreme Scale Workshop at LRZ	01/03/16	01/03/16	[Scientific Community (higher education, research)] [Customers]	30
Allinea - 2. Attendance at Extreme Scale Workshop with UCL partners	01/03/16	04/03/16	[Scientific Community (higher education, research)]	30
Ulf Schiller - Talk at 13th International Workshop on Multiscale Modeling and Simulation	06/06/16	08/06/16	[Scientific Community (higher education, Research)]	25

### 2.5.2.3 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
Saad Allowayed (UvA) - CERI annual review lectures, KACST - Saudi Arabia	21/06/16	21/06/16	[Scientific Community], [General Public]	40
Derek Groen - Keynote lecture at the User Day of the Flemish Supercomputer Centre	01/12/15	01/12/15	[Scientific Community (higher education, Research)], [Industry]	95
Derek Groen - Invited lecture at London School of Economics (statistics department)	01/06/16	01/06/16	[Scientific Community (higher education, Research)]	25
Olivier Hoenen - NMPP Seminar presenting the ComPat Fusion Application	06/09/16	06/09/16	[Scientific Community (higher education, Research)]	10 to 20
Ulf Schiller - Invited Talk at Clemson University Research Symposium	04/05/16	04/05/16	[Scientific Community (higher education, Research)]	40

## 2.6 Proposed Actions for Year 2

Our proposed action in the second year 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)

Deliverables for the second year are as follows:

- D7.3 Second annual Dissemination Report (M24)

Milestones for the second year are as follows:

- Milestone 9 – ComPat training event (M20)

Concerning Tasks 7.2 and 7.3, the website and twitter account will continue to be updated with project activity. In terms of events, we have identified some conferences and workshops where we plan to have a ComPat presence in some form (more will be added during the year):

- 26-28 October 2016, 1st Conference of the European Association of Systems Medicine (EASyM), Berlin
- 14-17 November 2016, Supercomputing (SC16) – Utah
- 10-12 April 2017, “The 5th International Conference on Computational and Mathematical Biomedical Engineering (CMBE17), Pittsburgh, USA
- 17-21 April 2017, Materials Research Society Spring Meeting & Exhibit (2017 MRS) – Phoenix
- 15-19 May 2017, HPC Summit Week 2017 – Barcelona

The second workshop to be organised by ComPat will take place in the second year of the project, around May 2017. It will be organised with the Lorentz Centre and the theme will likely be on High Performance Multiscale Computing Driven by Applications (also multiscale computing patterns). The workshop will have the objective of promoting ComPat 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.

Additionally, Simon Zwart is the scientific organizer for an astronomy workshop at the Lorentz Center on “Formation of the Solar System and the Origin of Life”, it will run from 20 Feb 2017 through 24 Feb 2017.

### **3 Conclusions**

There was a substantial amount of dissemination activity in the first year 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. 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 many stakeholders across the globe. We aim to expand further on this in years 2 and 3 of the project.

We believe that, through our dissemination activities, expected impacts will be accelerated and strengthened. Through the dissemination of ComPat research findings and the evangelisation of its open-source software to academia and industry alike, we will contribute 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 between our scientific community and the encouragement of collaboration activities, in addition to our training agenda, we will accelerate European excellence in mathematics and algorithms in a multi-disciplinary fashion. Also, we believe that through the effective communication of our work to standardisation bodies, we will be able to jointly develop new standards where they do not exist.

## 4 Annexes

### 4.1 Life's Rocky Start on PBS



Figure 11: Advert for Life's Rocky Start on PBS.

### 4.2 Solvay Symposium



Figure 12: Solvay Symposium Image 1.



**Figure 13: Solvay Symposium Image 2.**



**Figure 14: Solvay Symposium Image 3.**

4.3 Multiscale Workshop at ICCS 2016

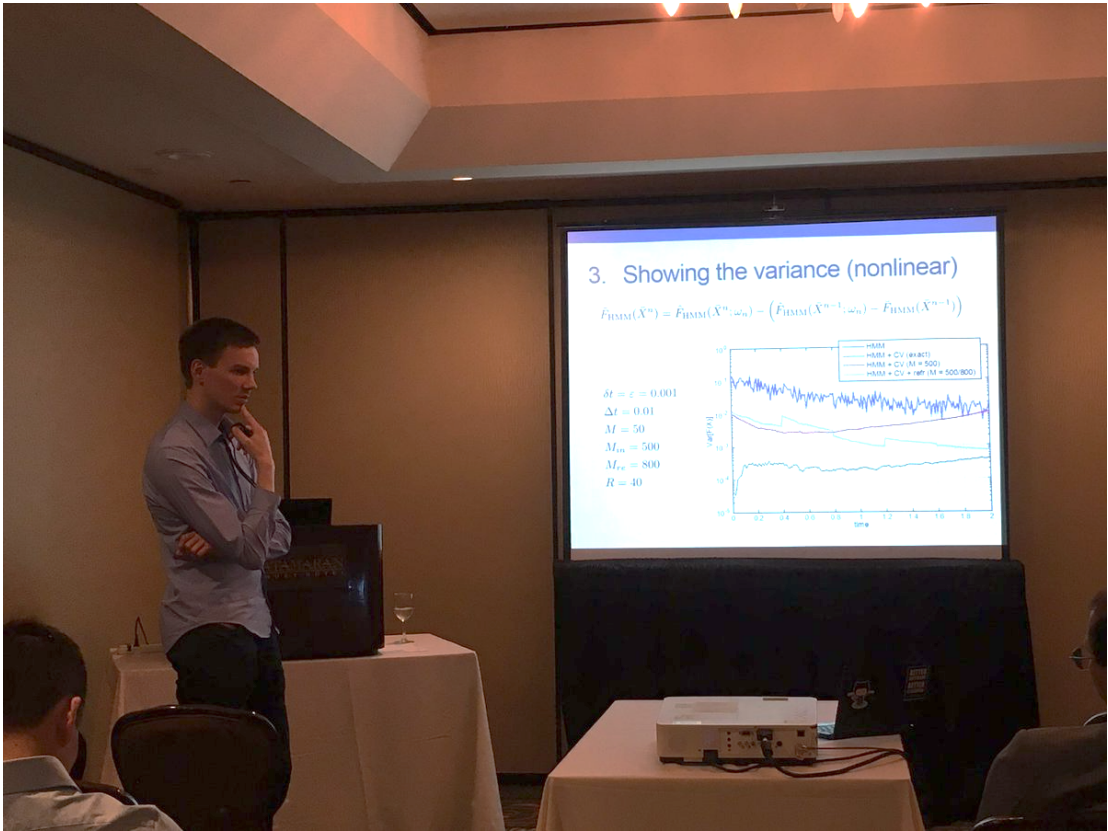


Figure 15: Multiscale Workshop Image 1.

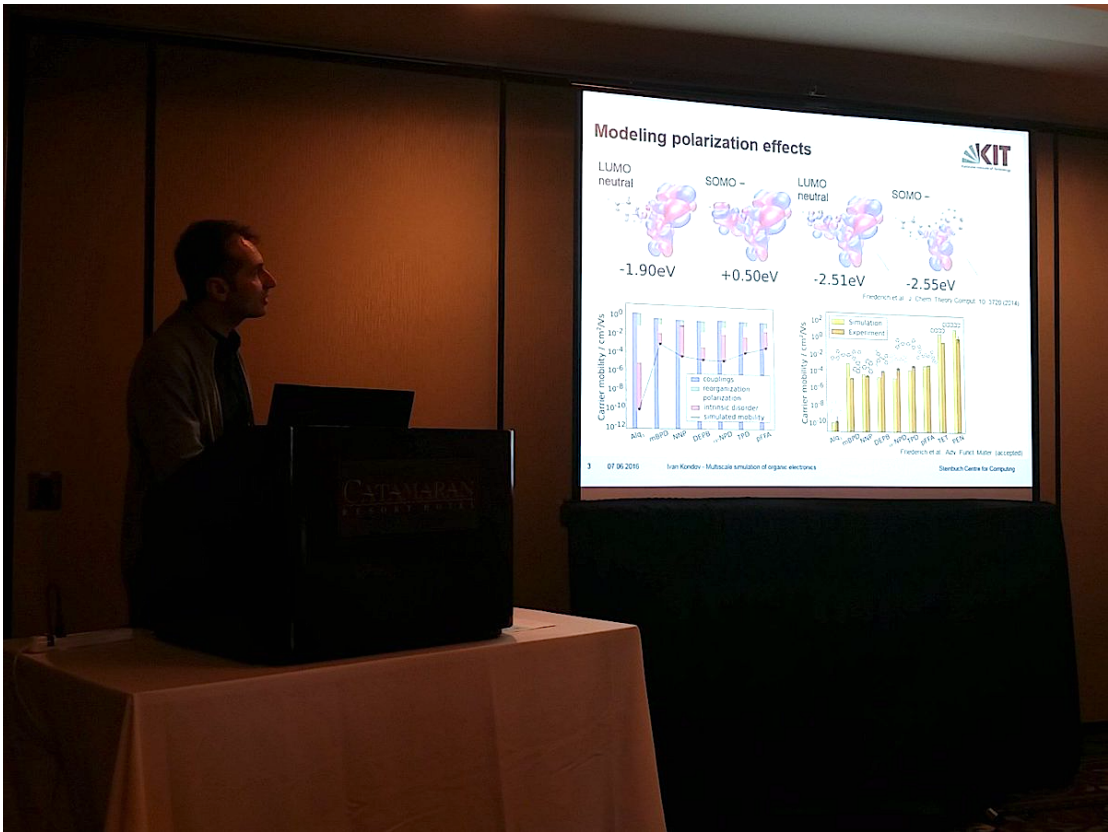


Figure 16: Multiscale Workshop Image 2.

4.4 PRACEdays16



Figure 17: PRACEdays16 Image 1.

4.5 New Scientist Article



Figure 18: First 2 pages of Simon Zwart's New Scientist Article.

## 4.6 Leidsch Dagblad Article

WOENSDAG 10 FEBRUARI 2016

**Getal van de week**

# 1,1

**miljoen euro**

Het LUMC en het Nederlands Kanker Instituut hebben samen twee subsidies van het KWF ontvangen. De ruim 11 miljoen euro wordt gebruikt voor onderzoeken naar de genetische component van kanker.

**Verschoorlezing Sunny Bergman**

**Leiden** Documentairemaker en schrijver Sunny Bergman houdt op 8 maart de Annie Romein-Verschoorlezing. Ze zal ingaan op de vraag of mannen en vrouwen van nature verschillend zijn, of dat opvoeding hen verschillend maakt. De lezing wordt jaarlijks rond Internationale Vrouwendag gehouden. Aanvang 20.00 uur, Academiegebouw. Toegang gratis.

**Physicaprijs voor Leidse hoogleraar**

**Leiden** Michel Orrit krijgt de Physicaprijs 2016. Deze prijs wordt toegekend aan een natuurkundige die in Nederland werkt. De Leidse hoogleraar wordt gelauwerd voor zijn werk op het gebied van één-molecul-spectroscopie. In 1990 was hij de eerste die het fluorescentiesignaal van een enkel molecuul waarnam. Zijn inzicht leidde tot een nieuw valgebied.

**Regionaal 11**

**Leidse wetenschap**

## Waarom zoeken naar planeet negen?

**Iris Nijman**

**Leiden** Planeet negen; in de afgelopen weken kon niemand er omheen. Sterrenkundigen van het California Institute of Technology (Caltech) publiceerden in januari een artikel waarin zij zeggen sterk bewijs te hebben voor het bestaan van deze planeet. Besluit planeet negen echt?

Sterrenkundigen Simon Portegies Zwart en Lucie Jilkova van de Universiteit Leiden zijn sceptisch, maar blij met de opgelaste interesse in het onderzoek naar het onbekende, buitenste gedeelte van ons zonnestelsel. Jilkova: „Sterrenkundigen kijken met telescopen naar objecten in het heelal die miljarden lichtjaren ver weg staan, maar we weten eigenlijk bijna niets over onze eigen huiskamer: ons zonnestelsel.”

**Planeet X**

Het idee van een extra planeet in ons zonnestelsel, planeet X, is niet nieuw. Laat bestaan werd al vermoed na de ontdekking van Neptunus in 1846. Pluto mocht een tijdlang de naam van planeet negen dragen, maar moest deze in 2006 afstaan nadat er grotere ijzachtige objecten werden gevonden. Deze dwergplaneten bevinden zich voornamelijk in een ring voorbij Pluto: de Kuiper gordel. Sinds meer objecten werden in en voorbij de Kuiper gordel gevonden, zelfs tot aan de Oortwolk, die ons zonnestelsel omringt met ijsachtige kometen.

De reden dat sterrenkundigen omkruis nadenken over het bestaan van een negende planeet, is het vreemde gedrag van objecten die zich tussen de Kuiper gordel en de Oortwolk bevinden. Deze objecten bewegen in banen die moeilijk te verklaren zijn zonder de invloed van een extra planeet. Een van die objecten is dwergplaneet Sedna, ontdekt in 2004. Sedna trok de aandacht van Portegies Zwart en Jilkova omdat ze in een soortgelijke baan beweegt als een andere dwergplaneet. „Dat is gek, want bijvoorbeeld de banen van Aarde en Jupiter zijn heel anders”, zegt Portegies Zwart. Vorig jaar ontdekten hij en Jilkova dat Sedna vroeg tijdens het ontstaan van ons zonnestelsel waarschijnlijk van een andere ster moet zijn gekomen. „Tijdens het ontstaan van het zonnestelsel bevond onze zon zich in een groep met andere sterren”, legt Portegies Zwart uit. „De sterren hebben mogelijk objecten uitgewisseld toen ze langs elkaar heen scheerden.”

Maar dat alleen zou niet de gekke banen van deze objecten verklaren; er is nog iets vreemds aan de hand. „Waarom blijven deze objecten zo netjes in hun baan?”, vraagt Portegies Zwart zich af. „We zouden verwachten dat de dwergplaneten steeds een snijk verschuiven door de aantrekkingskracht van Neptunus, maar dat doen ze niet. Daarom hebben wij ook al aan een negende planeet gedacht, die ze in balans houdt.”

**Chaos**

Portegies Zwart vindt de theorie van de negende planeet best plausibel, maar het biedt volgens hem en Jilkova niet een magische verklaring voor alles. Helas kunnen we de planeet in de komende jaren nog niet waarnemen. Het object is te ver weg, te klein en te zwak. Bovendien weten sterrenkundigen niet waar ze moeten zoeken. Het meest belangrijk vinden Portegies Zwart en Jilkova dat er nu weer meer belangstelling komt voor ons eigen zonnestelsel. Portegies Zwart: „Onderzoek binnen ons zonnestelsel was nooit zo spectaculair omdat iedereen dacht dat ons zonnestelsel netjes is ontstaan. Dit is verre van waar. Waarschijnlijk was de geboorte van ons zonnestelsel een heel chaotische gebeurtenis, met veel ontmoetingen met andere sterren.” Op dit moment proberen Portegies Zwart en Jilkova het ontstaan van het zonnestelsel te simuleren met de milieuvriendelijke computer in Japan. De eerste filmpjes verwachten ze eind 2016.

**or teleurstelling zorgen**

## Altijd al pragmatisch

is een belangrijker thema geworden. Al veel langer waren niet alle Nederlandse politieke spelers daar even positief over, merkt Vollaard op. Ook vandaag de dag blijven meningen verdeeld. De PVV en in mindere mate SP zijn de politieke tegenstanders van de huidige koers van Europese integratie en vooral de PVV weet vaak de aandacht te trekken. Vollaard: „Maar Nederland is meer dan Wilders alleen. De achterban van D66 denkt anders over Europese integratie dan die van de PVV en SP.”

**Referendum**

De meeste Nederlandse politici en kiezers houden vast aan de pragmatische houding en geven geen gehoor aan een roep om de EU te verlaten. „We zien dat het moeizaam loopt, maar voor veel mensen is er geen beter alternatief”, verklaart Vollaard. Toch verwacht Vollaard weinig toezichtelijkheid van de Nederlandse kiezer tijdens het aankomende referendum. „De voorstanders in het debat hebben het moeilijk want zij moeten betogen dat de economische samenwerking met een corrupt land als Oekraïne voordeliger oplevert voor Nederland.”

Hoewel het referendum kiezers de mogelijkheid biedt om zich uit te spreken over een Europese kwestie, denkt Vollaard dat het vooral teleurstelling gaat veroorzaken. „Ook al stemmen kiezers tegen, er zijn veel EU-landen die al voor het verdrag hebben gestemd. Dan wordt het lastig om met een Nederlandse neo-stem rekening te houden”, legt hij uit.

Zonder Nederlandse goedkeuring treedt het verdrag formeel niet in werking, maar gezien de huidige verhoudingen zullen er maar weinig aanpassingen voor Nederland worden gemaakt. Vollaard: „Ik denk dat de regeringsleiders zich meer afvragen of zij als burgers nog invloed kunnen uitoefenen op Europese besluitvorming.”

De bundel Van Aanval! Naar verdedigen? wordt donderdag gepresenteerd op de Campus Den Haag van de Universiteit Leiden. Voor meer informatie: <http://www.montesquieu-instituut.nl/>

**Een impressie van hoe planeet negen eruit zou kunnen zien. Illustratie Caltech**



Figure 19: First page of Leidsch Dagblad article “Waarom Zoeken Naar Planeet Negen”

## 4.7 Sky &amp; Telescope Magazine



Figure 20: First 2 pages of "What Caused The Great Eruption?".

## 4.8 NRC Article

O&DIO Wetenschap

# Het nieuwe, ruige zonnestelsel

**Astronomie** Het zonnestelsel begon veel wilder en dramatischer dan gedacht. Planeten schoven, gesteente werd heen en weer gekatapulteerd. En een naburige ster kapte ons stelsel af.

Zon Mercurius Venus Aarde Mars

0 AU 1 AU

**Waarom is Mars zo'n kleine planeet?**

Het in 2000 ontwikkelde Nice-model kan de roerige geschiedenis van het zonnestelsel in vijf lijnen simuleren. Maar het kan een aantal dingen niet verklaren. Bijvoorbeeld waarom de gasreuzen niet dichtbij de zon staan. De typische afstand is 1 of 2 Astronomische Eenheden (AE). Alessandro Morbidelli, medebedenker van het Nice-model, doet nu zijn modellen, en uit waarnemingen aan exoplaneten.

In 2011 kwamen Morbidelli en collega's met een mogelijke oplossing. Wanneer Jupiter en Saturnus vroeg in de geschiedenis van het zonnestelsel met elkaar in resonantie raakten, stuwden ze met hun magnetische velden Jupiter en Saturnus daarna om en bewogen vervolgens naar hun huidige posities - het zogeheten Grand Tack-scenario (vernoemd naar de Engelse leen voor de koerswijziging van een zeeschip).

Dit Grand Tack-scenario heeft ook meteen een oplossing voor een ander probleem: waarom Mars zo klein is in vergelijking met de aarde. In 2009 kwam astronoom Brad Hansen al met een voorstel hierover. Hij liet een simulatie zien dat Mars klein bleef wanneer er geen planetoiden waren op een afstand groter dan 1,5 tot 2 AE, zegt hij. Op die manier werden zij het gebied waar Mars ontstond schoon.

Er bleef genoeg materiaal over voor de huidige planeten Jovianen, en de migratie van de planeten zorgde ervoor dat planetoiden mengden, iets dat we vandaag terugzien in de Kuiper gordel.

Morbidelli sloeg daarop aan het rekenen. "Ik ging simulaties draaien waar de reusplaneten van Jupiter en Saturnus sloopten op ongeveer 1,5 tot 2 AE", zegt hij. "Op die manier werden zij het gebied waar Mars ontstond schoon."

Maar het Nice-model zet wel het klassieke beeld van het zonnestelsel, dat planeten statische dingen zijn, op zijn kop.

Als astronomen het zeggen: op een afstand van 40 Astronomische Eenheden (AE). Al in 2009 publiceerde Portegies Zwart in het vakblad *The Astronomical Journal* zijn oplossing. "Ik denk dat een ander planetenstelsel het zonnestelsel op 40 AE heeft afgelapt", zegt hij.

Als Portegies Zwart gelijk heeft, maakte een jonge ster met bijbehorende planeten in het verleden alle materie in de buitenste delen van het zonnestelsel weg. Dat proces vond plaats vóórdat de Oortwolk, de huidige verste uiterwaarde van het zonnestelsel, ontstond. Portegies Zwart: "Dit is de laatste fase van het zonnestelsel misschien zo'n 100 AE groot."

Dit akkoord blijft noodzakelijk wanneer je met een simulatie het huidige zonnestelsel wilt reproduceren. Dat blijkt uit het werk van astronoom Alessandro Morbidelli, verbonden aan het Observatoire de la Côte d'Azur en medebedenker van het zogeheten Nice-model. Dat model is vernoemd naar de stad waar Morbidelli's instituut huist, werd in 2005 gepubliceerd in *Nature*. Het geldt onder astronomen tegenwoordig als de breedst geaccepteerde theorie over onze lokale kosmische geschiedenis. "Het model werkt alleen als het zonnestelsel wordt afgelapt", zegt Morbidelli. Als de grens verder ligt, zou het er dankzij de zwaartekracht van de planeten anders uitzien. "De planeten zouden bijvoorbeeld verder uit elkaar liggen", zegt hij.

**Afkapping**

Een botsing met een ander planetenstelsel bleef volgens Morbidelli een goede verklaring voor de afkapping. "Maar het is ook denkbaar dat een heftigere botsing de buitenste delen van het zonnestelsel letterlijk verdampte."

Maar het Nice-model zet wel het klassieke beeld van het zonnestelsel, dat planeten statische dingen zijn, op zijn kop.

Door George van Hal

**V**eel duidelijker kan astronoom Simon Portegies Zwart van de Universiteit Leiden niet worden. Van de ideeën die in de school boeken staan, moeten we zo snel mogelijk af", zegt hij.

Hij doelt op de geschiedenis van het zonnestelsel. Die is namelijk veel rooier dan in de boeken staat, zoveel is de afgelopen jaren wel duidelijk geworden. Het statische beeld, dat de planeten zijn ontstaan waar ze nu staan, klopt niet.

In die schoolboeken staat het nu ongeveer zo: In een uitloopt van de Melweg zweefde 4,6 miljard jaar geleden een onbezield gaswolk. Op één plek was de dichtheid van waterstof, helium en kosmisch stof net iets hoger dan in de gebieden eromheen. Daar trok de gaswolk, onder invloed van de zwaartekracht, samen en viel ineen. Met een flits ontstond de zon. Erontstond een protoplanet. Daaruit vormden zich de planeten. Dichtbij de ster was het bloedheet, zodat water en ijs verdampen en rotsachtige planeten zoals de aarde ontstonden. Verderop was het kouder en ontstonden kille reuzen van gas en ijs: Jupiter, Saturnus, Uranus en Neptunus. Elke planeet ontstond kortop op zijn huidige locatie.

Maar zo is het dus niet. Kijk alleen maar eens naar de maan. Zijn pokdalige oppervlak suggereert dat hij ooit flink onder vuur is genomen door rondvliegend kosmisch gesteente. Maar dat valt in een stabiel zonnestelsel moeilijk voor te stellen. Of denk aan de groeiende verzameling (middelen ruim 3.500) exoplaneten die astronomen de afgelopen decennia buiten het zonnestelsel hebben ontdekt. Deze week nog werd bekend dat een planeet is ontdekt bij Proxima Centauri, de dichtstbijzijnde ster. Exoplaneten staan vaak in een totaal andere rangschikking om hun ster - dus niet zoals bij ons, vanaf de zon gezien, eerst rotsplaneten, dan ruimtegruis, gasplaneten en weer ruimtegruis. Hoe kan dat zo afwijken?

Portegies Zwart realiseerde zich een jaar of acht geleden dat niemand rekening hield met het feit dat een ster als de zon vrijwel nooit alleen ontstaat. De gaswolk die dienst deed als onze kosmische broedkammer barste vermoedelijk ook andere sterren, als het ware de broers en zussen van de zon. De onderlinge zwaartekracht hield hen gedurende de eerste tien miljoen jaar van hun leven allemaal dicht bij elkaar, waarna ze naar hun huidige locaties schoven. Wie het huidige zonnestelsel wil begrijpen, moet volgens Portegies Zwart met die andere sterren rekening houden.

**Ruimterotsen en dwergplaneten**

In dat huidige zonnestelsel zweven vlakbij de zon de aarde, en andere rotsachtige planeten. Daarnaast zit een gordel vol ruimtegesteente, de zogeheten planetoidengordel. In het buitenste deel van het zonnestelsel vinden we eerst de gasreuzen, met grofweg in de baan van Jupiter nog een tweede koudde kosmisch gruis: de trojansen. Achter Neptunus, vanaf de zon tweemaal de afstand van de aarde tot de zon, treffen we de Kuiper gordel, vol met ruimterotsen en dwergplaneten zoals Pluto. Dan volgt een hele tijd slechts een sporadisch stuk gesteente of verdwaalde dwergplaneet totdat op zo'n tienduizendmaal de afstand van de aarde tot de zon een bolvormige schil van ruimterots opduikt: de Oortwolk.

Toen Portegies Zwart rekening ging houden met de broertjes en zusjes van de zon, kon hij een deel van die complexe toestand direct verklaren - het feit dat de Kuiper gordel eindigt op zo'n veertigmaal de afstand van de aarde tot de zon. Of zo-

Figure 21: First page of "Het Nieuwe, Ruige Zonnestelsel".