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1 Version Log

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V0.1	31/01/2017	Marc Boonstra (UvA)	First Draft
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3 Definition and Acronyms

Acronyms	Definitions
CoE	Centre of Excellence
DBMS	DataBase Management System
DoA	Description of Action
GPU	Graphics Processing Unit
HPC	High Performance Computing
MOOC	Massive Open Online Course
PRACE	Partnership for Advanced Computing in Europe
SSC	Student Selected Component
TP	Training Plan
VPH	The Virtual Physiological Human

4 Executive Summary

We conceive the Centre of Excellence to be a hub for training in Computational Biomedicine, with emphasis on high performance computing in the context of the three specific research areas of CompBioMed: cardiovascular, molecularly-based and neuro-musculoskeletal medicine. The CompBioMed Training Plan should:

- bridge High Performance and Cloud Computing communities to biomedical communities
- offer a roadmap to access to High Performance and Cloud Computing for Biomedicine
- assess High Performance and Cloud Computing code useful for Biomedicine and find exemplars for training
- reduce the complexity of Computational Biomedicine for novices
- cater for diverse user bases including trainers (and train the trainers)

During the first six months of the project we have translated our vision and ambition into a training plan, to be executed in the remainder of the project. We have identified our target audience and the consortium who will be offering the training - both within CompBioMed and in collaboration with partner Centres of Excellence like BioExcel. We have extensively mapped out currently available training programs at partner institutes and analysed opportunities to tailor these specifically towards training in Computational Biomedicine. The CompBioMed training overview table is presented in Annex 1.

The ComBioMed training plan proposes:

- Two major training events in / around M24 and M30 (see section 8.2.1)
- Bi-monthly webinars (see section 8.2.2)
- University Courses (Y1, 2, 6) for medical students at UCL, the MSc in Computational Medicine at the University of Sheffield and academic partner courses modelled on each of these exemplars over the lifetime of the project (see section 8.2.3)
- At least one joint workshop with other Centres of Excellence (the first of these will take place in M8; see section 8.2.4)

The implementation of the training plan will be carried out in Task 3.5 “Training Coordination, Development, and Delivery”.

The training plan will be tuned appropriately in accordance with user and trainer feedback following each of the training events that takes place.

5 Introduction

An important pillar of the ComBioMed project is training. Our goals are ambitious. We intend to train a diverse set of stakeholders (from computational scientists to medical students) on a wide range of topics (from high performance computing to the basics of modelling and the simulation of biomedical systems). During the first six months of the project we have translated our vision and ambition into a training plan to be executed during the remainder of the project. This deliverable D3.3 describes in some detail the training plan for CompBioMed. We have aligned this vision with the plans as formulated in the Description of the Action, and with current priorities, opportunities and available resources, resulting in a training plan with

clearly formulated activities, including deadlines. We consider this training plan as a ‘living document’ that we intend to update regularly (on a yearly basis).

5.1 Task

CompBioMed significantly invests in dissemination and training. The commitments made towards the CompBioMed CoE are the focus of this Training Plan and it is our task to set this up in a thorough and sustainable manner.

The Training Plan consists of:

1. An outline of the curriculum for the training events that we have in mind;
2. A plan for how to turn existing material into tailored material for CompBioMed; and,
3. A plan for how to curate and sustain training material as it is produced by the consortium. We will align activities in WP3 with the plans set out in WP4 (Innovation and Sustainability) to create a sustainable training program that will have relevance, value and utility after the project’s end.

As such, the training plan identifies:

- Individuals and groups with the requisite experience to deliver training,
- Partner organisations at international and national levels (such as HPC centres) to collaborate with in the delivery of training,
- Specific user communities and the training they require.

5.2 Approach

Developing the Training Plan was initiated by UvA with project partners UCL, UPF, UEDIN, BSC and SARA and further elaborated upon by all consortium members.

We tested our proposed ideas and investigated possible approaches to the Training Plan to then converge towards the concept of a training offer that is rooted in and feeds back into the Centre of Excellence.

Using the six-W method we touched upon:

[WHY]

- The aims and goals of what the CoE should be and how the training plan will be an intrinsic part of this.

[WHO]

- Identifying at whom we direct the training plan and what will motivate them to pursue CompBioMed training. Likewise, we defined our expertise and motivation to offer training programs. Finally, we identified other CoEs, for example the Centre of Excellence for Computational Biomolecular Research (<http://bioexcel.eu>), with whom we could potentially team up in delivering training activities.

[WHAT]

- What training modules are on offer by consortium members already and how we can make these relevant for the CompBioMed Training Programme. This involved an analysis of what approach to take, e.g.
 - o application driven,
 - o infrastructure driven,
 - o (computational science) educational driven,
 - o skills driven, et cetera.

- Which dimensions the Training Plan should address, such as:
 - o user community (academia, clinic, industry),
 - o focus (cardiovascular, molecularly-based and neuro- musculoskeletal medicine),
 - o High Performance Computing (HPC) – savviness (novice, aware, expert),
 - o topic for training (modelling + simulation, visualisation, workflows, et cetera).

We found that we could best apprehend these dimensions when translated into an overview table that we present below.

[HOW]

- Which approach and what form of knowledge transfer (classroom, MOOC [Massive Open Online Course], webinar, other) will best satisfy the training needs our user communities. This we have also included in the overview table.

[WHEN and WHERE]

- What events or other occasions do we best connect to and with which programmes.

We invited all CoE members to comment our approach and to add to the inventory of training programs and materials in the overview table. From there, further discussion has shaped this first version of the Training Plan.

The present ComBioMed Training Plan is a living document, since the Centre of Excellence will evolve within (and after) the lifetime of this three-year project. The subsequent periodic CompBioMed project reports (October 2017, 2018 and 2019) will contain updates to the current plan.

5.3 Document

The setup of this current CompBioMed Training Plan is as follows:

- **Vision** (Section 6). How we position the Centre of Excellence as a hub for training in Computational Biomedicine with a link to HPC. Who are its trainees and who are the trainers?
- **Dimensions** (Section 7). We propose a Training overview table to define the different aspects underpinning the training programs (user communities, levels, topics, training forms).
- **CompBioMed Training Plan** (Section 8). Current training modules from project partners are presented in table form to enable a gap analysis. We then enfold the training offer for development and delivery in T3.5.
- **Implementation** (Chapter 9). Describes the Training Portal, the Online Repository and training timeline.
- **Sustainability** (Chapter 10). Training materials and outputs will be sustained beyond the project lifetime of the CoE.

6 Vision

We conceive the Centre of Excellence to be a hub for training in Computational Biomedicine, with emphasis on high performance computing in the context of the three specific research areas of CompBioMed: cardiovascular, molecularly-based and neuro-musculoskeletal medicine. The CompBioMed Training Plan should :

- bridge High Performance and Cloud Computing communities to biomedical communities
- offer a roadmap to access to High Performance and Cloud Computing for Biomedicine
- assess High Performance and Cloud Computing code useful for Biomedicine and find exemplars for training
- reduce the complexity of Computational Biomedicine for novices
- cater for diverse user bases including trainers (and train the trainers)

Below we seek to characterize the main factors in any transfer of knowledge: the trainees and the trainers.

6.1 Target Audience

The Centre of Excellence is to train future generations of scientists within the field of Computational Biomedicine by running training courses as well as training medical practitioners in the basic medical and clinical contexts of HPC simulation. We aim at the user groups that lie at the heart of CompBioMed: academic and industrial researchers, and clinical users.

6.2 Trainers

CompBioMed is a unique and extended collection of partners and associate partners throughout Europe that together offer vast knowledge on Computational Biomedicine and advanced computing. In our training activities, we will leverage as much as possible this knowledge and capabilities, as well as more importantly, the associated human resources. Most staff at partners of CompBioMed are not only expert in Computational Biomedicine and/or advanced computing, many of them are also experienced teachers at the graduate and post-graduate levels. In what follows, we briefly describe the relevant expertise of each CompBioMed partner in relation to the training activities we propose for CompBioMed.

UCL

University College London has experience in training users from a diversity of backgrounds (academic, industrial and clinical researchers, postgraduate and postdoctoral researchers, undergraduate and medical students). Training is provided in the application of computational approaches to address questions of biological and medical relevance.

UvA

Universiteit van Amsterdam has experience in academic teaching the broad field of Computational Science, including advanced computing, on the graduate and postgraduate level.

UPF

UPF has experience in teaching applications of molecular dynamics simulations in drug-discovery. UPF also teaches postgraduate students from different backgrounds for the master of bioinformatics at UPF on the subject of molecular simulations in general.

EPCC

EPCC has extensive experience providing training on a variety of HPC and data topics. Their experience ranges from postgraduate training (taught MSc) to a range of academic courses open to students and academics across Europe. Topics range from introductory courses on using HPC facilities, software engineering and data carpentry, to advanced courses in parallel programming techniques (e.g., Advanced parallel programming methods using MPI, hybrid coding and novel HPC architectures).

BSC

BSC has experience in training on computational mechanics and parallelization through its own research projects. In biomechanics, for example, the relevant project is the "Alya Red Cardiac Computational Model", which is a paradigmatic example of HPC-based simulation at the organ level.

SARA

SURFsara has experience in training users who are not familiar with the HPC concepts and/or HPC systems and would like to use it for their research. The topics of the trainings range from Unix, cluster and supercomputing, scientific data management to data-intensive applications with Spark & Hadoop, deep learning/machine learning with GPUs and visualization.

UOXF

The University of Oxford is a stimulating organisation, which enjoys an international reputation as a world-class centre of excellence in research and teaching. The Computational Cardiovascular Science (CCS) group has a Strong commitment to training postdocs and graduate students in an interdisciplinary, dynamic and flexible research environment to help them acquire the necessary skills for future jobs in academia, industry or government.

UNIGE

The Computer Science Department at the University of Geneva is a multidisciplinary oriented research team. Through research and education activities, it promotes a conceptual and theoretical approach, together with a commitment to real life applications. The Scientific and Parallel Computing Group is a research-lab member of the Computer Science Department and can offer to CompBioMed training on modeling methods "Modeling and simulation of natural phenomena" (MOOC and workshop), Advanced Computing: Introduction to HPC (yearly 3-day seminar) and Application code: tutorial on Palabos.

USFD

The University of Sheffield has a formidable record in computational life sciences research. With the recently established Insigneo Institute for in-silico Research – a joint venture between the faculties of Medicine and Engineering together with Sheffield's very large NHS Hospital Trust – it is Europe's largest single facility dedicated to the investigation of computational healthcare, and now provides unified access to all aspects of simulation-based medical research. With expertise across medical science, the Institute focuses particularly on orthopaedic, cardiovascular, oncological and neurological research, with an increasing role in

genetics and its associated large-volume data-processing. USFD can offer modelling and *in silico* medicine university courses to the CompBioMed Training Program.

7 Dimensions

To move from our initially proposed ideas and our six-W-method exercise towards the formulation of our Training Plan it was necessary to indicate the aspects underpinning its design. We laid out two dimensions in a basic table, horizontally listing the target groups, including their expert level, and listing the topics vertically (see Figure 1). The matrix entries are colour coded according to existing and/or future training formats. As seen in Figure 1, as an example, Topic a is training directed towards novice clinical users (e.g. medical students), Topic b is training directed at semi-expert academic users; this method of illustrating the users for whom training is being delivered is used in Annex 1, which summarises the existing training programmes of the CompBioMed partners.

Topics	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Topic a	√								
Topic b					√				
Topic c									√
et cetera			√						

Legend:

Face2Face
Webinar
MOOC
Online self-drive

Figure 1: layout of overview table.

7.1 User Community

The user communities (the trainees) are defined above (6.1).

7.2 Level

The Training Program addresses two pyramids of expertise simultaneously: one assessing the level of complexity and background in Biomedicine and one in computational science and high performance computing. Each ranges from novice (BSc / MSc / medical student) level to PhD (semi) to expert level.

7.3 Topics

We identified the following topics to be of specific interest both to Computational Biomedicine *and* within the realm of the consortium partners that will deliver the training programs. The list is not meant to be exhaustive and will be updated as the CoE evolves.

Advanced (HPC, GPU) Computing

High-performance computing (HPC) is a fundamental technology used in solving scientific problems. Concepts covered in HPC and GPU training include:

- the motivation for the use of parallel supercomputers in computational science
- the main models of parallel programming and parallelisation methods for standard problems
- Using MPI for scientific computing:
- Introductory: point-to-point communication, non-blocking operations, derived datatypes, virtual topologies, collective communication and general design issues.
- Advanced: communicator management, non-blocking and neighbourhood collectives, MPI-IO, single-sided MPI and the new MPI memory model
- Threaded programming:
- Introductory: fundamental concepts of threaded programming, the shared variables model, syntax and semantics of OpenMP and how it can be used to parallelise real programs
- Advanced: nested parallelism, OpenMP tasks, the OpenMP memory model, performance tuning, hybrid OpenMP + MPI, OpenMP implementations, and upcoming features in OpenMP 4.0
- How to effectively use GPUs: advantages of GPUs, using ‘accelerators’ in conjunction with CPUs, and how to get good performance.

All HPC and GPU training will provide practical experience, information on performance and the future of HPC. These courses will provide a background to appreciate the relevance of HPC in the CompBioMed field and equip attendees with the tools to start making effective use of HPC facilities. We are aware that such training is offered by many centres, as well as by PRACE (Partnership for Advanced Computing in Europe). We intend, however, to put this training in the context of Biomedicine, by working with example problems that are of interest to our community.

Using the command line for scientific programming

Using cloud based and HPC resources for scientific simulation often requires using Linux, Unix and the command line. This topic covers the basic concepts of using Linux or Unix, executing programs via the command line, file input and output, using useful Unix concepts such as awk and sed and scripting for processing data.

Modelling and simulation

The main concepts behind a simulation code, from the biomedical system and its mathematical description to the algorithms of discretization are covered within this heading. This is very broad and we intend to select specific topics based on our applications portfolio.

Application codes

Biomedical research presents a very challenging modelling and simulation scenario. Multiscale, multidisciplinary, great variability, large uncertainties, numerical issues, validation difficulties and complex mathematical models are the common features of Computational Biomedicine codes.

Large scale data processing

The increasing availability and the growing rate of biomedical information (i.e. genomics, clinical health, patient records) have resulted in the generation of large data sets of increasing volume and complexity, which are often very difficult to process with 'standard' HPC or DBMS (database management system) technology. Currently large-scale data processing is

particularly popular in the field of Biomedicine. Open-source frameworks such as Apache Spark and Hadoop have been developed with this challenge in mind and can be of great benefit for data-intensive computing.

Cloud Computing

Computational Biomedicine is characterised by a growing need for computational resources in term of power, ease of use of resources and flexibility of access, cybersecurity, and availability of resources. Cloud computing offers a solution to these requirements and may provide additional advantages such as cost saving, on demand access, and elasticity.

Data Management

Better and more effective approaches to managing digital research data are becoming increasingly important in computational science and beyond. The scientific datasets that underpin research papers can now occupy many gigabytes of storage, and are increasingly complex and challenging to work with. Topics covered will introduce the ideas, methods and techniques of modern, digital research data management.

How to obtain access and use resources (hands-on)

In order to fully exploit the capabilities of modern supercomputer we need to understand the basic steps required to manage, submit and analyse large parallel multi-process applications, including the structure of a supercomputer and how to access it as well as how to create batch script and how to submit a simple job.

Using and creating scientific workflows

Creating scientific workflow applications is complex but enables the control and flow of data and computational requirements associated with a scientific application. This topic discusses commonly required workflow tasks and how to execute workflow tasks and data transfer.

Visualisation

The visual representation of scientific data has been a key component of science. Nowadays, the field of scientific visualization is growing fast, thanks to the technological explosion and a renewed interest of society in design and aesthetics.

Research area specific

Applications of the preceding topics will be provided in the specific context of the three research areas of CompBioMed: cardiovascular, molecularly-based and neuro-musculoskeletal medicine.

7.4 Forms of Training

Face to face training

Face to face training will be provided in the form of workshops and seminars. Credit-bearing taught courses for medical students and novice (undergraduate) biomedical researchers (education) will be used to supplement training for existing users.

Webinars

Use cases for specific training topics will be delivered in regular (the aim is bi-monthly) webinars, providing training in both methodologies and their application to biomedical research areas.

Massive Open Online Course (MOOC)

An online virtual learning environment will be used to deliver self-guided training programmes and content to users. CompBioMed will research the option to provide forums for asynchronous discussion and use these to guide user navigation through this content. Use of the online self-drive assessment, below, will enable users to select the appropriate self-guided training programme for their needs and interests.

Online self – drive

EPCC / University of Edinburgh has developed the Online Self – Drive. The diversity of user backgrounds will be addressed using an online self-drive test - an online assessment tool that will enable an evaluation of each user’s familiarity with computation and HPC and ascertain the specific area of biomedical computation of greatest relevance to them. EPCC will study the possibilities of developing an Online Self – Drive that is tailored towards Computational Biomedicine.

7.5 Multiplicity

Our overview table presents different possible aspects able to be used to provide a more tailored approach to training. Our training will be delivered by creating programmes from appropriate combinations of these existing training modules - an approach that affords great flexibility in accommodating user needs. In the section on the actual training programs that we propose, we will characterize the training modules described within the matrix.

8 Towards the Training Plan

In the sections below we map the training modules that partners within and outside of CompBioMed are currently offering. We then used this to formulate a Training Plan that the Centre of Excellence will implement in the next 2.5 years.

8.1 Existing Training Plan

In Annex 1, we reproduce the CompBioMed overview training table. Each entry is based on an existing course.

From this overview we have identified – and will be addressing in the CompBioMed Training Plan – the following points:

- There is an abundance of training offered by the HPC – centres and academic institutions and almost all topics in computation(-al science) are covered. However, only a small proportion of this is tailored towards the realm of Computational Biomedicine. The CoE will address this in implementing its Training Plan.
- Most existing training is directed towards novice and semi-expert users and training for expert users will need to be developed (for any of the user groups).
- There is an overwhelming emphasis on face-face training. The advantages of personalised training are obvious, but this places significant constraints upon the place, time and number of persons that can be addressed for each training event. The CompBioMed training plan seeks to address these limitations by proposing regular webinars, and producing MOOCs and online self-drive formats.

8.2 Training Plan

Initially, as described in the DoA, we planned to organise three major training events that would provide targeted training to the three user groups, through a mixture of plenary and parallel sessions. The timing of these events was to be arranged around M18, M24 and M30 of the project and, where possible, alongside a relevant conference or meeting. The first event was to be a relatively small event, mainly focused on the researchers in need of training drawn from within the CompBioMed partners and their immediate associates in related projects. For the second and third events we planned to open up and target the broader CompBioMed community, liaising with the VPH Institute and with the Avicenna Alliance, as well as seeking active collaboration with relevant EU funded projects.

During the first six months of the project, however, while working on the Training Plan and in liaison with project partners, we were provided with an unprecedented opportunity to expand the reach and scope of our training programme and have elected to take advantage of this to provide an exciting and innovative training programme that will reach a greater number and variety of users. This approach enables us to provide a training programme that is enhanced beyond the description provided in the DoA. We have opted for a mix of face-to-face training events and webinars. On top of that we will deliver training by engaging with university courses in subject areas related to the CompBioMed research areas - initially through the provision of Computational Biomedicine to medical students and Computational Medicine to postgraduate (MSc-level) researchers. In addition to this, we contribute to training events in collaboration with other Centres of Excellence.

We now propose to deliver:

- Two major training events in / around M24 and M30 (see section 8.2.1)
- Bi-monthly webinars (see section 8.2.2)
- University Courses (Y1, 2, 6) for medical students at UCL, the MSc in Computational Medicine at the University of Sheffield and academic partner courses modelled on each of these exemplars over the lifetime of the project (see section 8.2.3)
- At least one joint workshop with other Centres of Excellence (the first of these will take place in M8; see section 8.2.4)

8.2.1 Major Training Events

The next conference on the Virtual Physiological Human, VPH2018, will be held in September 2018 in Zaragoza, Spain (in M24 of the project). We consider this to be a major event for at least a part of our community and CompBioMed will have a strong presence. We will organise our first training event alongside or during this event (details to be finalised). Although this is the first event, we will open it up for external users, as described in the DoA for the second training event.

Partner BSC organises yearly winter schools, and we intend to align our second event with their 2018/2019 winter school (in M28, slightly in advance of M30 of the project). The objective of the winter school is to give a panorama on the use of HPC-based computational mechanics in Engineering and Environment through the projects BSC are carrying out. This panorama includes a survey of the basics underpinning the main tools: computational mechanics and parallelization. We are considering hosting an additional event alongside the 2017/2018 winter school at BSC, but this will depend upon available resources and will be balanced against the bi-monthly seminars that we also wish to provide. We will explore this option at the forthcoming All Hands Meeting of the consortium, which is planned for 11-12 April 2017.

All events will be recorded and, where possible, the recordings will be enriched with teaching material and hands-on exercises, then made freely available (through an appropriate platform) as MOOCs.

8.2.2 Bi-monthly webinars

Instead of organising three large face-to-face meetings, as originally proposed, we have decided to exploit the options offered by the internet, and we now propose to expand the reach of our training programme through the delivery of regular (the aim is bi-monthly) webinars, on a range of topics, for a range of audiences, as identified in our training overview table. The Virtual Physiological Human institute is already organising webinars, and we intend to collaborate with them, creating synergy between the training potential and ambition in the project, and the extended network of the VPH institute. We will also engage with the Avicenna Alliance, in order to tap into their extended industrial network.

All webinars will be recorded and, where possible, the recordings will be enriched with teaching material and hands-on exercises, then made freely available (the medium with which we will do remains to be chosen) as MOOCs.

We intend to have the first webinar in June 2017, dedicated to Cardiac Modelling and HPC (tentative assignment, to be confirmed). Other topics and a detailed schedule will be decided upon within the consortium in the period M7-M9 of the project.

8.2.3 Training integrated with University Courses

8.2.3.1 Training for medical students at UCL

The Student Selected Component (SSC) of UCL's Medical School Curriculum provides an opportunity to educate medical students in Years 1, 2 and 6, which are the years of study for which the medical school runs these SSCs. This is an ideal scenario for providing a training capability that can be used to support relevant BSc degrees at UCL. This training flow will also support the establishment of new clinical specialisations

centred around the use of data science and high performance computing-based biomedical modelling. The integration of this teaching endeavour within the CompBioMed training programme will afford an unprecedented opportunity to engage medical students taking these SSCs with the clinical, industrial and academic partners in CompBioMed. We have developed an SSC workflow that has a primary focus on genomics in Year 1, on cardiovascular and blood flow modelling in Year 2 and in modelling-informed stent design and fabrication in Year 6.

The workflow described above is not restricted to medical students, but can be used to deliver workshops for more advanced training of active scientists/researchers. Ultimately, recipients of the proposed workflow would include medical students, undergraduate and postgraduate students, early career researchers and established senior scientists seeking to incorporate computational biology in their programmes of research. With Year 1, 2 and 6 SSC running with 20 students in each year, 60 medical students would be able to benefit from the CompBioMed training programme per annum. It is estimated that additional training events at UCL would provide a further 60 students per annum, for a total of 120 participants involved in the CompBioMed training programme each year. This training programme will be of relevance and able to be delivered by UCL and other partners (especially HPC partners in CompBioMed) beyond the lifetime of the grant. Certain elements of the training programme and expansion of the range of SSC modules offered will be facilitated through collaboration with BioExcel, a sister Centre of Excellence with a strong track record of training in the use of high-end computing in biomolecular research.

8.2.3.2 Training for postgraduate researchers at the University of Sheffield

Over the last five years the Faculty of Engineering at the University of Sheffield has invested heavily in *in silico* medicine with the creation of the INSIGNEO Institute, aimed at realising the scientific ambition behind the Virtual Physiological Human international initiative, and, in collaboration with Sheffield Teaching Hospitals NHS Foundation Trust, producing a transformational impact on healthcare. The MSc in Computational Medicine is a cutting edge programme of study designed to form a new generation of scientist, using computerised techniques to improve disease diagnosis and treatment in the healthcare sector. Real biophysical and biological processes are simulated in a virtual environment and the course provides the opportunity to apply engineering solutions to the human body.

There is a growing need for computer-aided medicine and personalised treatment within the health care service. It is becoming a crucial consideration in the testing of new drugs and treatments. This course has been developed in response to this new and emerging trend and provides training for novice academic researchers. This course will educate the first generation of subject-specific modelling specialists for this emerging industrial sector, providing hands-on training in modelling of the human body using the most advance technologies available to date.

8.2.4 Collaborative Training with BioExcel

We will be seeking opportunities to provide training in collaboration with other Centres of Excellence, where this would enhance the user base. In the first instance, we are planning, with BioExcel, to offer a collaborative training workshop entitled Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences. This two day meeting, with a

particular focus on the prediction of ligand-protein binding affinities, will take place on 30-31 May 2017 (M8) and is divided into two parts. On Day One, the workshop will be limited to about 40-50 participants mainly, if not exclusively, drawn from our two Centres of Excellence (CoEs), with a focus on scientific and technical discussions pertaining to the theory, algorithms and their implementation on high performance architectures. Day Two will be a public meeting featuring speakers from both CoEs as well as other invited experts working across the full domain of theory and applications ranging across academia, industry and healthcare sectors. We will aim for a maximum of around 100 participants, and so we are advertising externally as well as within our projects.

This event will be recorded and, in combination with (additional) teaching material, made publically available as a MOOC. Day 1 will be a training event, Day 2 will comprise outreach.

9 Implementation

9.1 Training Portal and Repository

The Training Portal will be part of the project website (www.compbioMed.eu) and will be maintained by those project partners who take part in the preparation of training material. The portal will contain a list of the future and past training events organized within the CompBioMed project and a repository for all of the training material associated with each of the courses (this includes copy of the course slides, code examples, exercises and when available a record of audio and/or video of the training event).

9.2 Certification

CompBioMed will explore options to award training certificates for participants who have completed training courses. These certificates will describe the learning outcomes achieved and provide a base for clinical, academic and industrial researchers to collate a portfolio of achievement in Computational Biomedicine.

9.3 Timeline

As we have indicated above we have a clear initial timeline for the training plan. To summarize:

Training Events

1. Co-located with VPH2018, September 2018, Zaragoza, Spain
2. Winter school at partner BSC, winter 2018/2019
3. Tentative Winter school at partner BSC, winter 2017/2018

Bi-monthly seminars

Starting in June 2017, every two months (exact schedule to be decided)

University courses for medical students at UCL and Sheffield

Starting in academic year 2017-2018.

Joint training event with BioExcel

30-31 May 2017, Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences: see <http://tinyurl.com/lvgrrlw>

10 Sustainability

To ensure sustainability of the training materials and outputs beyond the end of the CoE, WP3 will sustain the following:

- Online provision of training materials including slides, practical problem sheets and relevant software examples/submission scripts. This will be handled under a suitable license for future use (e.g. the Creative Commons License). The content will be archived in alignment with the sustainability plan (WP4) for all CoE outputs.

Where possible, video/audio recordings of each course type will be taken to provide online resources in alignment with the CoE's sustainability plan.

11 Conclusion

UvA, UPF, UEDIN, BSC, SARA and UCL have closely worked together to establish the Training Plan for the CompBioMed Centre of Excellence. The Training Plan holds contributions from all CoE members that provide training, including UNIGE, UOXF and USFD. Moreover, it connects to expertise in the field and with PRACE, VPH and the BioExcel Centre of Excellence.

Early in January 2017, we gathered in Amsterdam to define our approach towards training in Computational Biomedicine and determine what the CompBioMed Centre of Excellence should add to this realm. Since then, we have mapped out and analysed existing training programs and identified opportunities for tailored training that will meet the specific needs of our users. The Training Plan identifies relevant topics, user communities, trainers, training levels and methods. It defines a timeline for the provision of the training on offer and describes how we will curate and sustain training materials. With this plan in hand the CoE can now move towards its next phase in training: the development and delivery of bespoke training in Computational Biomedicine.

COMPBIOMED Existing Training Programs
Alphabetical on Institute

Legend:	Face2Face
	Webinar
	MOOC
	Online self-drive

Organisation	BSC								
Title of training	Introduction to Computational Mechanics (BSC iCM)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				v	v	v			
Short description	Main concepts behind a simulation code. The Physical system and its Mathematical description. Discretization: algorithms and codes.								
Announced through (url-s)	https://www.bsc.es/education/training/patc-courses/patc-course-hpc-based-simulations-engineering-and-environment-2/								
Training dates	14-Feb-17								
Recurring	Frequency:	Every year							

Organisation	BSC								
Title of training	Parallel algorithms for Computational Mechanics (BSC PATCM)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				v	v	v			
Short description	Paradigms and scenarios of parallelization in a simulation code. Description of parallelization schemes. Parallel algebraic solvers and solving strategies.								
Announced through (url-s)	https://www.bsc.es/education/training/patc-courses/patc-course-hpc-based-simulations-engineering-and-environment-2/								
Training dates	14-Feb-17								
Recurring	Frequency:	Every year							

Organisation	BSC								
Title of training	Introduction to Computational Solid Mechanics (BSC iCSM)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				v	v	v			
Application codes									
Short description	A general view of the most used and useful approaches and constitutive theories applicable to the deformation and fracture of metals, composite and biological materials, covering the general aspects of the modelling and solution								
Announced through (url-s)	https://www.bsc.es/education/training/patc-courses/patc-course-hpc-based-simulations-engineering-and-environment-2/								
Training dates	15-Feb-17								
Recurring	Frequency:	Every year							

Organisation	BSC								
Title of training	Introduction to mesh generation for simulation (BSC iMesh)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				v	v	v			
Application codes									
Short description	Introductory course in: geometrical representations, meshing methods, element types, boundary approximations, quality measures, sizing approaches and software packages. Intended to facilitate the election of the proper mesh generation								
Announced through (url-s)	https://www.bsc.es/education/training/patc-courses/patc-course-hpc-based-simulations-engineering-and-environment-2/								
Training dates	15-Feb-17								
Recurring	Frequency:	Every year							

Organisation	BSC								
Title of training	Scientific visualization (BSC SciVis)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Visualisation				v	v	v			
Data Management									
Short description	Course to improve graphical communication skills. It explores elements of computer graphics, human-computer interaction, perceptual psychology and design in addition to data integrity. The aim is to learn how to present the data to								
Announced through (url-s)	https://www.bsc.es/education/training/patc-courses/patc-course-hpc-based-simulations-engineering-and-environment-2/								
Training dates	16-Feb-17								
Recurring	Frequency:	Every year							

Organisation	CompBioMed and BioExcel Joint Workshop CBM-BE joint workshop								
Title of training	Free Energy Calculations from Molecular Simulations: Applications in Life and Medical Sciences								
Topic(s) + Address (choose topic (s) from matrix and indicate address)	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation		√	√		√	√		√	√
Short description	prediction of ligand-protein binding affinities: theory, algorithms and implementation on high performance architectures								
Announced through (url-s)	http://www.combiomed.eu/free-energy-calculations-from-molecular-simulation-applications-in-life-and-medical-								
Training dates	30-31 May 2017								
Recurring Y/N	NO								

Organisation	EPCC, University of Edinburgh								
Title of training	Supercomputing (EPCC-SupComp)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation	√			√			√		
Intro Computing	√			√			√		
Short description	<p>This free online course will introduce you to what supercomputers are, how they are used and how we can exploit their full computational potential to make scientific breakthroughs.</p> <p>Over five weeks, we'll look at:</p> <p>supercomputers: introducing supercomputing terminology and some of the largest machines in the world.</p> <p>parallel computers: how they are built from hundreds of thousands of CPUs, each similar to those in a desktop PC.</p> <p>parallel computing: using parallel processing to harness the power of all of those CPUs for a single calculation.</p> <p>computer simulation: how we can perform virtual experiments to make real-life predictions.</p> <p>case studies: how supercomputing is making scientific breakthroughs that were never possible before.</p>								
Announced through (url-s)	https://www.futurelearn.com/courses/supercomputing								
Training dates	March 6th 2017								
Recurring	Frequency:			TBD					

Organisation	EPCC, University of Edinburgh								
Title of training	Scientific Computing (EPCC SciComp)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation	√	√		√	√		√	√	
Advanced computing (HPC, GPU)	√	√		√	√		√	√	
Short description	<p>This course covers the fundamental concepts of numerical simulation, and how modern parallel supercomputers are used in computational science.</p> <p>At the end of the course, attendees should be able to:</p> <p>explain the motivation for the use of parallel supercomputers in computational science</p> <p>describe the main models of parallel programming and propose parallelisation methods for standard problems</p> <p>understand the way real numbers are stored on a computer and the way that this affects the accuracy of results</p> <p>explain why random numbers are used in many simulations</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#sci_comp								
Training dates	June 2017, Edinburgh								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Message Passing Programming with MPI (EPCC MPP-MPI)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced computing (HPC, GPU)						√			√
Short description	<p><u>Video recordings of all the MPI lectures from the 2014 ARCHER Summer School.</u></p> <p>Associated course materials including slides, exercises and coding examples.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/online/								
Training dates	N/A – online, self-drive								
Recurring	Frequency:			N/A – online, self-drive					

Organisation	EPCC, University of Edinburgh								
Title of training	Introduction to HPC (EPCC introHPC)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced computing (HPC, GPU)					√			√	
Short description	<p>This material covers topics relevant to HPC and Parallel Computing as a whole, although ARCHER is often used as a All material comes from a run of the Hands-on Introduction to HPC course, held at EPCC in summer 2016. All the Videos See this playlist on the ARCHER YouTube channel which is a complete recording of the course.</p> <p>Slides Slides are available from the Past Course Materials Repository.</p> <p>Exercises Exercises are available from the Past Course Materials Repository.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/online/								
Training dates	N/A – online, self-drive								
Recurring	Frequency:			N/A – online, self-drive					

Organisation	EPCC, University of Edinburgh								
Title of training	Introduction to ARCHER (EPCC Archer)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced computing (HPC, GPU)				√	√		√	√	
How to get access to and how to use resources (hands-on)					√			√	
Short description	<p>This material gives details on the ARCHER hardware and software environment, and assumes familiarity with general HPC concepts (e.g. as covered in Introduction to HPC).</p> <p>Documentation</p> <ul style="list-style-type: none"> - The ARCHER Quickstart Guide is a good place to start for information on how to get up and running on ARCHER. - The first two sections of the ARCHER Data Management Guide give a general overview of file systems and data transfer mechanisms. <p>Slides</p> <ul style="list-style-type: none"> - Overview of material and high-level description of the ARCHER system - Details of how ARCHER is constructed from Intel CPUs and the Cray Aries interconnect, plus a high-level software overview - Details on compiling and submitting parallel jobs to ARCHER - Data management on ARCHER - Introduction to the Research Data Facility and Data Analytic Cluster <p>Videos</p> <p>These videos are recordings of the five lectures above.</p> <ul style="list-style-type: none"> - Overview of material - Details of how ARCHER is constructed - Details on compiling and submitting jobs - Data management on ARCHER - Introduction to the Research Data Facility and Data Analytic Cluster <p>These videos are recordings of ARCHER Virtual Tutorials covering relevant topics.</p> <ul style="list-style-type: none"> - PBS Job Submission - ARCHER Filesystems 								
Announced through (url-s)	http://www.archer.ac.uk/training/online/								
Training dates	N/A – online, self-drive								
Recurring	Frequency:			N/A – online, self-drive					

Organisation	EPCC, University of Edinburgh								
Title of training	Handson Introduction to High Performance Computing (EPCC h-onHPC)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				√	√		√	√	
Advanced computing (HPC, GPU)				√	√		√	√	
Short description	<p>High-performance computing (HPC) is a fundamental technology used in solving scientific problems. Many of the grand challenges of science depend on simulations and models run on HPC facilities to make progress, for example: protein folding, the search for the Higgs boson and developing nuclear fusion.</p> <p>The course runs for 2 days. The first day covers the the basic concepts underlying the drivers for HPC development, HPC hardware, software, programming models and applications. The second day will provide an opportunity for more practical experience, information on performance and the future of HPC. This foundation will give the you ability to appreciate the relevance of HPC in your field and also equip you with the tools to start making effective use of HPC facilities yourself.</p> <p>The course is delivered using a mixture of lectures and hands-on sessions and has a very practical focus. During the hands-on sessions you will get the chance to use ARCHER with HPC experts available to answer your questions and provide insight.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#hands_on_intro								
Training dates	To be announced								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Data Carpentry (EPCC DC)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				√	√		√	√	
Advanced computing (HPC, GPU)				√	√		√	√	
Data Management	√	√		√	√		√	√	
Short description	<p>In many domains of research, the rapid generation of large amounts of data is fundamentally changing how research is done. The deluge of data presents great opportunities, but also many challenges in managing, analysing and sharing data. Data Carpentry aims to teach the skills that will enable researchers to be more effective and productive. The course is designed for learners with little to no prior knowledge of programming, shell scripting, or command line tools.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#data_carpentry								
Training dates	9th – 10th May 2017								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Hands-on Porting and Optimisation Workshop: Making the most of ARCHER (EPCC h-on POW)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				√	√		√	√	
Advanced computing (HPC, GPU)				√	√		√	√	
Short description	<p>Instead of a typical ARCHER course consisting of alternating lectures + practicals, this workshop is designed to provide an opportunity for attendees to gain individually tailored hand-on help and advice from the ARCHER team / HPC specialists and to ask questions pertaining directly to your use of ARCHER.</p> <p>Each attendee will be assigned a technical advisor. This advisor will work closely with you throughout the day to help run your application and any associated essential software on ARCHER and to advise on how the system can be used most efficiently, to help evaluate the application's performance (providing guidance on the use of available tools if appropriate), and to suggest possible changes that could be made to the code to improve its performance.</p>								
Announced through (url-s)	https://events.prace-ri.eu/event/595/								
Training dates	4th April 2017 in Birmingham, UK								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Introduction to Scientific Computing with Python (EPCC Pyth)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				√	√		√	√	
Advanced computing (HPC, GPU)				√	√		√	√	
Short description	<p>This course is aimed at programmers with basic Python knowledge seeking to learn how to use Python for scientific computing. We will introduce Python's fundamental scientific libraries such as NumPy, SciPy and Matplotlib. We will also introduce how to interface Python with Fortran and C codes, and outline how to implement message-passing in Python with mpi4py.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#python								
Training dates	To be announced, location will be London								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Message Passing Programming with MPI (EPCC MPPwMPI)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation					√			√	
Advanced computing (HPC, GPU)					√			√	
Short description	<p>The world's largest supercomputers are used almost exclusively to run applications which are parallelised using Message Passing. This course covers all the basic knowledge required to write parallel programs using this programming model, and is directly applicable to almost every parallel computer architecture.</p> <p>Parallel programming by definition involves co-operation between processors to solve a common problem. The programmer has to define the tasks that will be executed by the processors, and also how these tasks are to synchronise and exchange data with one another. In the message-passing model the tasks are separate processes that communicate and synchronise by explicitly sending each other messages. All these parallel operations are performed via calls to some message-passing interface that is entirely responsible for interfacing with the physical communication network linking the actual processors together. This course uses the de facto standard for message passing, the Message Passing Interface (MPI). It covers point-to-point communication, non-blocking operations, derived datatypes, virtual topologies, collective communication and general design issues.</p> <p>The course is taught using a variety of methods including formal lectures, practical exercises, programming examples and informal tutorial discussions. This enables lecture material to be supported by the tutored practical sessions in order to reinforce the key concepts.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#mpp_with_mpi								
Training dates	15th – 17th February 2017 at UCL, London, Birmingham, UK 19th – 21st April 2017 at Southampton, UK								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Software Carpentry (EPCC SC)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + simulation				√	√		√	√	
Advanced computing (HPC, GPU)				√	√		√	√	
Short description	<p>Software Carpentry's goal is to help scientists and engineers become more productive by teaching them basic computing skills like program design, version control, testing, and task automation. In this two-day workshop, short tutorials will alternate with hands-on practical exercises. Participants will be encouraged both to help one another, and to apply what they have learned to their own research problems during and between sessions.</p>								
Announced through (url-s)	http://www.archer.ac.uk/training/courses/index.php#sw_carpentry								
Training dates	11-12 May 2017								
Recurring	Frequency:			To be announced					

Organisation	EPCC, University of Edinburgh								
Title of training	Practical Introduction to Data Science - MOOC (EPCC-PIDSmooc)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Data Management	√			√			√		
Short description	<p>This online course will introduce the important ideas and concepts of data science and will allow you to gain the basic skills that would be expected of a data scientist. It has two broad themes, namely the importance of looking after data (so that it can be analysed) and data analytics techniques. It's a practical course so you will get to try out these techniques and explore these ideas using common Data Science tools and languages including R and Python.</p> <p>This course is an assessed course, and on completion of this course you will receive a Postgraduate Professional Development Award of Academic Credit (corresponding to 20 SCQF credits) from the University of Edinburgh.</p>								
Announced through (url-s)	https://www.epcc.ed.ac.uk/online-courses/courses/online-courses/practical-introduction-data-science								
Training dates	January to May 2017 – online MOOC								
Recurring	Frequency:			To be confirmed, yearly					

Organisation	EPCC, University of Edinburgh								
Title of training	Practical Introduction to High Performance Computing - MOOC (EPCC PIHPCmooc)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling+Simulation	√			√			√		
Advanced Computing (HPC, GPU)	√			√			√		
Short description	Modern supercomputers are parallel computers, gaining their power from many thousands of individual processors. Developing software to run on these systems requires using new parallel programming technologies. The course will cover all the fundamental concepts that underpin modern HPC. The course is practical in the sense that you will explore these topics by running parallel programs on real HPC systems such as the UK national supercomputer ARCHER (link is external). The same techniques can also be applied to smaller systems such as multi-core desktops, graphics processors and computing clusters.								
Announced through (url-s)	https://www.epcc.ed.ac.uk/online-courses/courses/online-courses/practical-introduction-hpc								
Training dates	January to May 2017 – online MOOC								
Recurring	Frequency: To be confirmed, yearly								

Organisation	SURFsara								
Title of training	Introduction to Unix (Intro Unix)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Intro Computing	√			√			√		
Short description	<p>Content</p> <p>You'll learn about the structure of Unix operating systems and the basic commands. You'll practice working with the command line and giving a number of commands.</p> <p>Target</p> <p>Anyone who wants to have sufficient basic knowledge of Unix to be able to work with it on the national compute cluster Lisa or on the Cartesius supercomputer, for example. You are familiar with the Windows or OS X operating systems.</p>								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring	NO								

Organisation	SURFsara								
Title of training	Introduction to data management								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Data management	√			√			√		
Short description	<p>Content</p> <p>In this course we will give you an overview of the services available for researchers in the Netherlands. Specifically, we</p> <p>Target group</p> <p>Anyone who would like to get started with data management applications. You are familiar with the basics of programming and the Unix command line</p>								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring	NO								

Organisation	SURFsara								
Title of training	Introduction to GPU programming (GPU)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced computing						√			√
Short description	<p>Content</p> <p>You'll find out how NVIDIA GPUs and CUDA interact and you'll be introduced to a number of different parallel programming techniques. You'll learn to work with existing libraries which use GPU acceleration. You'll be given practical examples of most techniques, including GPU programming models such as OpenACC.</p> <p>Target group</p> <p>Anyone who would like to find out how GPUs work so that they can work with them themselves. You are familiar with the basics of programming and the Unix command line. You are familiar with the Unix command line and have experience of the programming languages C or Fortran.</p>								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring Y/N	NO								

Organisation	SURFsara								
Title of training	Introduction to Visualization (Visual)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Visualization		√			√			√	
Short description	<p>Content</p> <p>The concept of visualizing scientific data will be explained. Visualization gives you insights into remarkable phenomena in data and helps you check the accuracy of the results and present and communicate results in an understandable manner. You can, for example, display your research results using remote visualization, where datasets are too big and complex to be visualized locally (on your own laptop).</p> <p>Different types of data require different visualization methods, techniques and tools. You'll be given examples of 2D and 3D simulations, geographical data and networks. The visualizations comprise images and video materials and even interactive visualizations on the web. You'll practice with existing research data but you can also bring your own data with you.</p> <p>Target group</p> <p>Anyone who would like to find out how visualization helps in understanding research data. You are familiar with scientific research.</p> <p>Announced through (url-s)</p> <p>Beneficiary website and/or SURFsara mailing list</p> <p>Training dates</p> <p>On request</p> <p>Recurring Y/N</p> <p>NO</p>								

Organisation	SURFsara								
Title of training	Introduction to Machine Learning (Machine Learn)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced Computing						√			√
Short description	<p>Content</p> <p>You will learn how to login and use the GPU nodes on the Cartesius supercomputer for training large neural networks. You will learn how to use several libraries and tools designed to facilitate experiments and research in the area of machine-learning.</p> <p>Target group</p> <p>Anyone who would like to find out more about machine learning and is familiar with Unix command line and have experience in bash and python.</p> <p>Announced through (url-s)</p> <p>Beneficiary website and/or SURFsara mailing list</p> <p>Training dates</p> <p>On request</p> <p>Recurring Y/N</p> <p>NO</p>								

Organisation	SURFsara								
Title of training	Getting started with HPC Cloud (HPC cloud)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Cloud		√			√			√	
Short description	<p>Content</p> <p>You'll learn to work with SURFsara's HPC Cloud. The course includes everything from logging in to the virtual environment via OpenNebula to running a simple MPI program and the execution of distributed processes. You'll perform practical tasks on the HPC Cloud and set up a cluster yourself.</p> <p>Target group</p> <p>Anyone who would like to get started with HPC Cloud. You are familiar with the basics of programming and the Unix</p> <p>Announced through (url-s)</p> <p>Beneficiary website and/or SURFsara mailing list</p> <p>Training dates</p> <p>On request</p> <p>Recurring Y/N</p> <p>NO</p>								

Organisation	SURFsara								
Title of training	Getting started with the Hadoop cluster (Hadoop)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Big Data		√			√			√	
Short description	<p>Content</p> <p>You'll learn how to work with SURFsara's Hadoop cluster. And how to compute using MapReduce, Apache Spark, Hive, Pig and HBase. You'll practice on the Hadoop cluster yourself and locally on a virtual machine (VM).</p> <p>Target group</p> <p>Anyone who would like to get started with the Hadoop cluster so that they can perform Big Data analyses. You are familiar with the basics of programming and the Unix command line.</p> <p>Announced through (url-s)</p> <p>Beneficiary website and/or SURFsara mailing list</p> <p>Training dates</p> <p>On request</p> <p>Recurring Y/N</p> <p>NO</p>								

Organisation	SURFsara								
Title of training	Getting started with Grid computing (GRID)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advanced Computing		√			√			√	
Short description	Content								
	You'll learn how to work with SURFsara's Grid computing clusters and the associated data storage systems. You'll gain an overview of the basic concepts of Grid computing such as parallelizing on the Grid, task distribution, monitoring and data management. This course is also available online and you can complete it in your own time.								
	Target group								
	Anyone who would like to get started with Grid computing. You are familiar with the basics of programming and the Unix command line.								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring Y/N	NO								

Organisation	SURFsara								
Title of training	Getting started with the Cartesius/Lisa (HPC)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Intro Computing		√			√			√	
Short description	Content								
	You'll learn how to work with the Cartesius supercomputer and the national compute cluster Lisa. We explain when you need the supercomputer and what applications feature on the Lisa cluster. This hands-on course includes both an interactive part on the login nodes and a batch part on the worker nodes. You will use capability and capacity cluster computers.								
	Target group								
	Anyone who would like to get started with Cartesius and Lisa. You are familiar with the basics of programming and the Unix command line.								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring Y/N	NO								

Organisation	SURFsara								
Title of training	Getting started with iRODS and EUDAT data management (iRODS-EUDAT)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Data Management		√			√			√	
Short description	Content								
	You'll learn how to set up a data management infrastructure with applications such as iRODS (Integrated Rule-Oriented Data System) and PIDs (persistent identifiers). Through use cases you'll gain an understanding of how they work. You'll also practice with the applications yourself on virtual machines. We also present EUDAT (European Data Infrastructure)'s data management services.								
	Target group								
	Anyone who would like to get started with data management applications. You are familiar with the basics of programming and the Unix command line.								
Announced through (url-s)	Beneficiary website and/or SURFsara mailing list								
Training dates	On request								
Recurring Y/N	NO								

Organisation	UCL								
Title of training	From skin to metagenomics: exploring your microbiome								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Intro computing	√								
Linux command line	√								
Application codes (Python)	√								
How to get access to and how to use resources	√								
Advanced computing (HPC, GPU)	√								
Subject specific: molecularly-based medicine	√								
Short description	Participants will isolate genomic DNA from their skin bacteria and use state of the art NGS sequencing and computational resources to analyse the metagenome data obtained								
Announced through (url-s)	TBA								
Training dates	October - December 2017								
Recurring Y/N	YES								

Organisation	UNIGE nat pheno								
Title of training	Modeling and Simulation of Natural phenomena								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation		√		√	√			√	
Short description	MOOC								
Announced through (url-s)	www.coursera.org								
Training dates									
Recurring Y/N	YES								

Organisation	UNIGE cadmos								
Title of training	CADMOS HPC course								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Advance computing				√	√		√	√	
Short description	Introduction to HPC, MPI and scientific applications								
Announced through (url-s)	www.cadmos.org								
Training dates									
Recurring Y/N	YES								

Organisation	UNIGE Palabos								
Title of training	PALABOS Tutorial								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Application				√	√		√	√	√
Short description	Tutorial on how to use the open-source lattice-boltzmann solver Palabos								
Announced through (url-s)	www.palabos.org								
Training dates									
Recurring Y/N	YES								

Organisation	UOXF Elec Mech								
Title of training	MRI-based cardiac electromechanical modelling								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Application codes		√		√	√	√			√
Short description	Introduction to image analysis and processing to construct 3D heart geometries, to simulate the electromechanical activity from ionic level to tissue and heart.								
Announced through (url-s)	http://www.cs.ox.ac.uk/ccs/home								
Training dates	September 2017 - September 2018								
Recurring Y/N	YES annual								

Organisation	UOXF Chaste								
Title of training	Introduction to the multiphysics simulation software Chaste								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Application codes				√	√				
Short description	Webinar introducing the usage of Chaste focused on electrophysiological simulations at tissue and whole organ level								
Announced through (url-s)	http://www.cs.ox.ac.uk/ccs/home								
Training dates	September 2017 - September 2018								
Recurring Y/N	YES annual								

Organisation	UPF / Acellera								
Title of training	HTMD workshop (UPF HTMD)								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Application codes				√	√		√	√	
Short description	The aim of this workshop is to learn the latest developments of high-throughput molecular dynamics simulations with practical lectures and real data and to give scientists the opportunity to exchange their experiences. Hands-on session and training will be given using HTMD, a powerful programmable environment to prepare, handle, simulate and analyze molecular simulations, and efficient GPU-based MD simulations, and standard protocols to execute numerical experiments. There will be at the end of the workshop a session on applying what you have learned on your data/proteins.								
Announced through (url-s)	http://workshop.htmd.org/								
Training dates	November 2017(to be decided)								
Recurring Y/N	Yearly								

Organisation	USFD CM								
Title of training	MSc Computational Medicine								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	modelling and <i>in silico</i> medicine								
Announced through (url-s)	TBA								
Training dates	Oct 2017-Sept 2018								
Recurring Y/N	YES	annual							

Organisation	UvA								
Title of training	Introduction Computational Science								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Intro computing				√					
Linux command line									
Application codes (Python)				√					
How to get access to and how to use resources									
Advanced computing (HPC, GPU)									
Short description	Introduction to the basic concepts of modelling and simulation								
Announced through (url-s)	uva.nl								
Training dates	October - December 2017								
Recurring	YES	annual							

Organisation	UvA								
Title of training	Introduction Computational Science								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	Introduction to the basic concepts of modelling and simulation								
Announced through (url-s)	uva.nl								
Training dates	September - October 2017								
Recurring	YES	annual							

Organisation	UvA								
Title of training	Stochastic Simulation								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	Monte Carlo methods in modelling and simulation								
Announced through (url-s)	uva.nl								
Training dates	October - December 2017								
Recurring	YES	annual							

Organisation	UvA								
Title of training	Complex System Simulation								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	Modelling complex systems, network science, ABM, CA, etc.								
Announced through (url-s)	uva.nl								
Training dates	June 2017								
Recurring Y/N	YES	annual							

Organisation	UvA								
Title of training	Scientific Computing								
Topic(s) + Address	CLINICAL			ACADEMIA			INDUSTRY		
(choose topic (s) from matrix and indicate address)	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	numerically solving PDEs								
Announced through (url-s)	uva.nl								
Training dates	February - March 2018								
Recurring Y/N	YES	annual							

Organisation	UvA								
Title of training	Computational Biology								
Topic(s) + Address (choose topic (s) from matrix and indicate address)	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	introduction to computational biology								
Announced through (url-s)	uva.nl								
Training dates	April-May 2017								
Recurring Y/N	YES	annual							

Organisation	UvA								
Title of training	minor Computational Science								
Topic(s) + Address (choose topic (s) from matrix and indicate address)	CLINICAL			ACADEMIA			INDUSTRY		
	novice	semi	expert	novice	semi	expert	novice	semi	expert
Modelling + Simulation				√					
Short description	introduction to programming in python, numerical math, modelling and simulation, and selected applications								
Announced through (url-s)	uva.nl								
Training dates	September 2017 - January 2018								
Recurring Y/N	YES	annual							