# CompBioMed and EOSC-hub

## Opportunities and collaborations

**The HPC Centres of Excellence in the EOSC arena**

EOSC-hub Week 2019

Marco Verdicchio, Narges Zarrabi

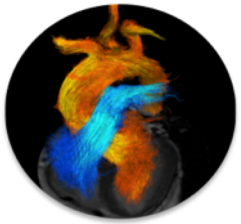
**SURFsara**

**11 April 2019**

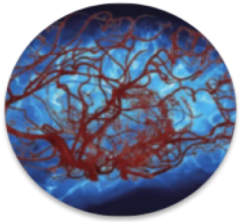
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 675451.

# User-driven biomedical modelling and simulation

## Targeting new and emerging biomedical research areas



Cardiovascular medicine



Neuro Musculoskeletal medicine

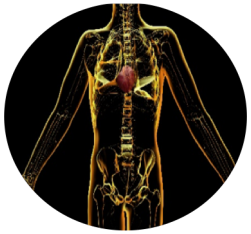
Molecularly based modelling

## Biomedical science across all scales

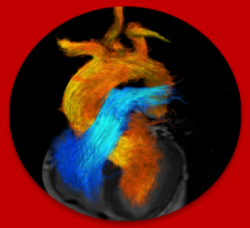
Molecular systems

Organs

The Virtual Human

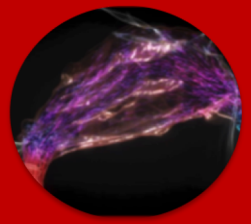


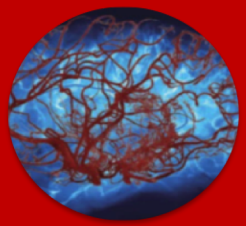
# CompBioMed Objectives



Cardiovascular medicine

Molecularly based medicine





Neuro Musculoskeletal medicine

**CompBioMed Applications**

**Computational Resources**

SURF SARA

epcc

Microsoft Azure

lrz

amazon web services™

CSCS

DNAnexus

# CompBioMed Core partners


Academic Partners

Clinical Partners

UCL

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES

UNIVERSITY OF OXFORD

upf. Universitat Pompeu Fabra Barcelona

The University Of Sheffield.

Industrial Partners

Bull atos technologies

janssen

evotec

SMEs

acellera

CBK

LifeTec Group

Supercomputing Centres

THE UNIVERSITY OF EDINBURGH

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

SURF SARA

# CompBioMed Associate partners


## Academic and Research Institute Partners

BIRMINGHAM CITY University
Brunel University London
ITMO UNIVERSITY
UNIVERSITY OF Southampton
Aix*Marseille université Initiative d'excellence
ULB UNIVERSITÉ LIBRE DE BRUXELLES
UNIVERSITY OF LEEDS
RUTGERS
جامعة زايد ZAYED UNIVERSITY
NHS National Institute for Health Research
Oxford Biomedical Research Centre
KINDI الكندي لبحوث الحوسبة Computing Research QATAR UNIVERSITY
INSTITUTE OF MOLECULAR BIOLOGY
Avicenna Alliance Association for Predictive Medicine
Hartree Centre Science & Technology Facilities Council
VPH Institute Building the Virtual Physiological Human
HITS
IT IS FOUNDATION
e-Cardiology ESC Working Group
diamond
مؤسسة حمد الطبية Hamad Medical Corporation HEALTH · EDUCATION · RESEARCH صحة · تعليم · بحوث
SCIENCE MUSEUM

## Supercomputing Centres

Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities
CYFRONET

## Cloud providers

DNAnexus
alcesflight
Microsoft

## Industrial Partners

DASSAULT SYSTEMES
Medtronic
ANSYS
gsk
PIE MEDICAL IMAGING
AstraZeneca
POZLAB

## SMEs

LIGHTOX
INSILICOTRIALS
norton straw engineering & management consultants
DiaVita Life Science
EnsembleMD

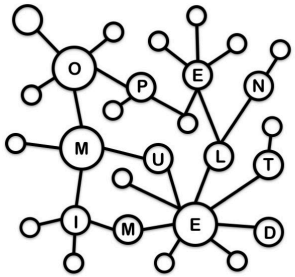
# CompBioMed Related Projects

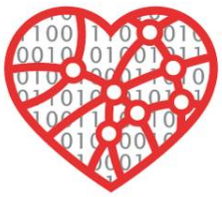
EOSC-hub




EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING


Human Brain Project

VHEARTSN

Red Española de Modelización Computacional Cardiaca




# CompBioMed Objectives

**CompBioMed user-driven CoE**

**Academic**

**Industry/SMEs**

**Clinical**

## Efficient computing capabilities

- HPC infrastructures
- Access to accelerators and new architectures (GPUs, etc.)

## Robust data services

- Long term storage facilities
- Integrated data management tools

## Secure and easy access

- Confidentiality of data and methods
- Instant/on demand access to resources
- Quality of Service

# CompBioMed resources

## HPC Infrastructure

- Supercomputers (Tier 0, Tier 1)
- Cluster computer (Tier 2, Tier 3)
- Accelerators (GPU, XeonPhi)
- Cloud computing

## Data Storage

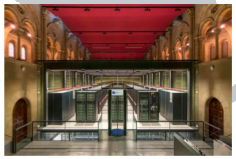
- Data archive (disk, tape)
- Backup systems
- Cloud Storage
- Data Management tools

## Security

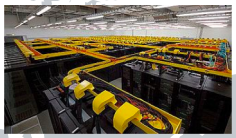
- Cloud providers and HPC centres certified to the international standard for information security, **ISO 27001**

# CompBioMed towards exascale


**MIRA**
Argonne Nat Lab
Alya



**MareNostrum IV**
BSC
Hemocell
Alya

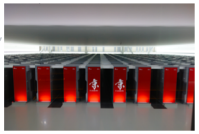


**Super MUC**
LRZ
BAC

**Blue Waters**
NCSA UIUC
HemeLB
BAC

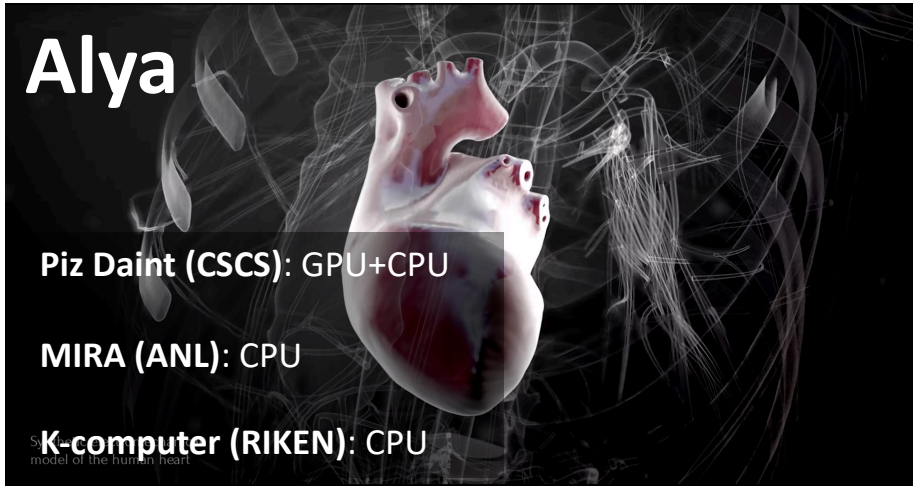
**Titan**
Oak Ridge Nat Lab
BAC

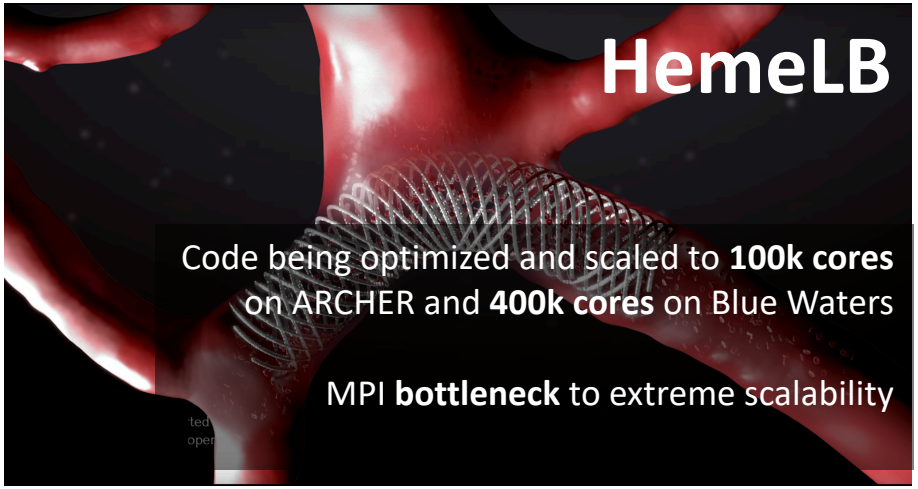
**Piz Daint**
CSCS
Alya
HemeLB
Palabos

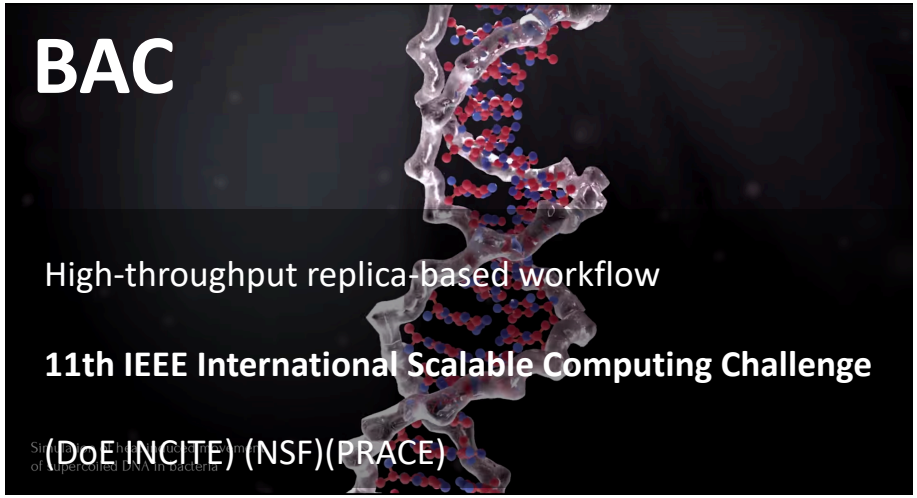


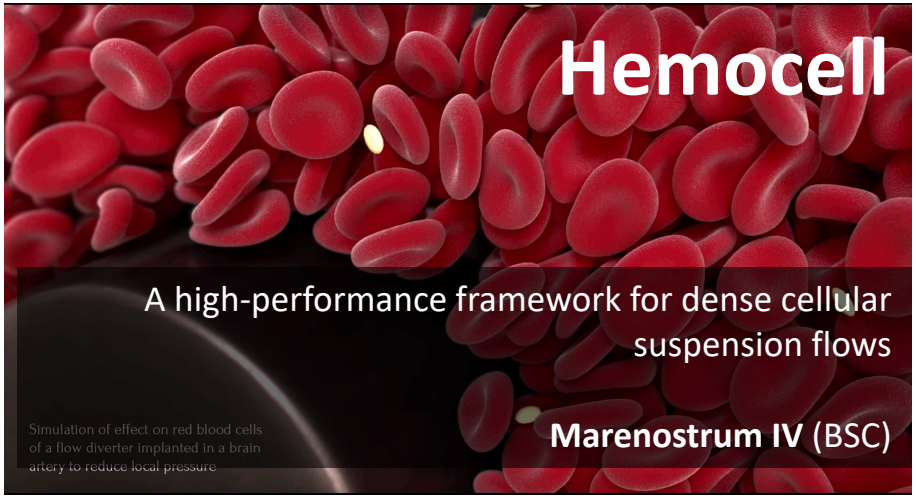
**K-computer**
RIKEN
Alya

# CompBioMed towards exascale



# CompBioMed and cloud computing

**Cloud computing** advantages:

- **Quality of service**
- **Urgent, on demand access**
- **Security**

## Cloud computing in CompBioMed

**SURFsara HPC cloud** allocation for CompBioMed partners

## CompBioMed and cloud partnership

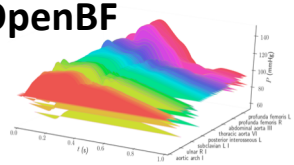
# CompBioMed and cloud computing


**BAC** Deployed and test on AWS, Azure HPC and DNAnexus services


**Alya** containerisation done with Singularity, Docker and Shifter (tests on Lenovo machine)

**Alya** tested on Oracle Cloud for HPC (tests on a bare-metal instance)

**OpenBF**



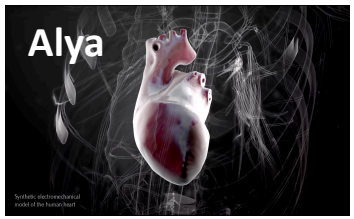
**OpenBF** 1D cardiovascular workflows deployed on SURFsara HPC cloud + HPC

**AceCloud**, from Acellera, offers access to on-demand cloud computing resources for MD simulations on the AWS marketplace.

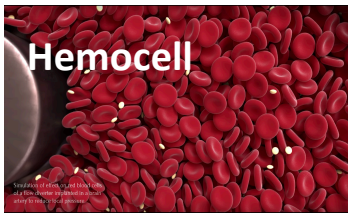
Acellera and UPF currently work on **PlayMolecule** platform to deploy and run applications in the Cloud

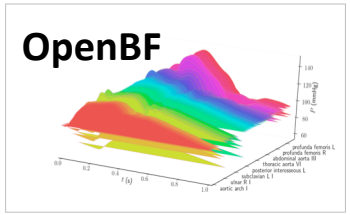
# CompBioMed and cloud computing

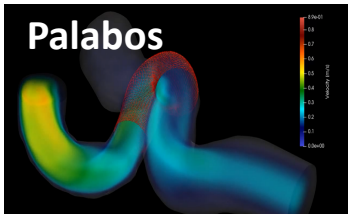
## Containers for biomedical applications







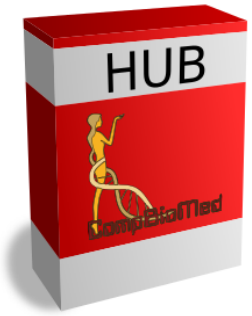




Charliecloud


docker

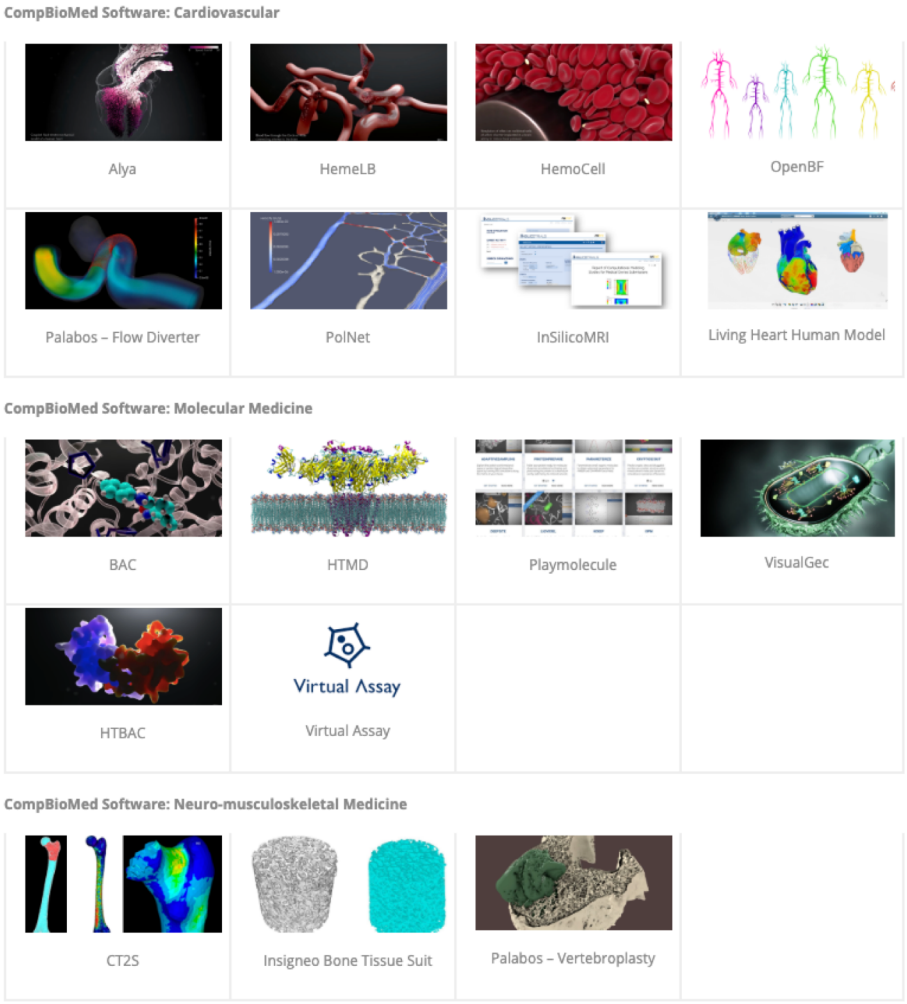
UDOCKER

# CompBioMed Software Hub




- ✓ Centralized access the resources developed and coordinated by the CompBioMed project.
- ✓ 12 end-user solutions + 5 from Associate Partners
- ✓ Accessible through EOSC catalogue

**http://www.compbiomed.eu/services/software-hub/**



# CompBioMed Data Intensive Research

## FAIR data in CompBioMed

- Typical datasets range from 100 MB-10 GB
- Total volume of data project partners want to store is around 20-25TB with significant growth expected
- 25% of users did not want to continue using their existing data storage systems

Need for a system capable of storing arbitrary data in many different file formats, which can be shared with other users and preserved for the long term.

## Intensive data transfer and storage

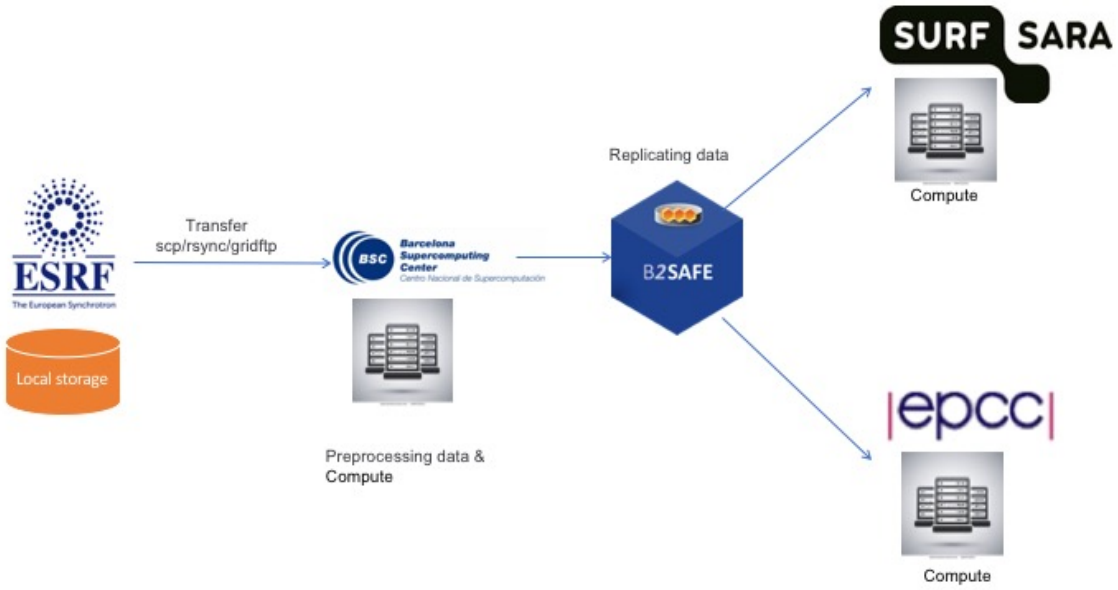
Pilot projects for experimental images transfer to HPC centres.

# CompBioMed Data Intensive Research

## Safe data replication with B2SAFE - Pilot

Safe data replication and large data transfer is one of the major requirements within the CompBioMed community

- **Step 1: Data creation and transfer**
- **Step 2: Data pre-processing**
- **Step 3: Data Replication**

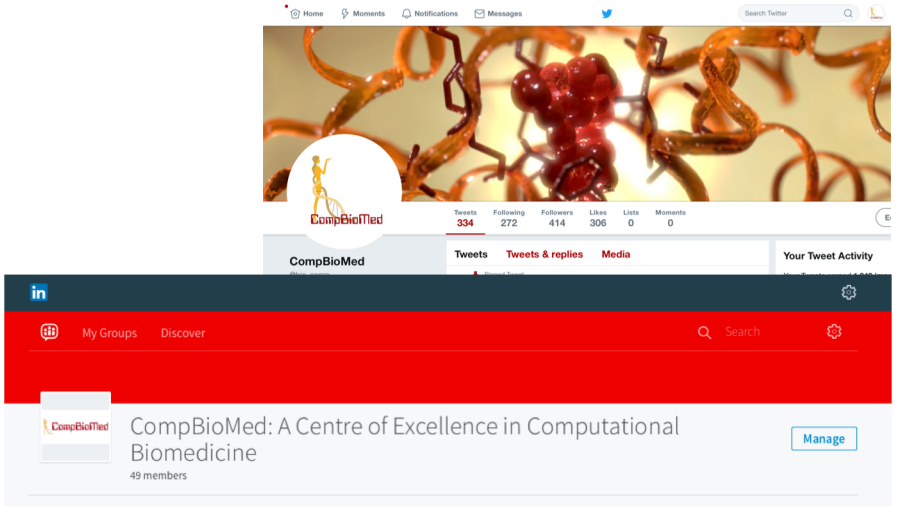


# CompBioMed Dissemination & Outreach

## CompBioMed Online presence

@bio_comp

#CompBioMed





- IMAX event at Science Museum, London
- Various showings at scientific presentations
- Won SCINEMA award for Technical Merit (Australian Science Film Festival)

# CompBioMed Training activities

## Training repository

- Partners' trainings available through CompBioMed
- Accessible through EOSC catalogue

## Courses and Workshop

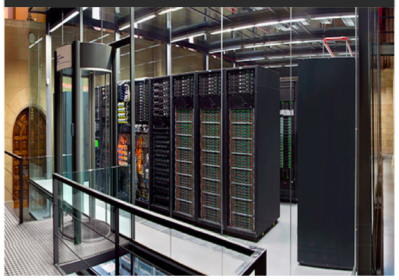
- Three major training events
- University based courses at UCL (life sciences & early-stage medical students), University of Sheffield and other academic partner courses
- Joint workshops with other related projects

## Webinars

- Bi-monthly webinars (started November 2017)

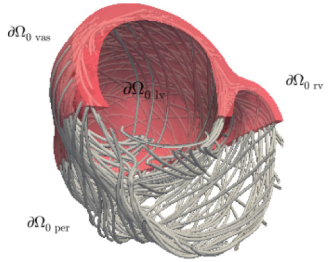
**CompBioMed Training:**
***Winter School 2019,***
*BSC, Barcelona*

**13-15 February 2019**



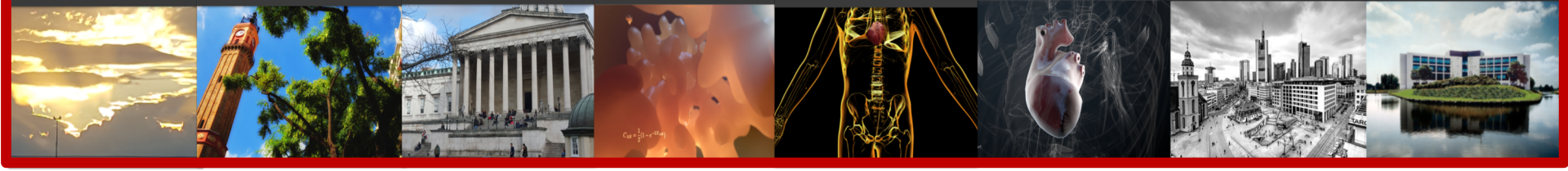
**CompBioMed Webinar Series:**
7. Sensitivity analysis of a strongly coupled cardiac electro-mechanical model

**20 March 2019**



# CompBioMed Conferences & Meetings

| Cloud & HPC in Biomedicine, London | CompBioMed at PRACEdays 2017, UPC, Barcelona | CompBioMed & Bioexcel, Free-energy Workshop, London | OpenMultiMed & CompBioMed Joint Workshop at EPMA 2017, Malta | The Virtual Human, IMAX event at Science Museum, London | CompBioMed & VHeart Joint Workshop UvA, Amsterdam | CompBioMed BoF at ISC-High Performace 2018, *Frankfurt, Germany* | CompBioMed Containerisation Meeting, *SURFsara, Amsterdam* |
|---|---|---|---|---|---|---|---|
| 27 April 2017 | 16 May 2017 | 31 May 2017 | 15 September 2017 | 27 September 2017 | 28 March 2018 | 27 June 2018 | 28-29 March 2019 |



**25 - 27 September 2019**

**Institute of Engineering & Technology, Savoy Place, London, UK**

CompBioMed Conference 2019

**www.compbiomed-conference.org**

# Interactions CompBioMed & EOSC-hub

- **Uptake of CompBioMed services**
  - Promoting and offering CompBioMed services (technologies) through EOSC-portal.
  - Service “life cycle”
- **Infrastructure usage alignment Cloud + HPC**
  - Usage of EGI compute services (EGI fat node clusters, High-Throughput compute, Services for sensitive data)
- **Data management services:**
  - User Support
  - Storage services (EGI Archive and Online storage, secure file sharing and storage)
  - Moving toward FAIR data and open access (data + software)
- **Interactions between EU projects on common challenges (trainings, workshops).**
  - Sharing knowledge and experience with other communities (often communities have common needs)

# Thank you

Website: **www.compbiomed.eu**

YouTube: **Computational Biomedicine**

Twitter: **@bio_comp**

**www.compbiomed-conference.org**