

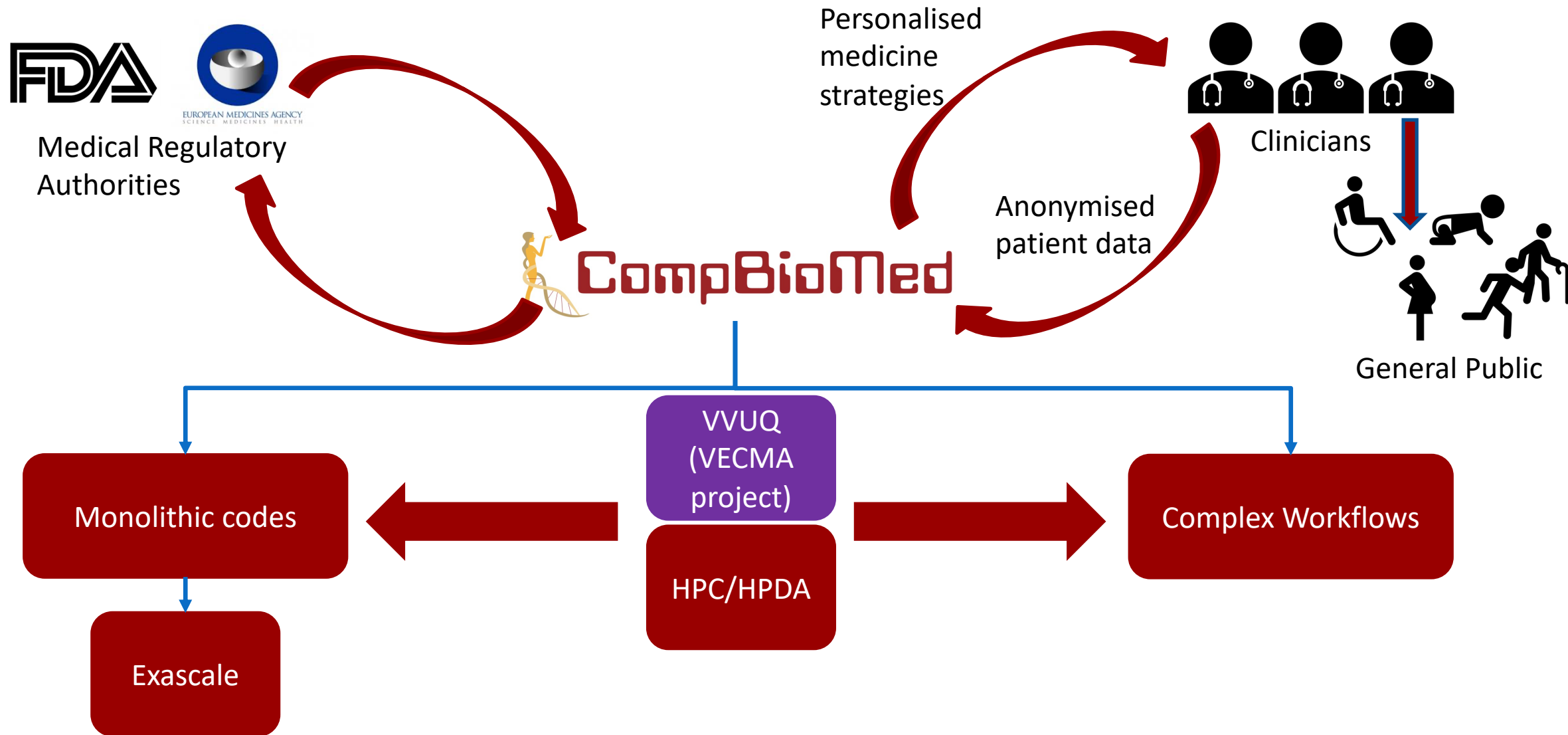
# CompBioMed

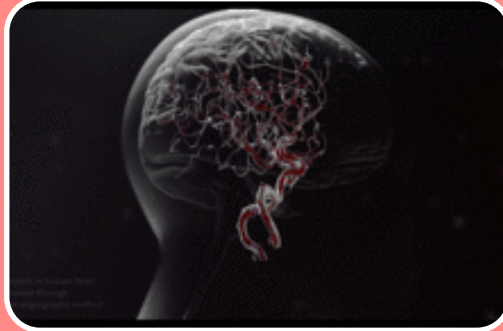
**17<sup>th</sup> June 2021**

<http://www.compbiomed.eu/>

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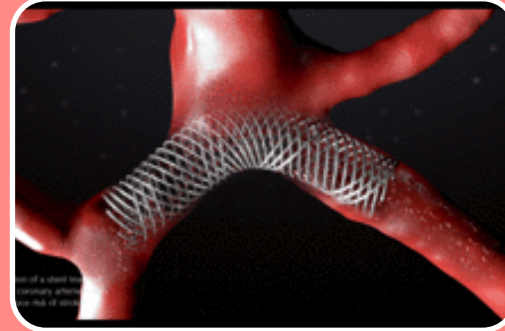
# Motivation and objectives





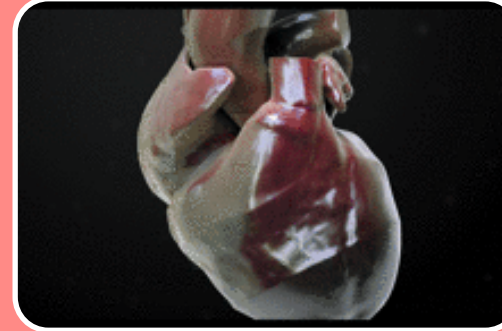
## Academic Users

- Conferences, Journals, Training, Software Hub
- Promoting use and uptake of results



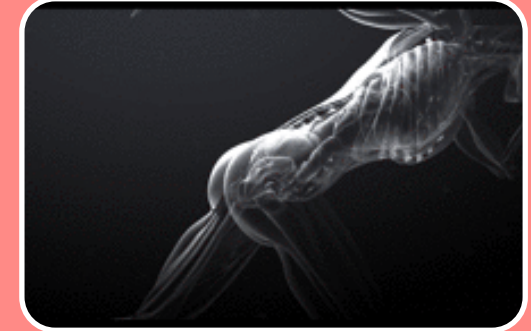
## Industrial Users

- Training (specifically webinars), IAB, access to HPC
- Awareness through to uptake



## Clinical Users

- Training (medical school courses), conferences, personal collaborations, HPC
- Awareness through to uptake



## General Public

- Virtual Human film, social media, television
- Awareness only

How CompBioMed is preparing users for HPC:

- **Scaling as a Service**

- Providing support to current HPC users for scaling and porting of applications

- **Training**

- Existing training program ongoing: Medics, Bioscience students and Advanced users
- Scaling of training to expand user engagement to include EU13 and HPC-poor countries: new initiative for July 2021

- **Dissemination**

- Engagement with the public and users in building a Virtual Human, through webinars, public talks, scientific engagement projects (Evidence Week 2021), written work showcasing the Virtual Human and a public event at Science Museum that builds on the success of our first Virtual Humans film

# Access and availability of CompBioMed codes

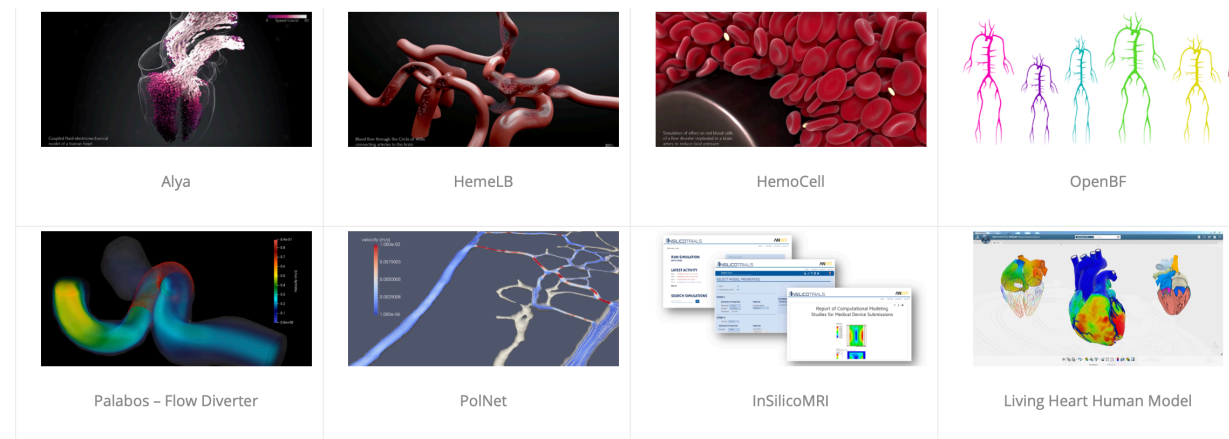


## CompBioMed Software Hub

### All about the software for the computational biomedicine research community

The CompBioMed Software Hub addresses the needs of the computational biomedicine research community, which can use the Hub to access the resources developed, aggregated and coordinated by CompBioMed.

#### CompBioMed Software: Cardiovascular



#### CompBioMed Software: Molecular Medicine

Offered By

**Use scenario**  
Non-clinical research; Clinical research; Clinical decision support; Design & optimisation for medical devices; In silico clinical trial.

**HPC motivation**  
Solve unreducible model; Multiscale model; Strongly coupled multiphysics model.

#### Relevant links

- [Alya official website](#)
- [Alya documentation](#)
- [HPC Multi-scale computational modelling using Alya Red](#)
- [CompBioMed Webinar: HPC simulations of cardiac electrophysiology using patient specific models of the heart \(using CHASTE and Alya\)](#)
- [Alya Red: A Computational heart](#)
- [CompBioMed Virtual Humans Film](#)

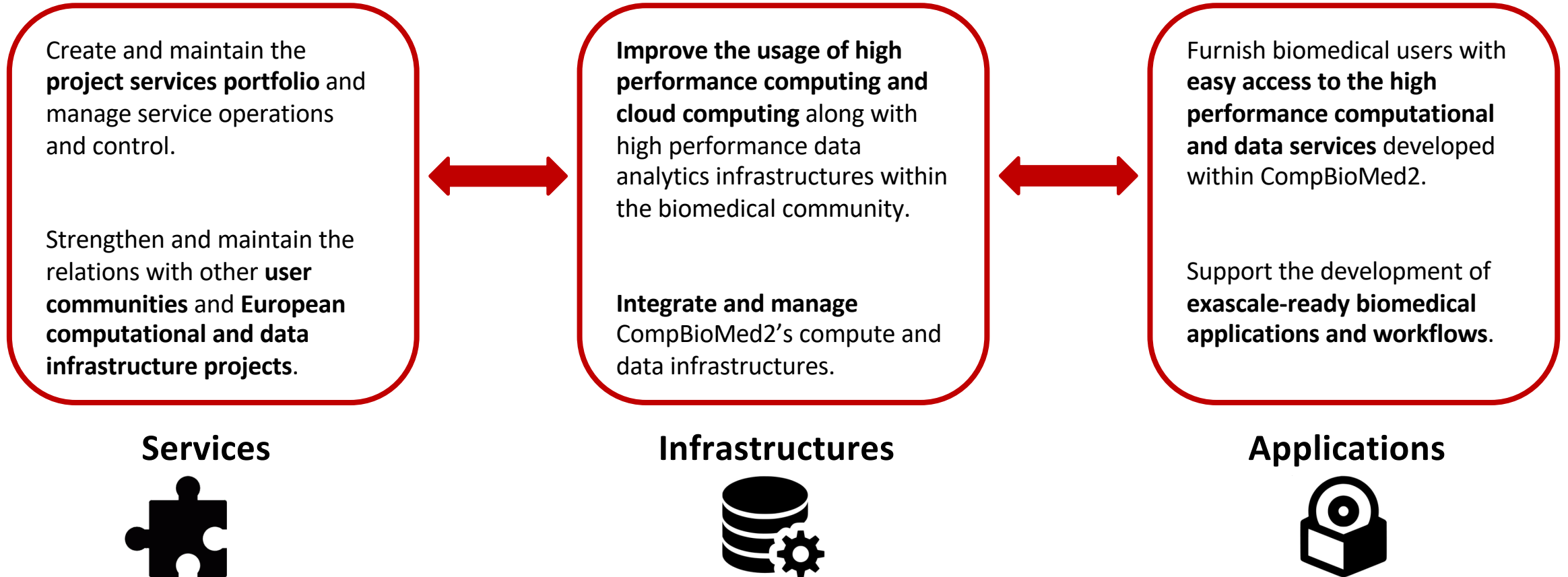
Proactive support for end users

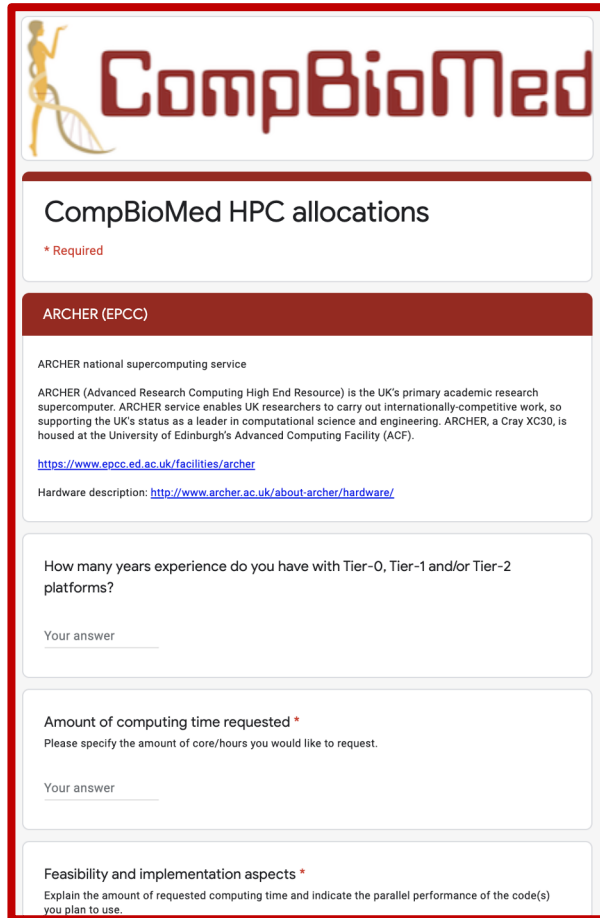
Open source codes

Software Hub - details the codes and where to download them

Developers details outlined in the application page

# Compute and Data Services



A screenshot of the CompBioMed HPC allocations application form. The form is titled "CompBioMed HPC allocations" and includes a red asterisk indicating required fields. It features a section for "ARCHER (EPCC)" with a description of the service and links to the EPCC website and hardware description. Below this, there are three input fields: "How many years experience do you have with Tier-0, Tier-1 and/or Tier-2 platforms?", "Amount of computing time requested \*" (with a sub-instruction to specify core/hours), and "Feasibility and implementation aspects \*" (with a sub-instruction to explain the amount of time and parallel performance).

**CompBioMed**

CompBioMed HPC allocations

\* Required

**ARCHER (EPCC)**

ARCHER national supercomputing service

ARCHER (Advanced Research Computing High End Resource) is the UK's primary academic research supercomputer. ARCHER service enables UK researchers to carry out internationally-competitive work, so supporting the UK's status as a leader in computational science and engineering. ARCHER, a Cray XC30, is housed at the University of Edinburgh's Advanced Computing Facility (ACF).

<https://www.epcc.ed.ac.uk/facilities/archer>

Hardware description: <http://www.archer.ac.uk/about-archer/hardware/>

How many years experience do you have with Tier-0, Tier-1 and/or Tier-2 platforms?

Your answer \_\_\_\_\_

Amount of computing time requested \*

Please specify the amount of core/hours you would like to request.

Your answer \_\_\_\_\_

Feasibility and implementation aspects \*

Explain the amount of requested computing time and indicate the parallel performance of the code(s) you plan to use.

- **CompBioMed HPC allocation programme (partners systems)**
  - Fast and flexible access (GPU, CPU) + support
  - About 7,000,000 core/hours already used
  - ARCHER2 “6-week free-period”, CompBioMed2 users consumed ~7,800,000 core hours
- **Access to Tier-0 systems**
  - PRACE allocations (HRLS, CSCS, JSC, CINECA, BSC)
  - US HPC systems (Summit ORNL, Frontera TACC)

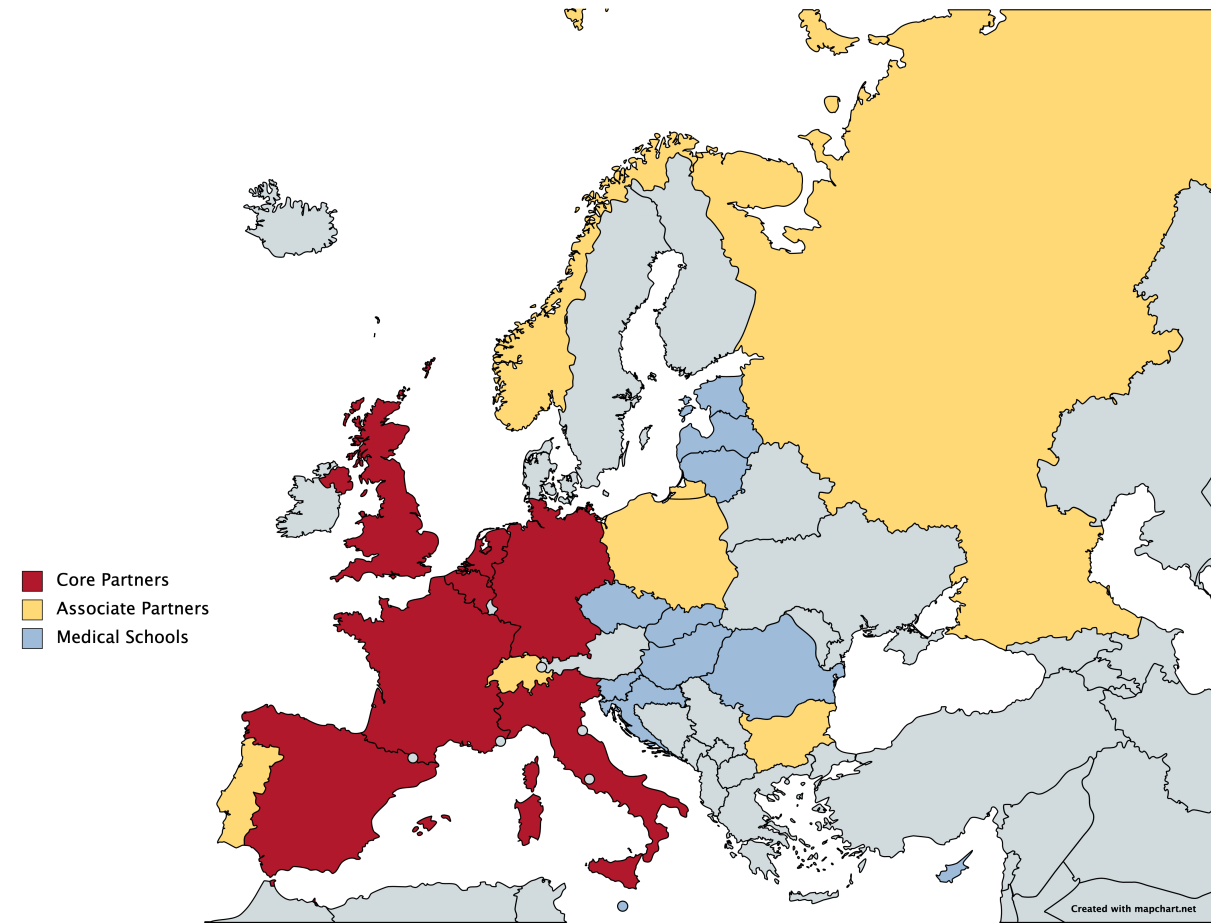
# CompBioMed Partners



Core Partners are located throughout Europe (Red countries)

Associate Partners are located in these countries as well as many others (Yellow countries)

We are working to expand our Associate Partners and collaborators within the EU13 (Medium blue countries) and HPC-under-represented countries.





Online Form: <https://www.compbioMed.eu/innovation/visitor-programme/>

Duration: 1 week to 3 months

Travel Costs: up to €5000

The proposal should include:

- A full description of the work (length as outlined above)
- An estimate of the anticipated HPC requirements and how they would be used
- Justification of the chosen host institute
- A proposal of the costs involved

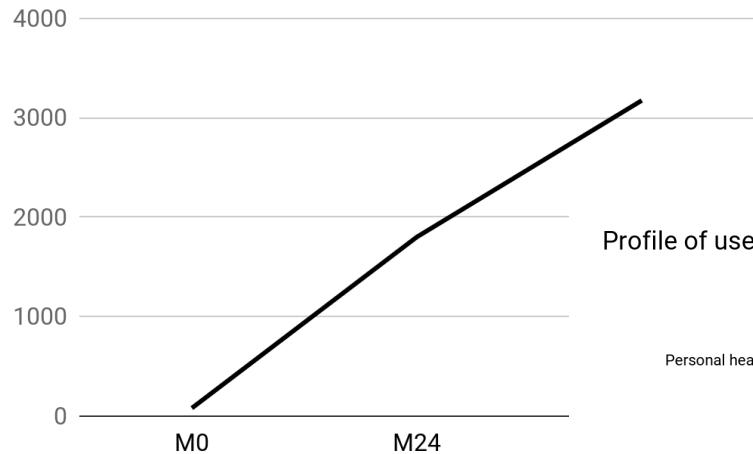
Following the application, the proposal will be reviewed by the selection committee, subject to the following criteria

- Alignment of the proposal with the strategic goals of CompBioMed
- Quality of the project proposal
- Potential impact of the project

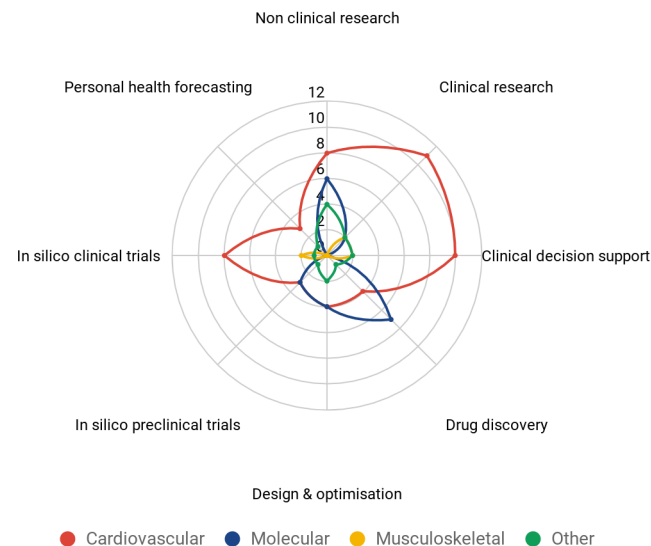


## CompBioMed (phase 1)

Total number of user: all solutions



Profile of users: across domains



## CompBioMed (phase 2)

- Advanced HPC training
  - 180 attendees (M24 KPI target -50)
- Medical students training
  - Embedded in 2 Medical Schools (target 4 at M46)
- HPC underrepresented EU countries
- Coaching users' communities on potential of HPC and exascale
- Total attendees/members so far: 750+
- D6.1 Establishment of the community engagement, and technical report



## In Silico World Community of Practice

**Community of Practice:** a safe pre-competitive space where experts from academia, industry, and regulatory agencies can request and exchange advices, join teams and collaboratively work on shared goals



- 400 members
- 14 private channels
- 10 public channels
- 10 volunteer admins
- 13000+ messages sent
- Review paper on In Silico Trials

### Expertise

The community is invitation only: in this way we ensure only interested experts have access

### Safe space

A pre-competitive space where experts from academia, industry, and regulatory agencies can ask for and exchange advices

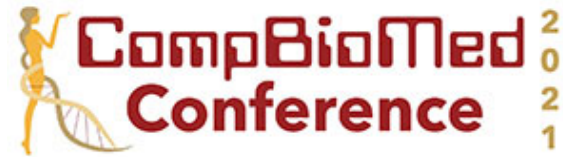
### Collaboration

Join teams and collaboratively work on shared goals, projects, concerns, problems or topics

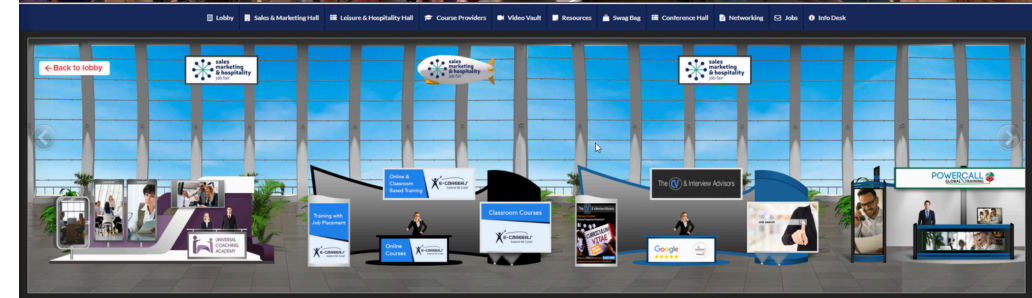
# Conference and Workshop Planning

AHM – CompBioMed All-Hands Meeting – External meeting  
23<sup>rd</sup> June 2021

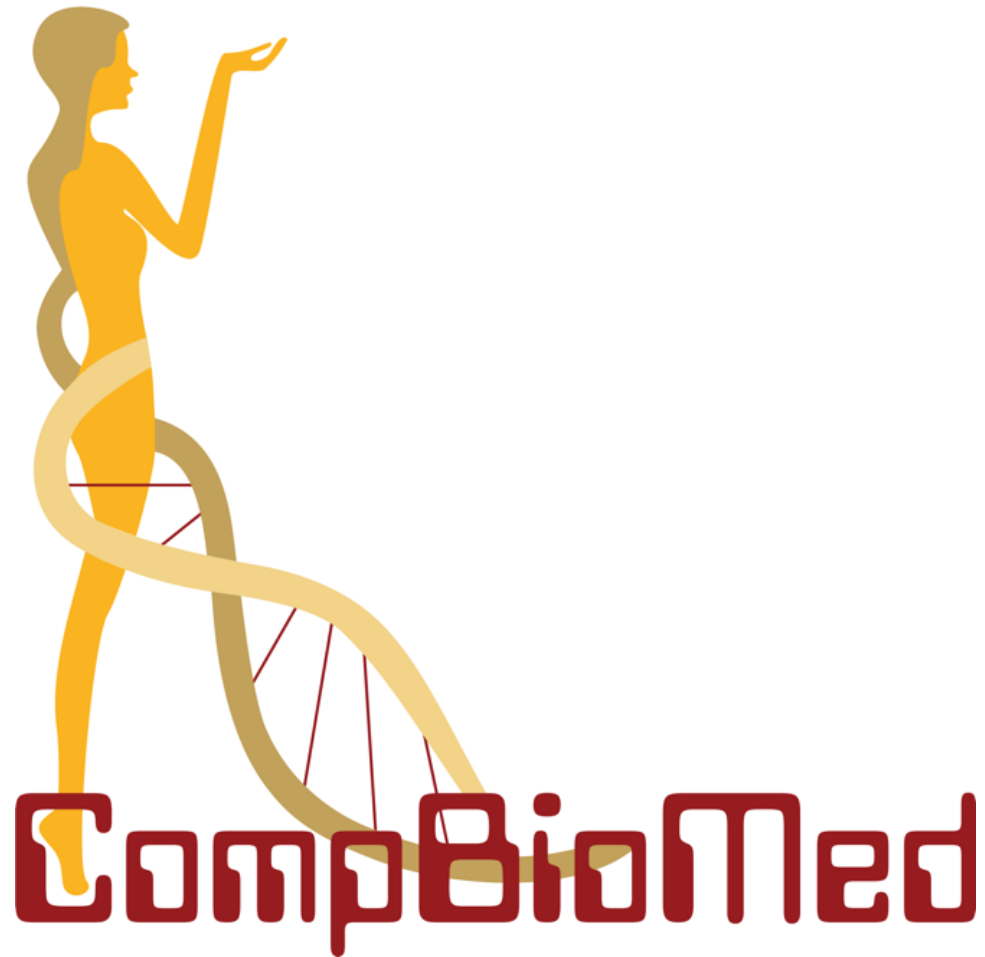
Conference – CBMC21, Online Conference, 15-17 September  
2021



Biomedical Applications	Methodology	Technology and Outreach
State of the art in Personalised Medicine (PerMedCoE)	Multiscale Modelling & Patterns of Compute	Imaging & Visualisation
Molecular Medicine & Drug Discovery	Building the Virtual Human	In Silico Trials: Challenges and Opportunities
Organ Modelling and Simulation	On the path to the Exascale	From desktop to HPC and beyond in the clinic
Covid & Immunology	Validation, Verification and Uncertainty Quantification	Innovation in Modern Biotechnology
HPC in Healthcare: Genomics & Oncology	The role of Quantum Computing in biomedicine	Public Awareness, Training and Education including Public Policy



# Thank you



Website: [www.compbioMed.eu](http://www.compbioMed.eu)

YouTube: **Computational  
Biomedicine**

Twitter: **@bio\_comp**