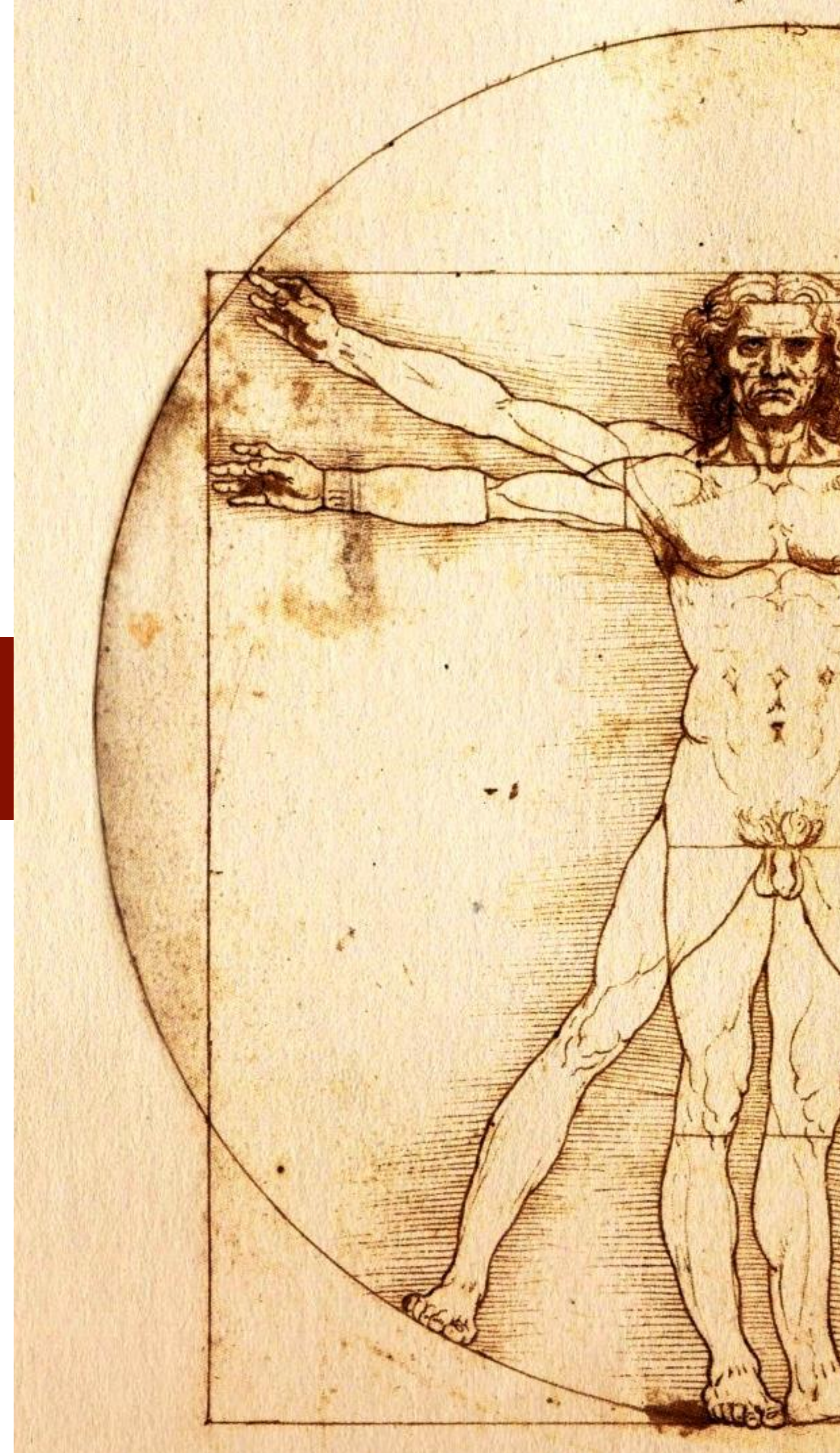




CompBioMed: The Center of Excellence for Computational Biomedicine



Together with BioExcell, one of the two bio-CoEs

Coordinated by P. Coveney (UCL)

Applications Manager: M. Vázquez (BSC)

Partners: BSC, University College London, Universities of Geneva, Edinburgh, Oxford and Amsterdam, surfSARA, Janssen Pharmaceutical.



Advance the role of computationally based modelling and simulation within
biomedicine

Predictive computational biomedicine

Applications that are comprised of multiple components, arranged into automated
workflows

High performance computing (HPC) as a fundamental cornerstone of
computationally assisted biomedical research

Identify user communities and their needs

Three initial targets:

Cardiovascular and respiratory systems

Musculo-skeletal system

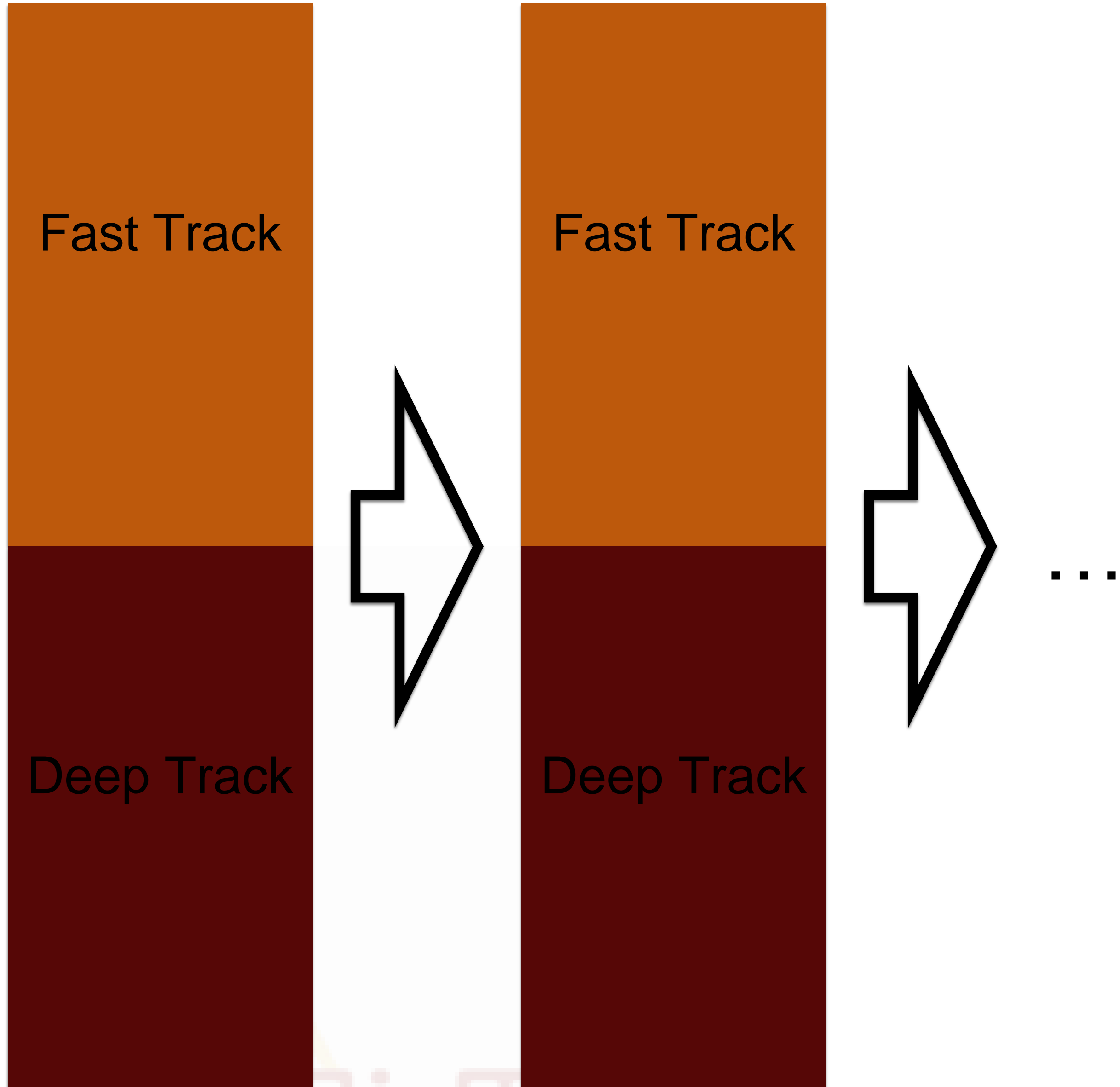
Molecular medicine

Develop complex biomedical simulation tools

Deploy these tools in supercomputing centers

Provide access and training to user communities (the Fast Track)

Improve and optimise simulation tools (the Deep Track)



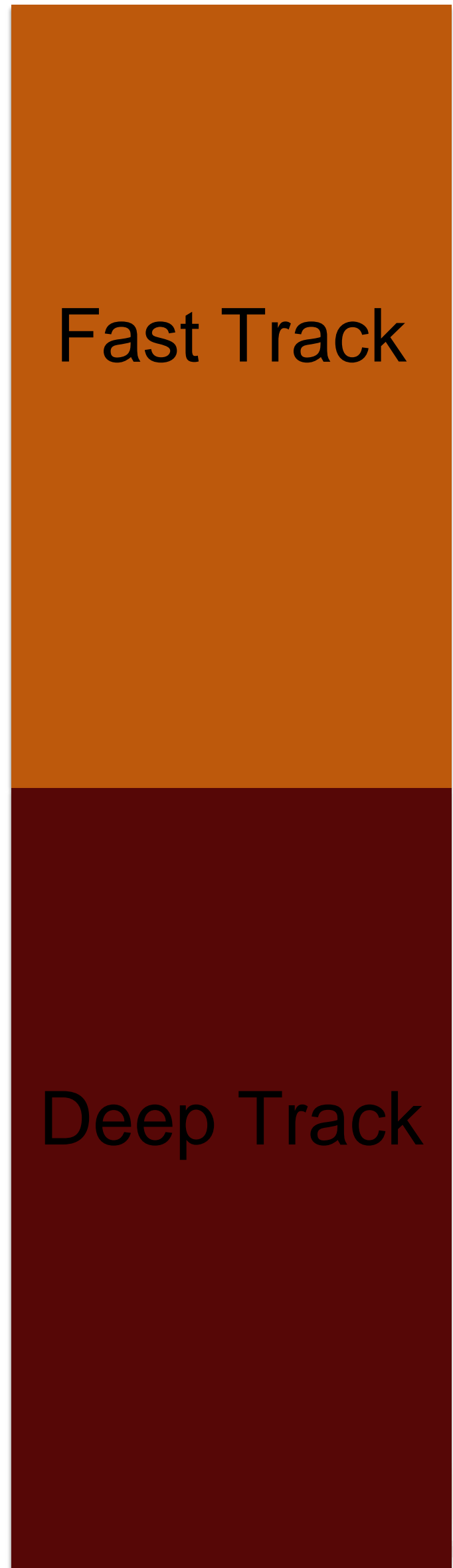
Applications structure in pipelined layers

CompBioMed defines the pipeline

Each layer could have a “FT” and a “DT”

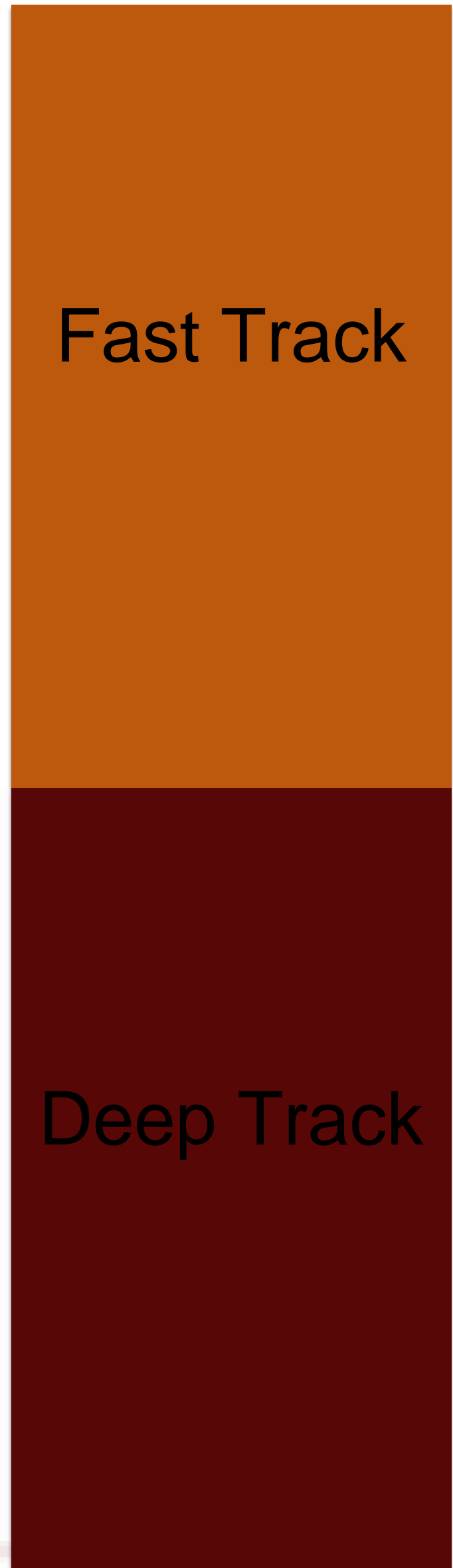
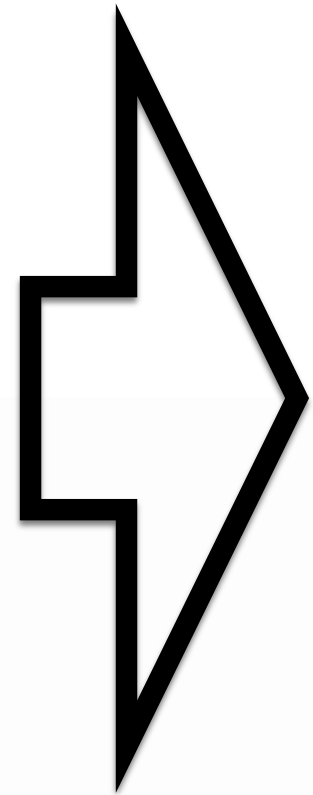
The FT is ready to go, with a relatively simple definition of the connecting pipeline and all the required software ready

The DT requires longer term research



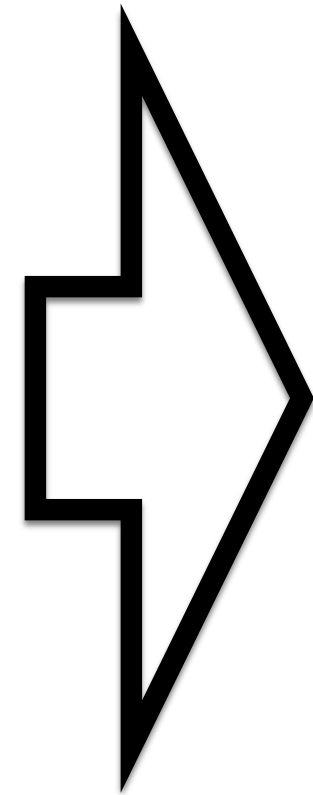
Fast Track

Deep Track



Fast Track

Deep Track



...

Each layer will use codes we are already using, with few modifications

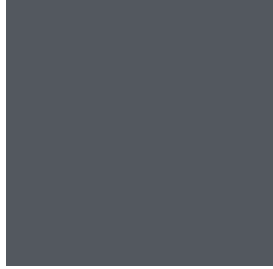

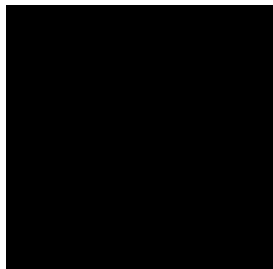
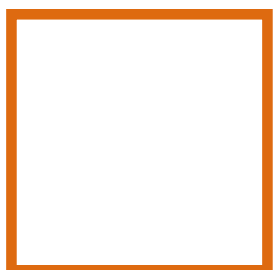
Codes could be commercial or academic, open source or not

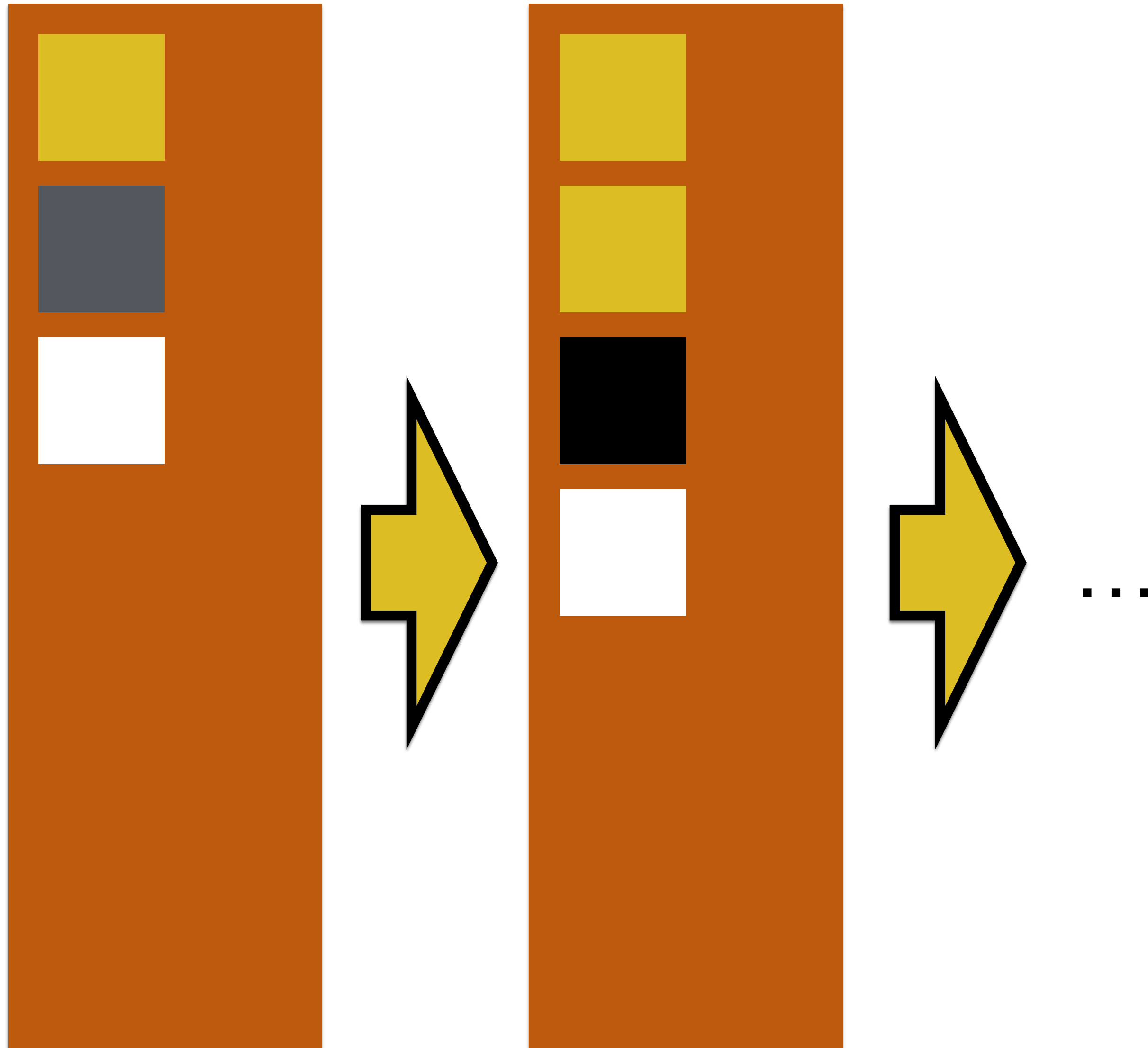
It is important to define the pipelined structure in a flexible way, carefully defining the interfaces in a standard and clear way, so different codes could be used at every point...

... even codes not already among our current tools.

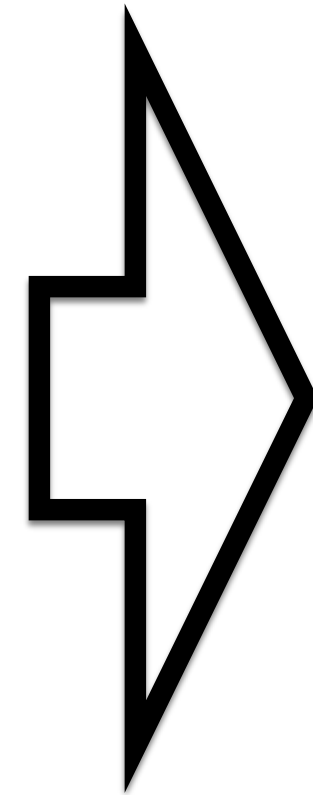
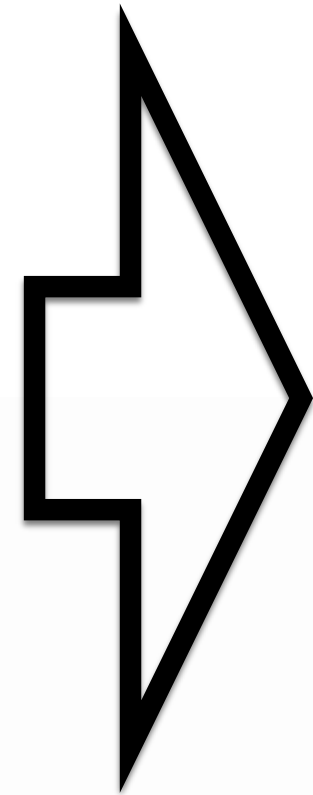
Example of a CompBioMed infrastructure

Codes integrated and deployed:

-  Open access (no sources)
-  Open source
-  Commercial
-  No code, just the interface defined



This infrastructure could be also available at a centralized Hub for deployment somewhere else, or at least, a part of it (at least at the development stage...)

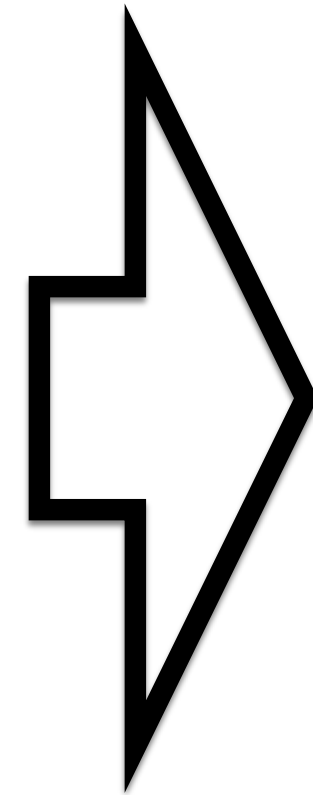
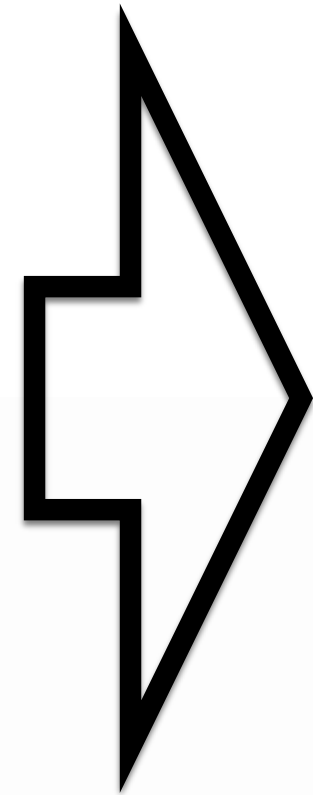


...

The applications pipeline should be deployed in the ComBioMed partners computational resources

For the supercomputing centers, in their supercomputers and accessible through the CompBioMed committed resources

In the case of commercial software users, the pipeline will be fully operational in those systems with the appropriate licences



...

It is highly desirable to have a “benchmark suite” where some specific and well-defined problems can pass through the full pipeline

The BS is to be defined according to each exemplar

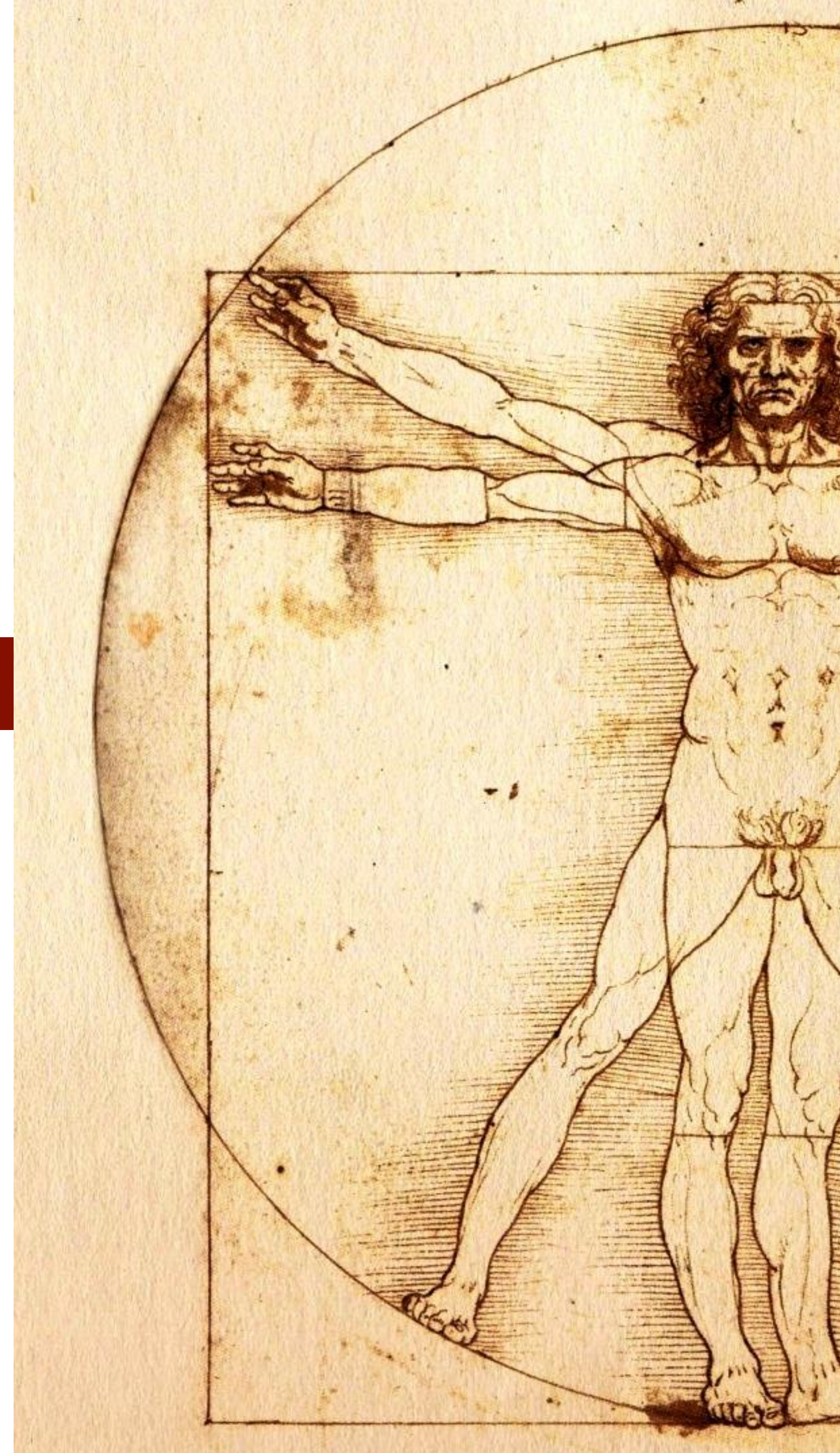
The CompBioMed web site will become a hub where users can:

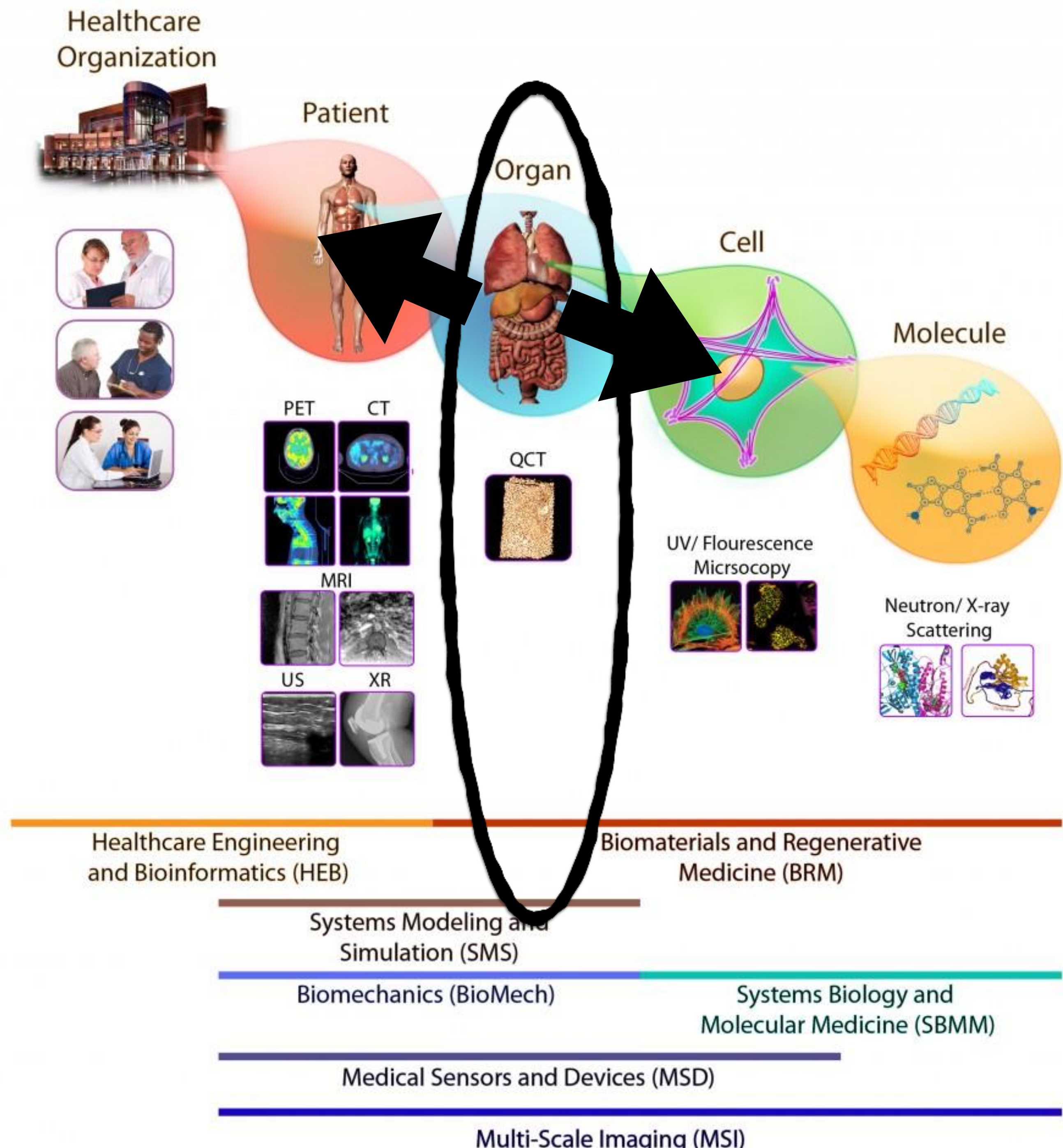
- Ask for expertise, training...
- Ask for the CompBioMed infrastructure
- Download documentation, benchmarks, datasets
- Some software will be there ready to be downloaded
- Some other software will be downloaded from third-parties sites, whose links will be in the CompBioMed repository





BSC role in CompBioMed





Alya

Multi-physics & multi-scale HPC-based simulation tool

Born 2004, born parallel, born multi-physics

Approx. 800K code lines

Approx. 40 developers

One code, no multiple versions

Centralized repository

Solvers in-house, no 3rd parties libraries (except METIS)

BSC involvement

WP2 Biomedical Research Activities:

- Activities Coordination
- Simulation software provider: *Alya / IRIS Mesh*
- Expertise in multi-scale / multi-physics coupling
- Expertise in HPC (esp. with coupling)
- Fast track & deep track for cardiovascular (mostly with Oxford)
- Visualization
- Coupling

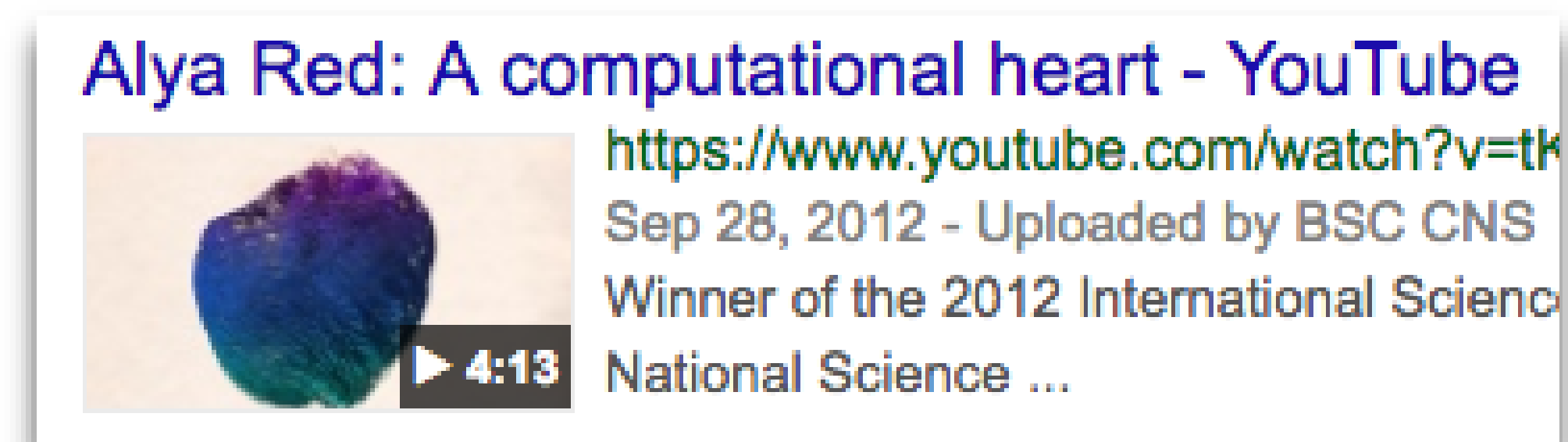
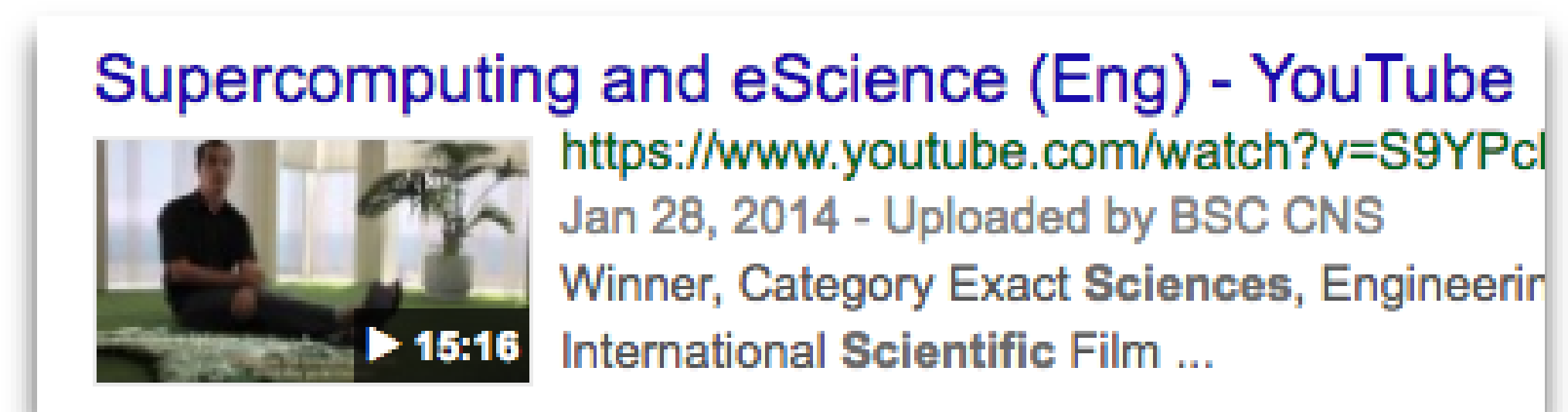
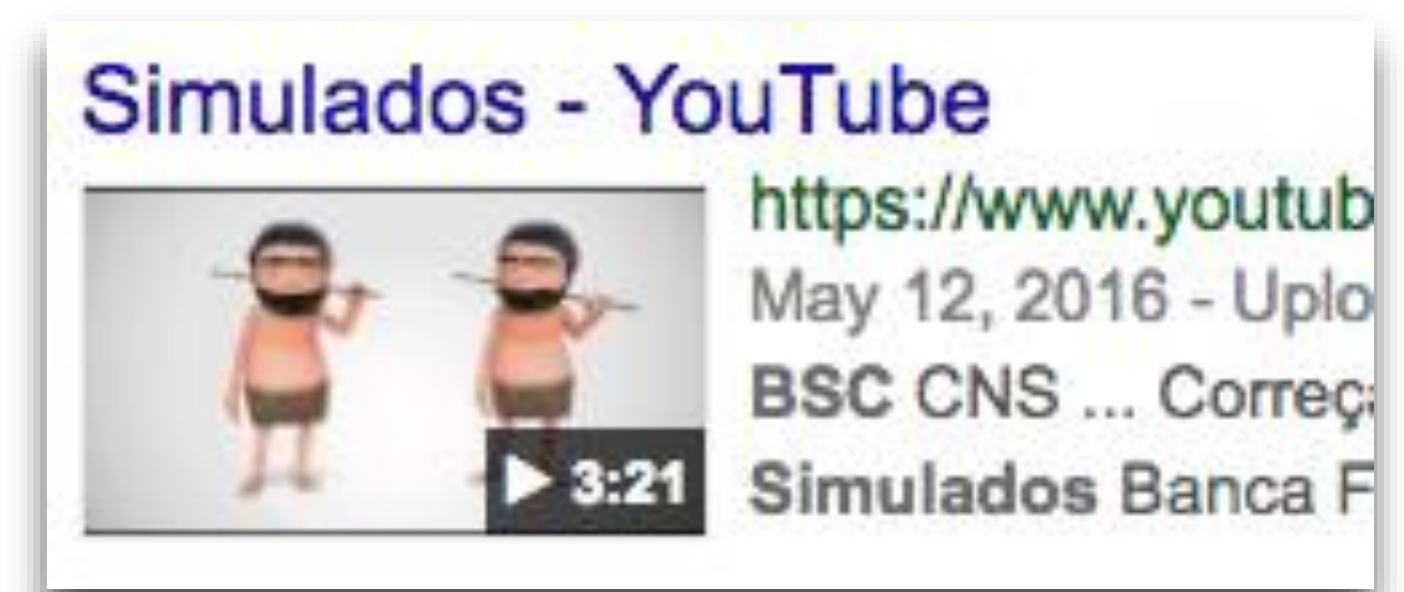
BSC involvement

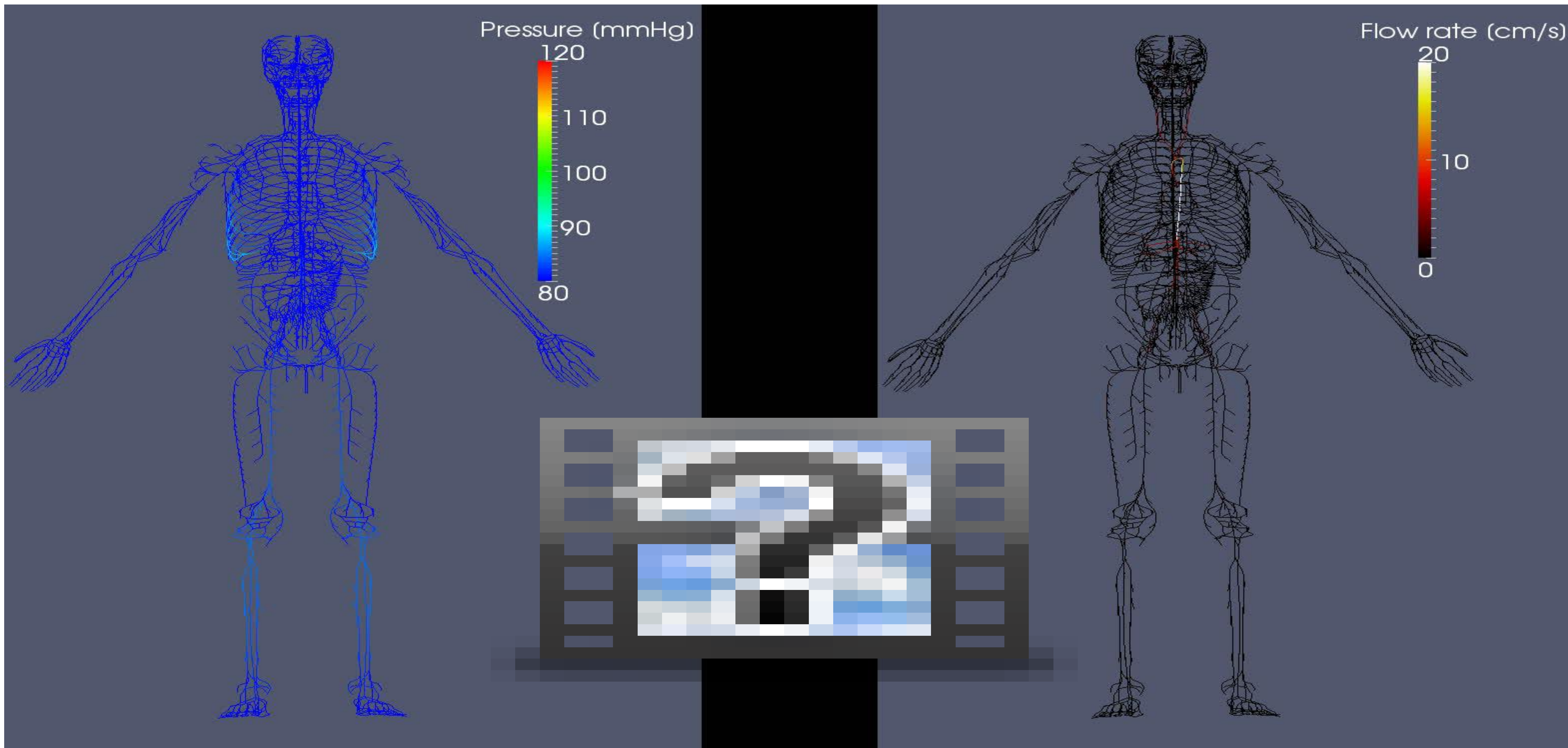
WP3 Training and dissemination:

- Produce dissemination material and work on training actions
- Examples: google “Alya Red computational heart” or “Supercomputing and e-Science” or “Simulados BSC”

WP4 Innovation and sustainability

- Help with the innovation plan







HPC-based Computational Biomechanics

M. Vázquez
Barcelona Supercomputing Center
Spain

CompBioMed Kick-off Meeting
London
3-4 October 2016

