Supercomputers & Biomedical research: High Performance Computational Biomechanics

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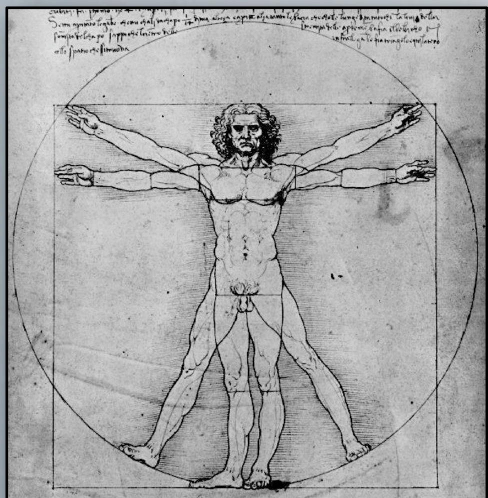
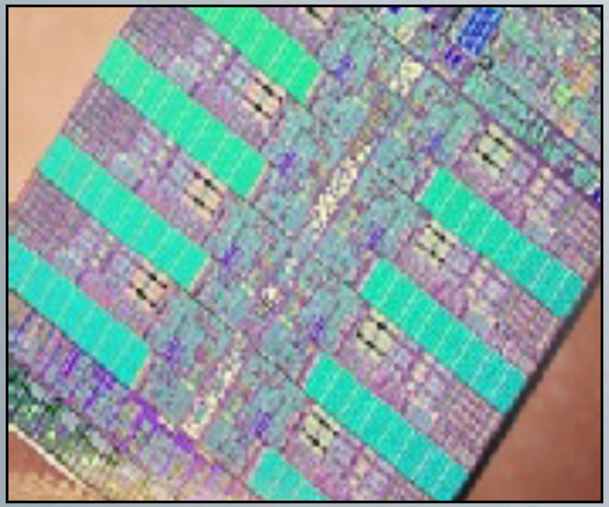
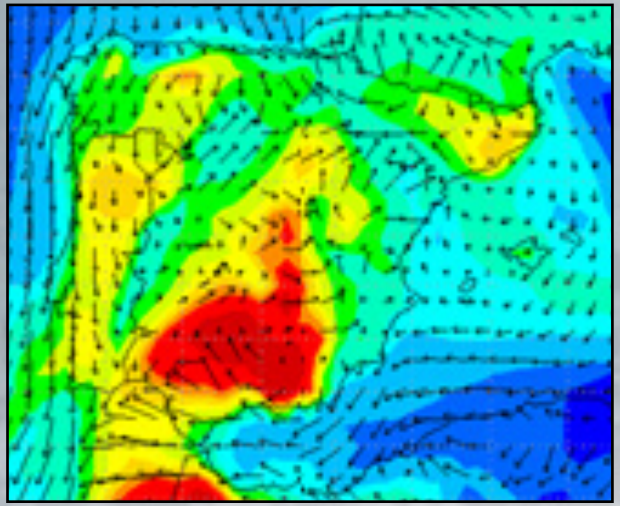


BSC & HPC in Biomedical Research



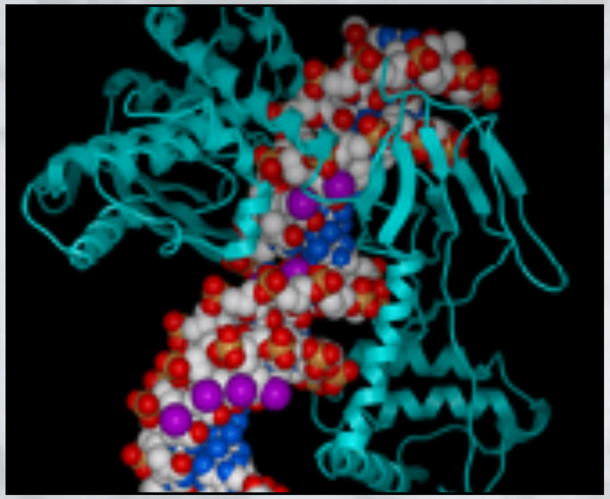
Computer Science

Performance tools
Computer architectures
Programming models



Earth Science

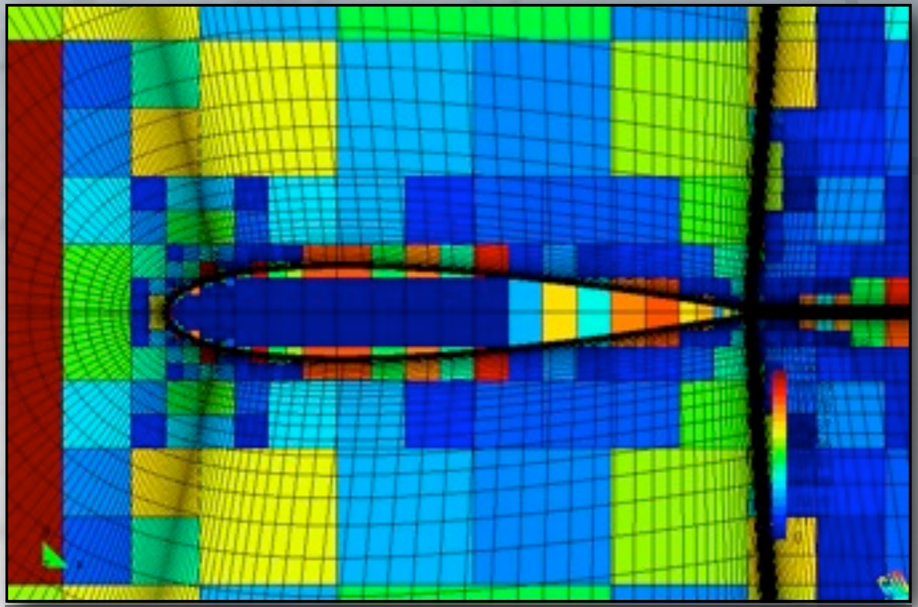
Air quality



Life Science

Genomics
Proteomics

Computer Applications in Science and Engineering
CASE



Environment

Energy

Aerospace

Trains and Automotive

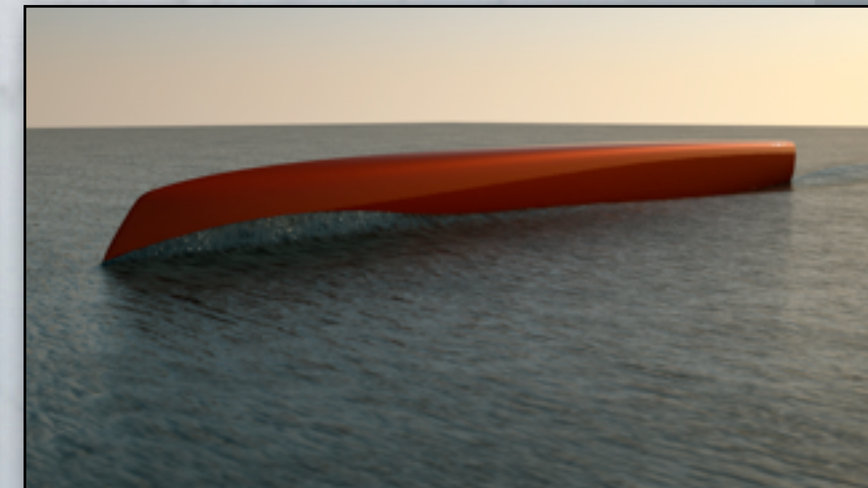
Oil and Gas

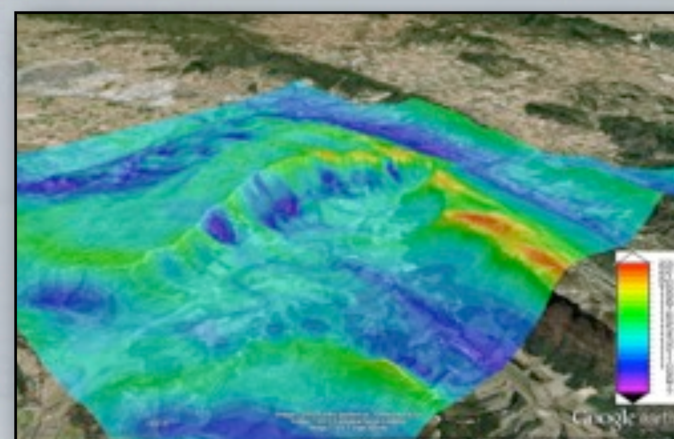
Artificial Societies

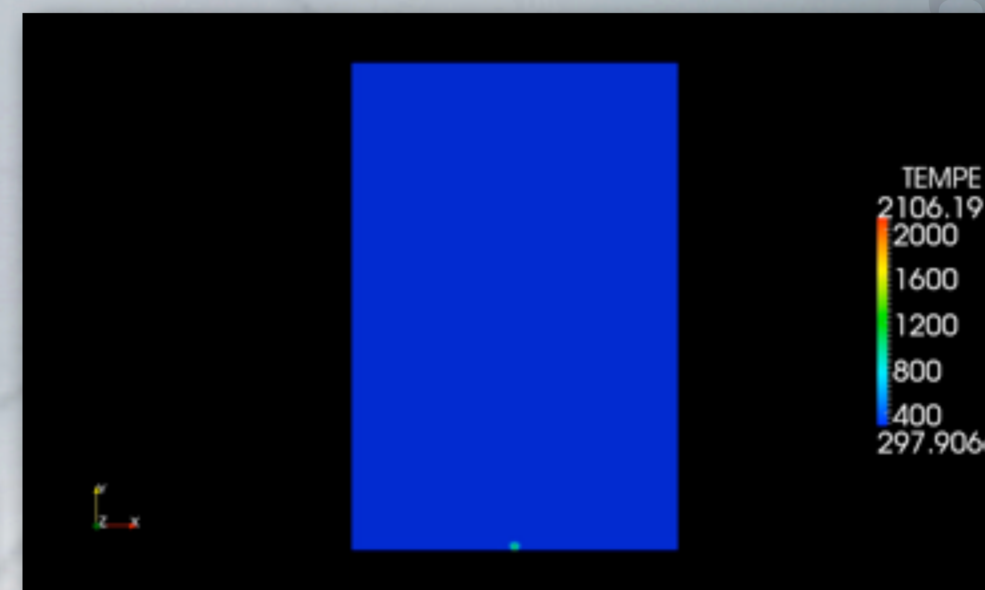
High Energy Physics

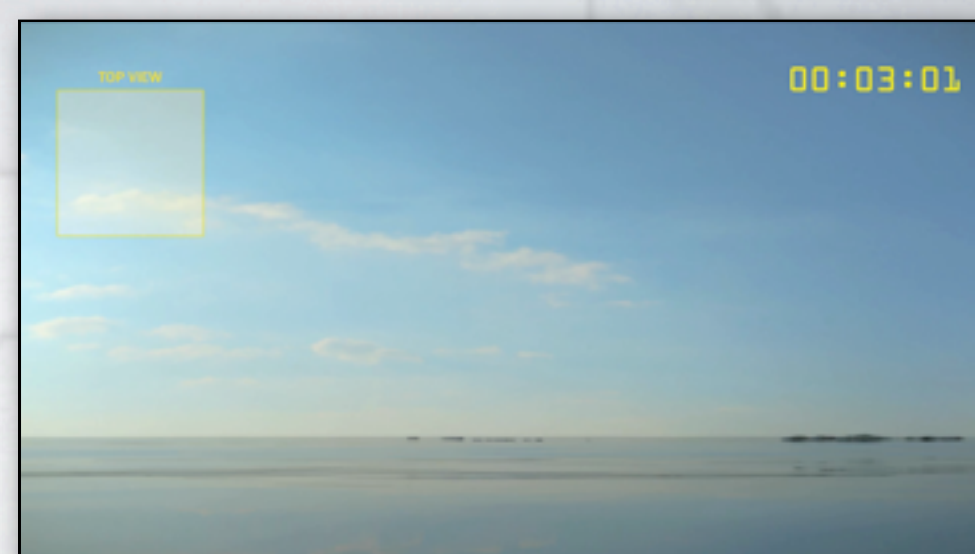
Materials Sciences

Biomechanics





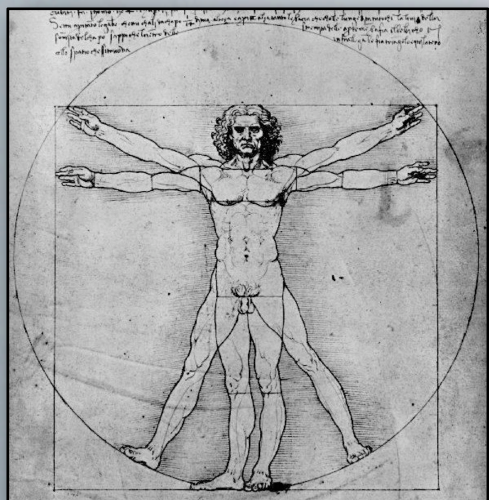




BSC-CNS is the only supercomputing center with +60 researchers devoted to HPC-based Biomedical Research:

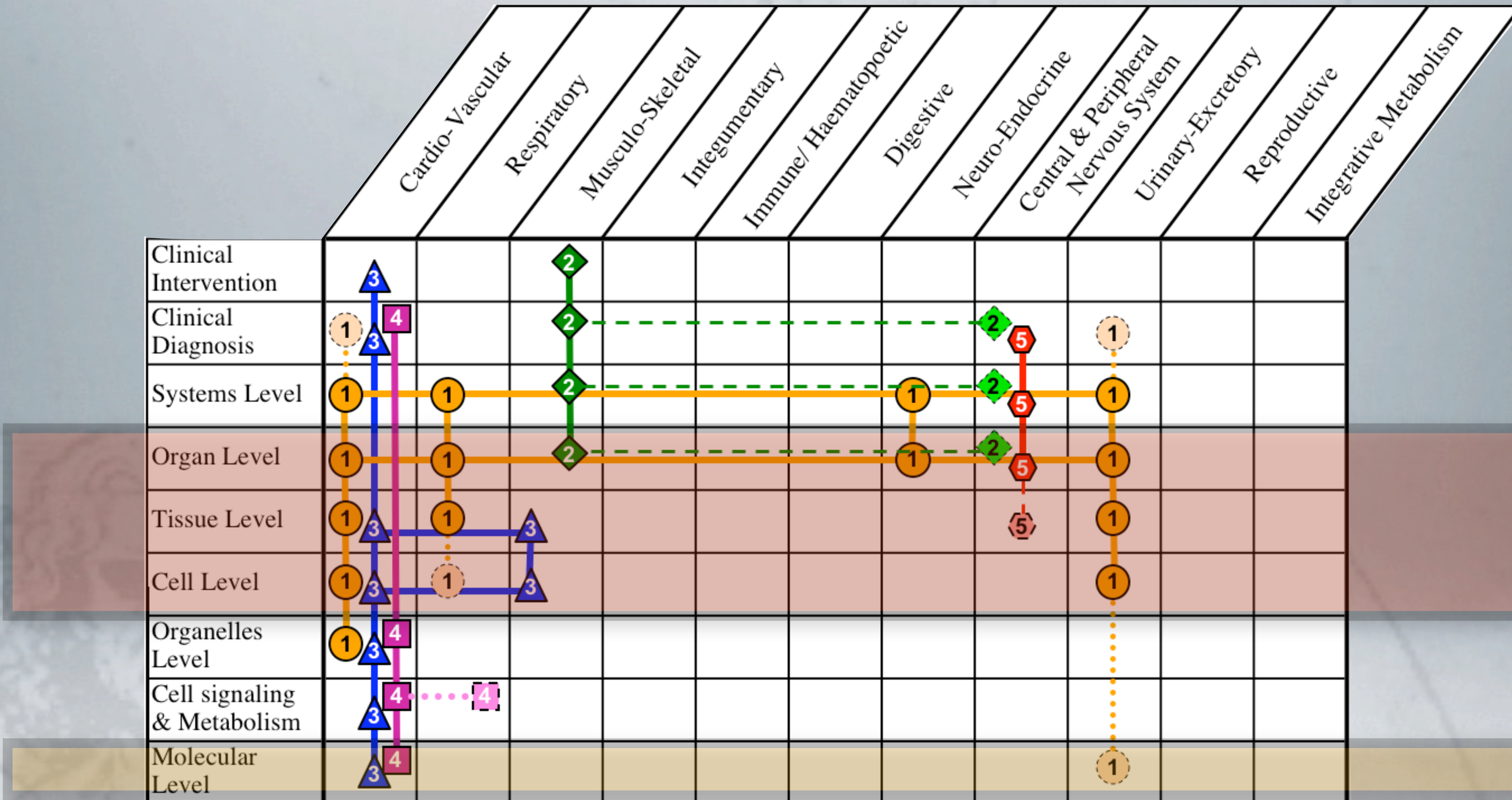
Bioinformatics (45 Life Science Department)

Biomechanics (15 - 20 CASE Department)



Computational Biomechanics

Barcelona Supercomputing Center



Organ Systems vs. Levels of Organizations

Extracted from S.R. Thomas et al., VPH Exemplar Project Strategy Document. Deliverable 9, VPH NoE. 2008

Drugs from the lab to the patients

A finished new drug: **12 to 15 years** to be obtained, can cost over **1 BEuros**

The idea of a target can come from **academia, clinical research or the commercial sector**

It may take **several years** to get a supporting volume of background for that target to be considered in the drug discovery programmes

Then suitable molecules which possess the necessary characteristics are screened to make the drugs.

From *Principles of early drug discovery. Br J Pharmacol. 2011 March, 162(6):1239-1249.*

Our goal: Speed up all the process, reduce costs and improve success rate.

Drugs from the lab to the patients

Why could a drug fail in the clinic?

- They do not work
- They are not safe.

Molecular interactions are **not the only set** of variables in a physiological system.

Reasons for fail or success:

- Overall interaction of various components
- Dynamical responses
- Non-directly related mechanisms
- Coupling with a larger system

Understanding biological systems

Biological systems are extremely complex

Strong variability

High degree of uncertainty in the Physiological models

Scarce experimental dada

Costly experiments

Test

Improve modeling

Predict behavior

Keywords

Drug action

Drug delivery

Treatment planning

Medical training

Design: prosthesis, stents, valves, bio-materials, experimental and manufacturing kits...

Study surgical procedures and treatments

...

Targets

Biomedical research: know better and deeper, improve diagnose and treatment

Pharma industry: reduce time and costs of “from-design-to-market” cycle

Medical devices manufacturers: design better devices

The research program

CASE Department: Biomechanics at organ level

Multi-scale & multi-physics problems where HPC is a must

Parallelization on supercomputers (regular use of thousands of cores)

Simulate complex biomedical problems

Deep commitment of MDs in all projects

Strong collaboration links with MDs, physiologists, clinical image researchers

A Computational Man: the best possible “dummy” for biomedical research

First, create the dummy. **Then**, adapt it to patients.

Medical doctors:

Healing is the final objective
Diagnose and treatment planning

Understanding biological systems
Physiological models

They provide the main motivation and insight to the problem

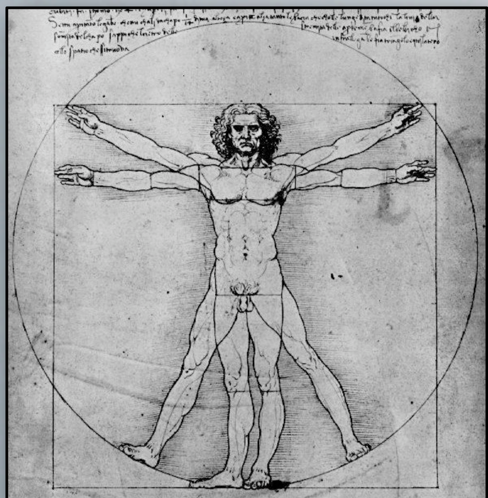
Computational scientists:

Developing computational tools to run simulations

Provide the required simulation capacity

Bio-engineers:

Develop the Physiological models
Deal with medical image processing
Design data acquisition tools



Alya Red
HPC-based Biomechanical Simulations

Cardiac computational models
Respiratory system
Cerebral aneurisms rupture risk
Long skeletal muscles
Biomaterials and tissue engineering

The Alya System

Multi-physics modular code for High Performance Computational Mechanics

Born in 2004

Designed from scratch to solve multiphysics problems with high parallel efficiency

Numerical solution of PDE's

Variational methods are preferred (FEM, FVM)

Hybrid meshes, non-conforming meshes

Explicit and Implicit formulations

Coupling between multi-physics (loose or strong)

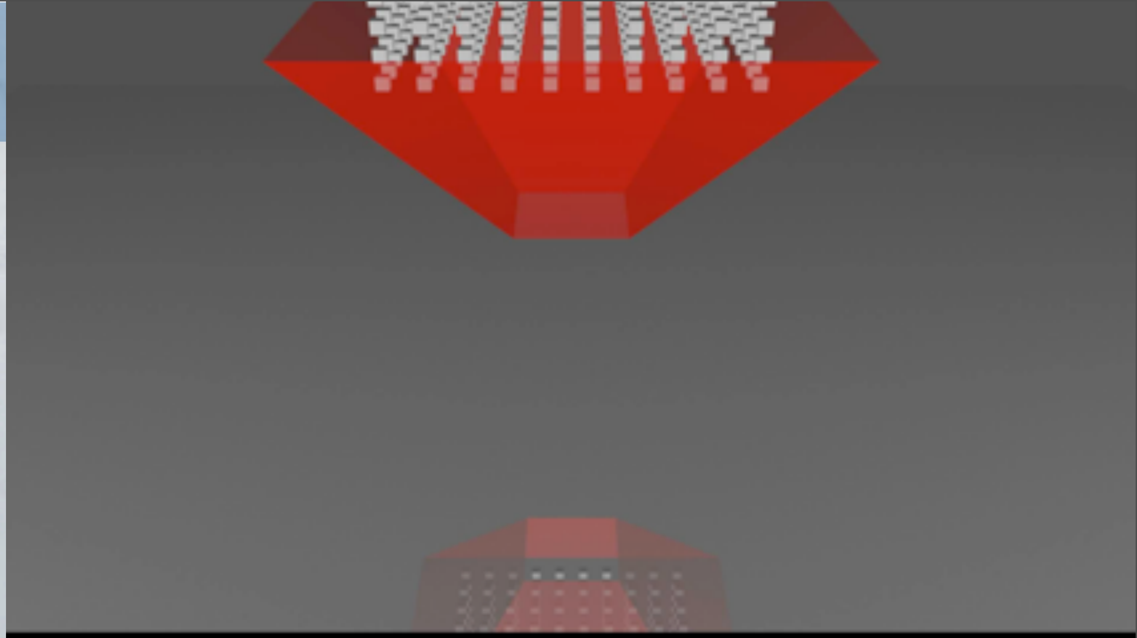
Advanced meshing issues

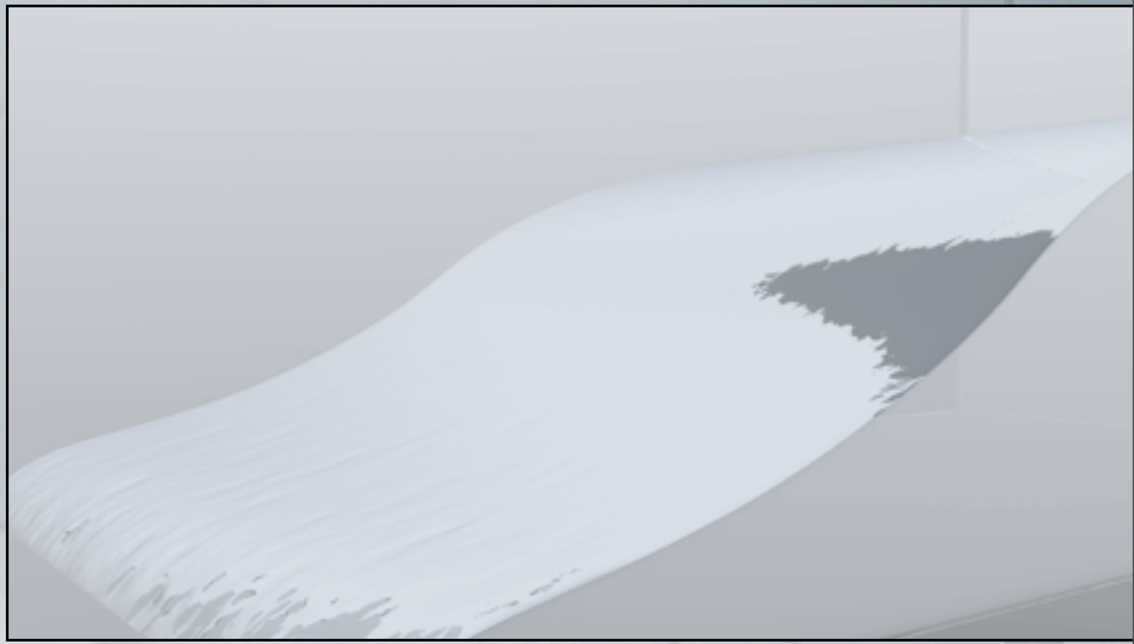
Parallelization by MPI and OpenMP

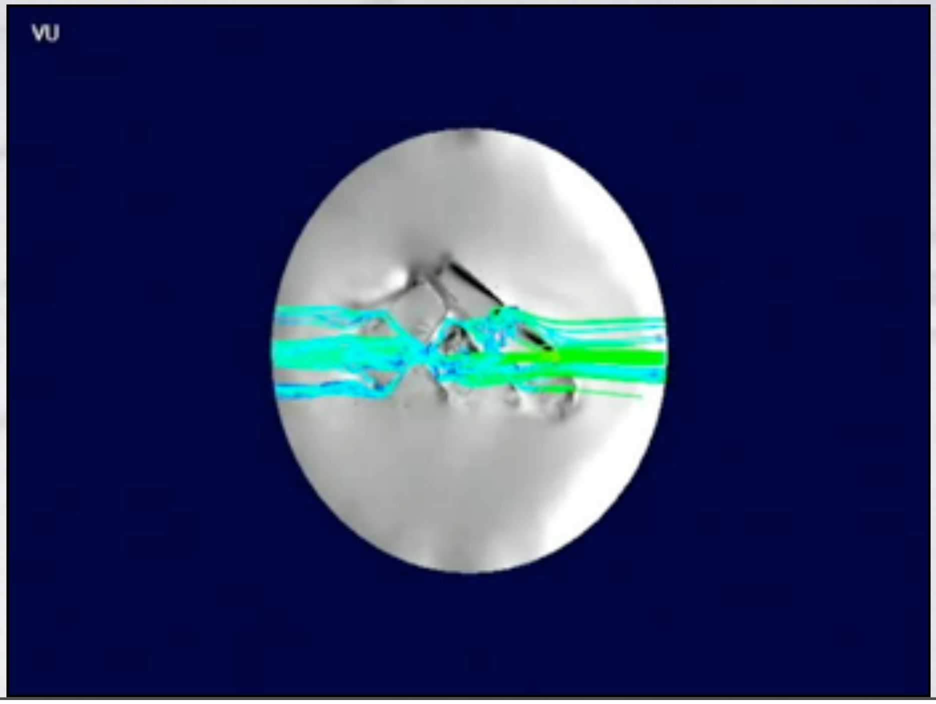
Automatic mesh partition using Metis

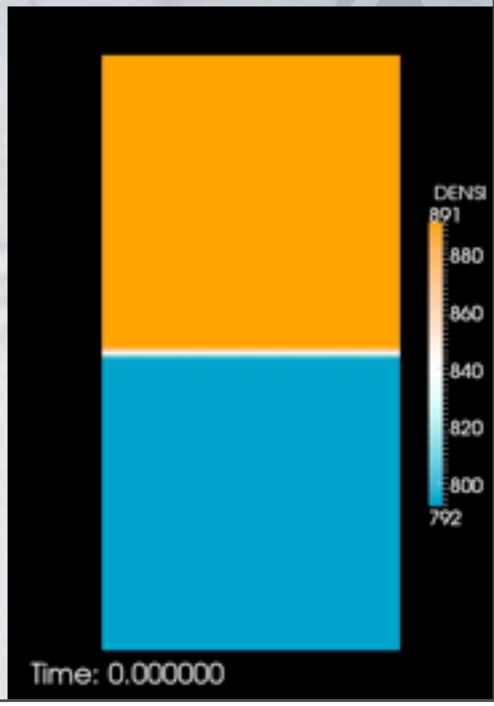
Portability is a must

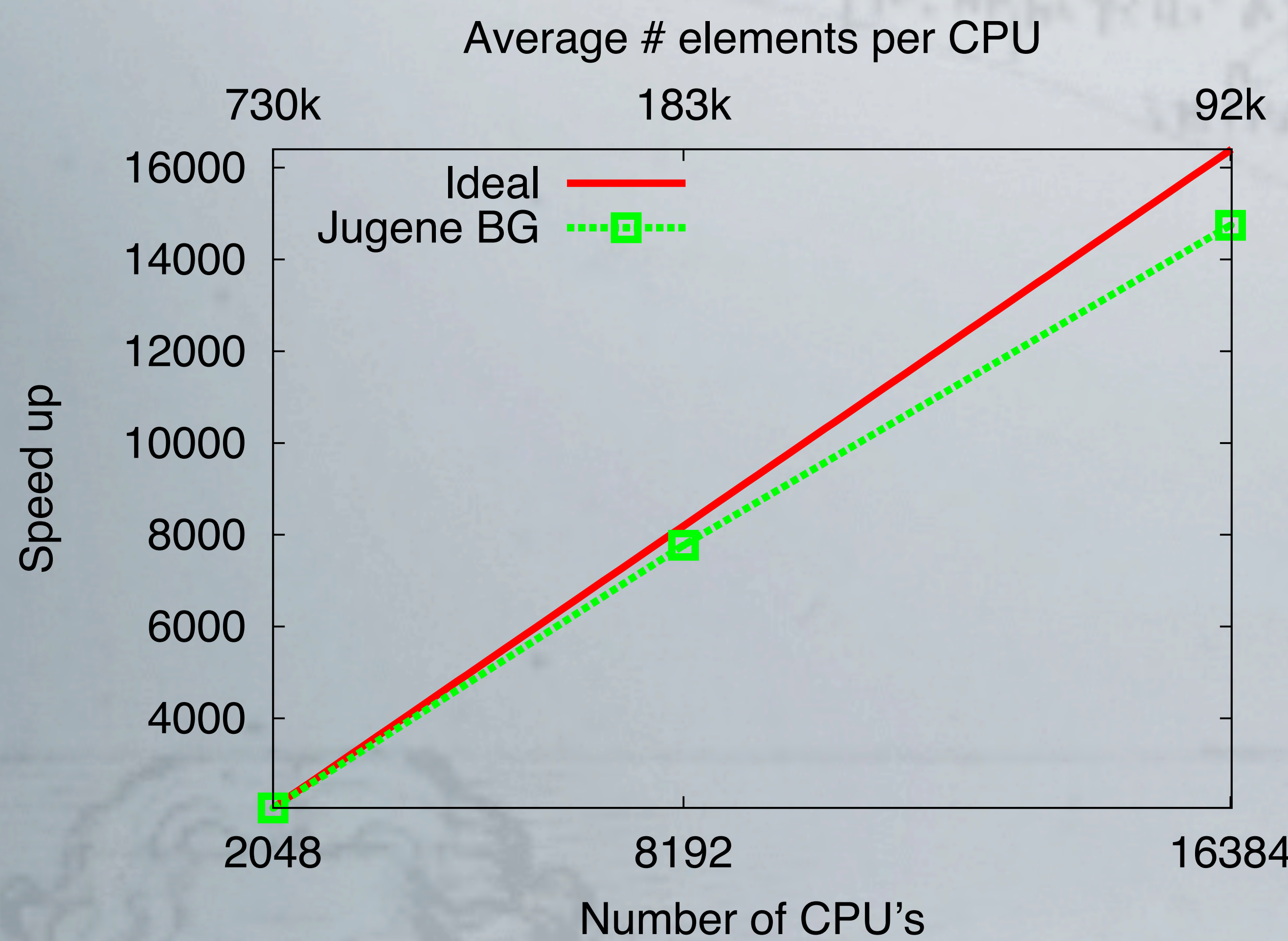
Porting to new architectures: MICs, GPUs, ...

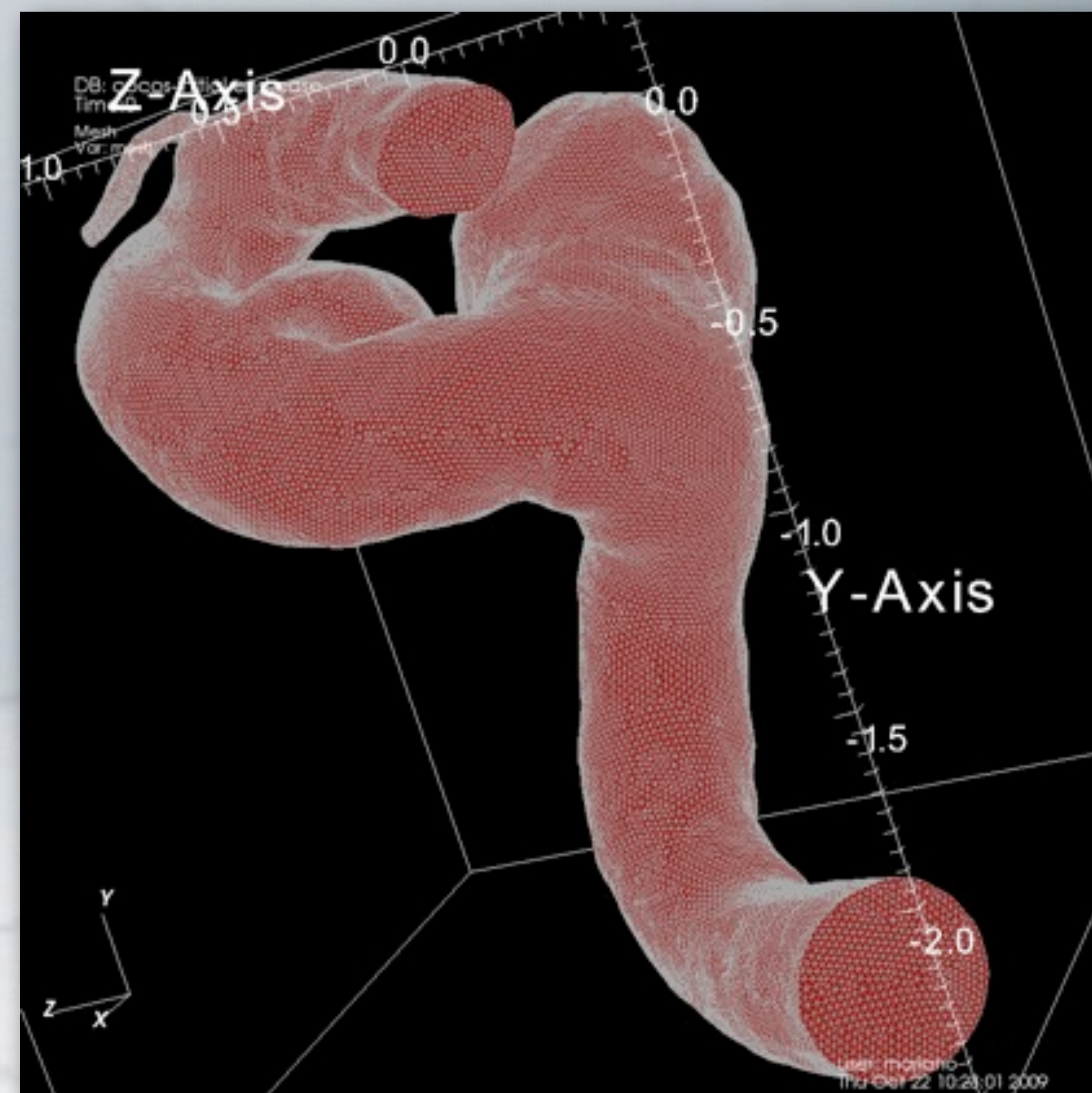












Benchmark

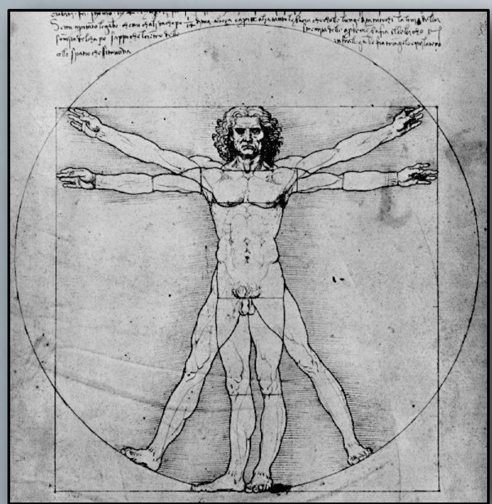
Aneurism geometry provided by R. Cebral

Uniform refinement up to 1.6B tetrahedra

Incompressible flow

Implicit formulation

Algebraic Fractional Step: BCGStab + Deflated CG



Alya Red

HPC-based Biomechanical Simulations

Cardiac computational models

Respiratory system

Cerebral aneurisms rupture risk

Long skeletal muscles

Biomaterials and tissue engineering

Cardiac Computational Model

Muscle pumping action of the heart

The Cardiovascular In-Silico Experimental Laboratory

Multiphysics - multiscale

Complex geometries

Very expensive computational modelling

HPC-based

As comprehensive as possible

Cardiac Computational Model

Muscle pumping action of the heart

The Cardiovascular In-Silico Experimental Laboratory

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As comprehensive as possible

The goals:

A computational scenario to implement models and analyze their behavior under different conditions

Study healthy hearts, pathologies, treatments, drugs action

Adapt the mean model to patients

Cardiac Computational Model

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Debora Gil, Ferrán Poveda and Agnés Borràs
Centro de Visión por Computador
Universitat Autonoma de Barcelona (Spain)

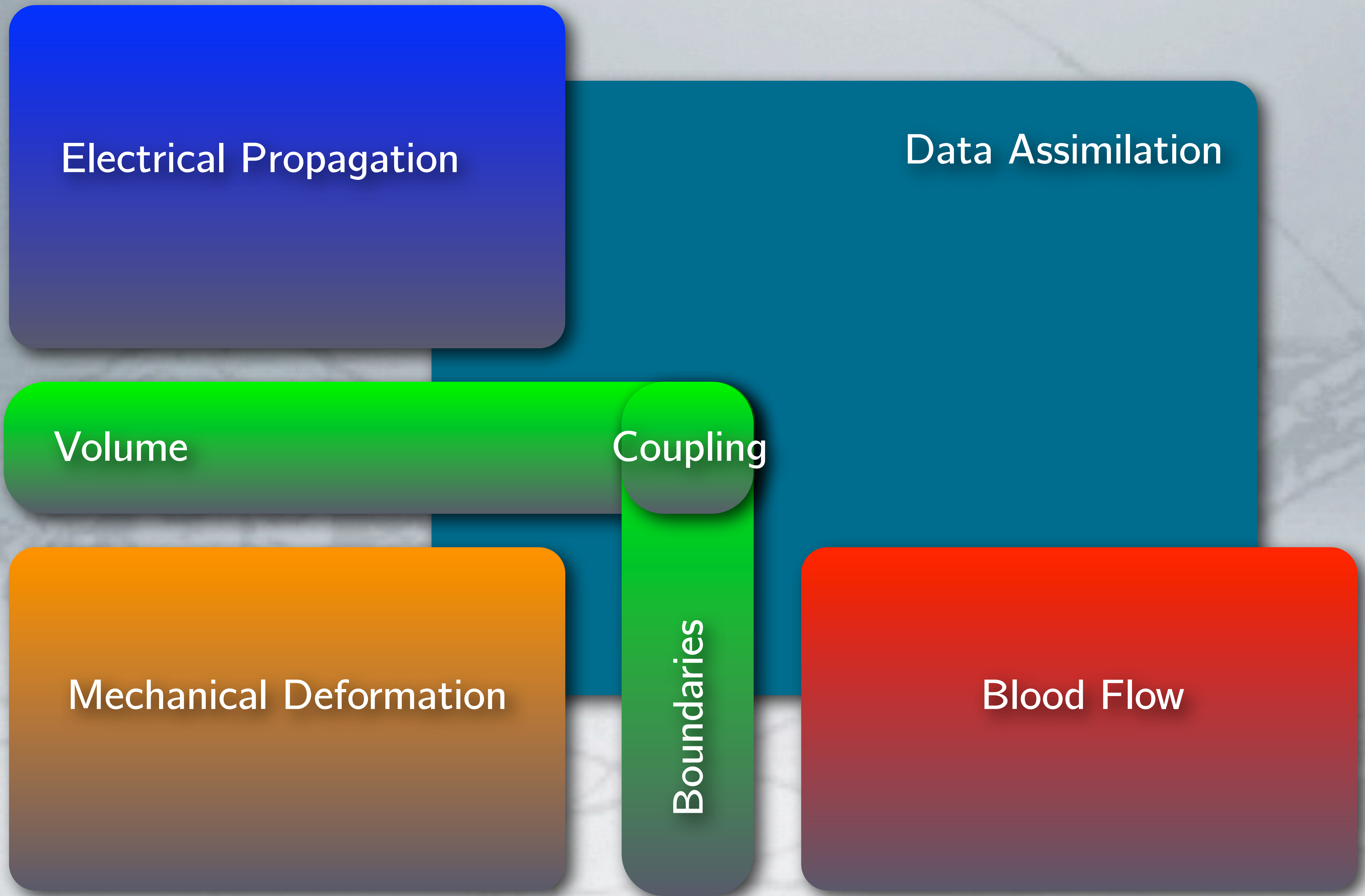
Pablo Blanco, Lab. Nac. de Cálculo Científico (Brasil)

Antoine Jerusalem, University of Oxford (UK)

Dan Einstein, Pacific Northwest National Lab (USA)

Pablo Lamata and David Nordsletten, King's College London (UK)

Cardiac Computational Model



Cardiac Computational Model

Electrical Propagation

Electrophysiology:

Linear anisotropic (fibers) diffusion + non-linear source terms

Volume

Electro-mechanical coupling, Ca+ is the key

ALE + Immersed Boundaries

Mechanical Deformation

Boundaries

Blood Flow

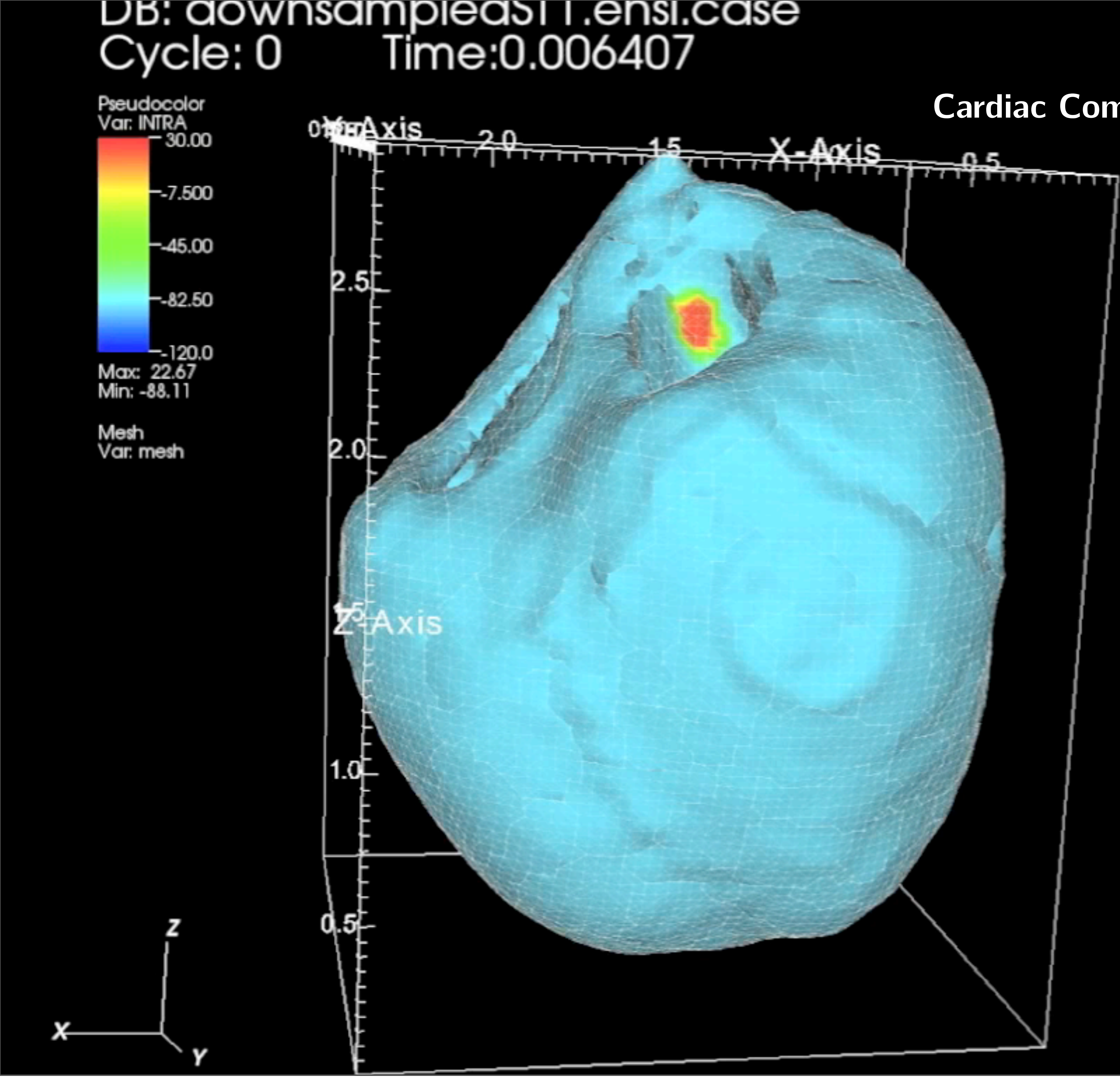
Mechanical deformation:

Large deformations + non-linear material models

Incompressible Flow

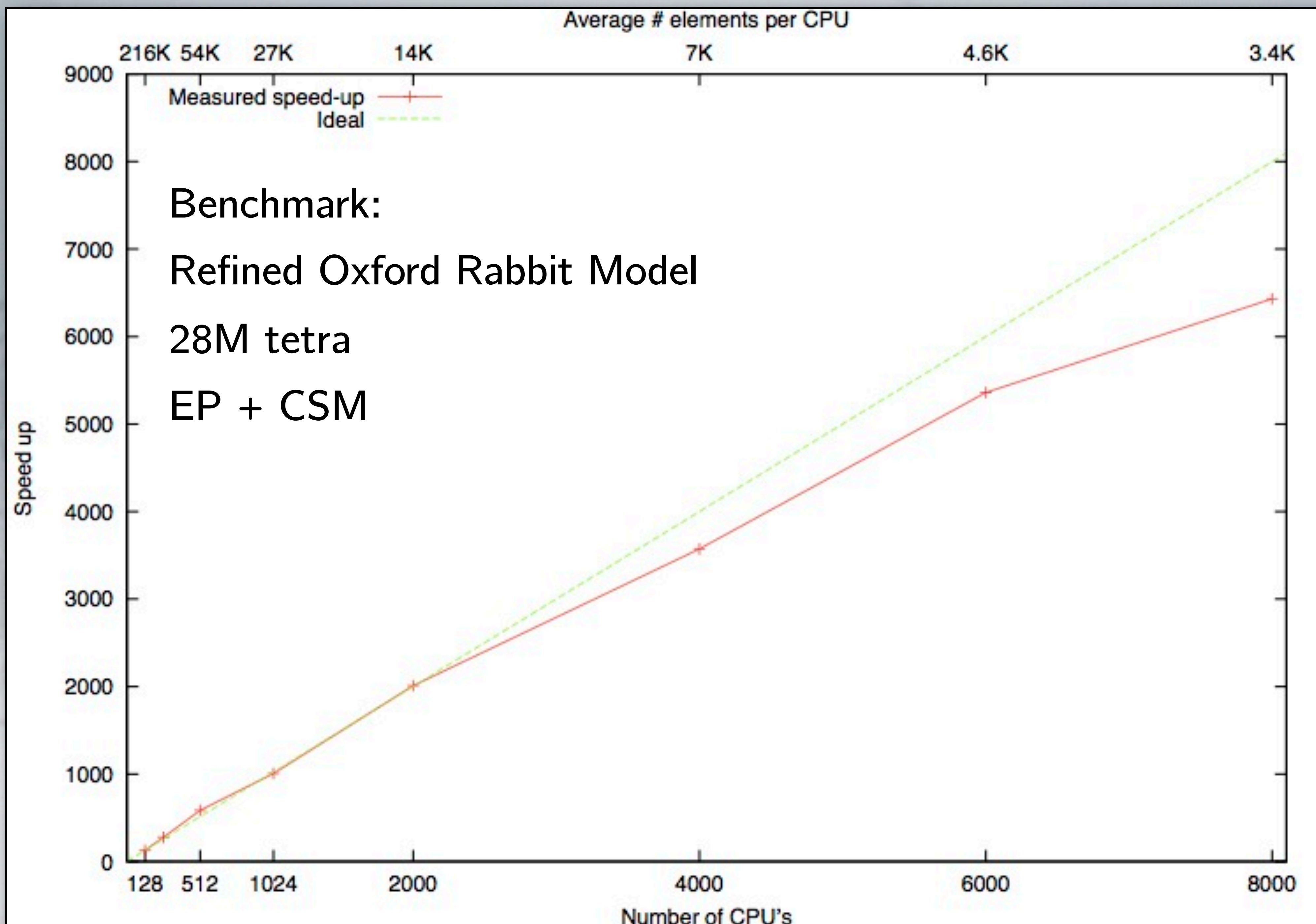
Biomechanics

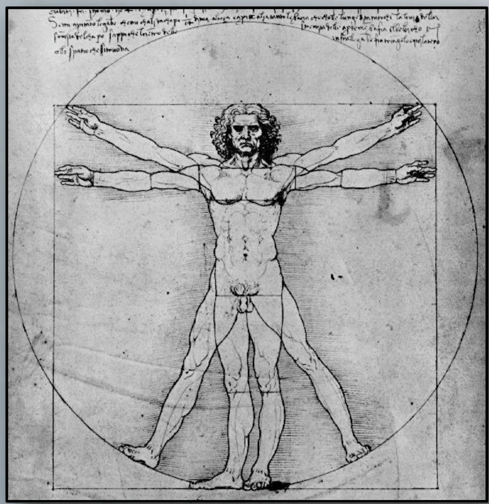
Cardiac Computational Model



Scalability: Electro - Mechanical problem

Marenostrum III - BSC





Alya Red

HPC-based Biomechanical Simulations

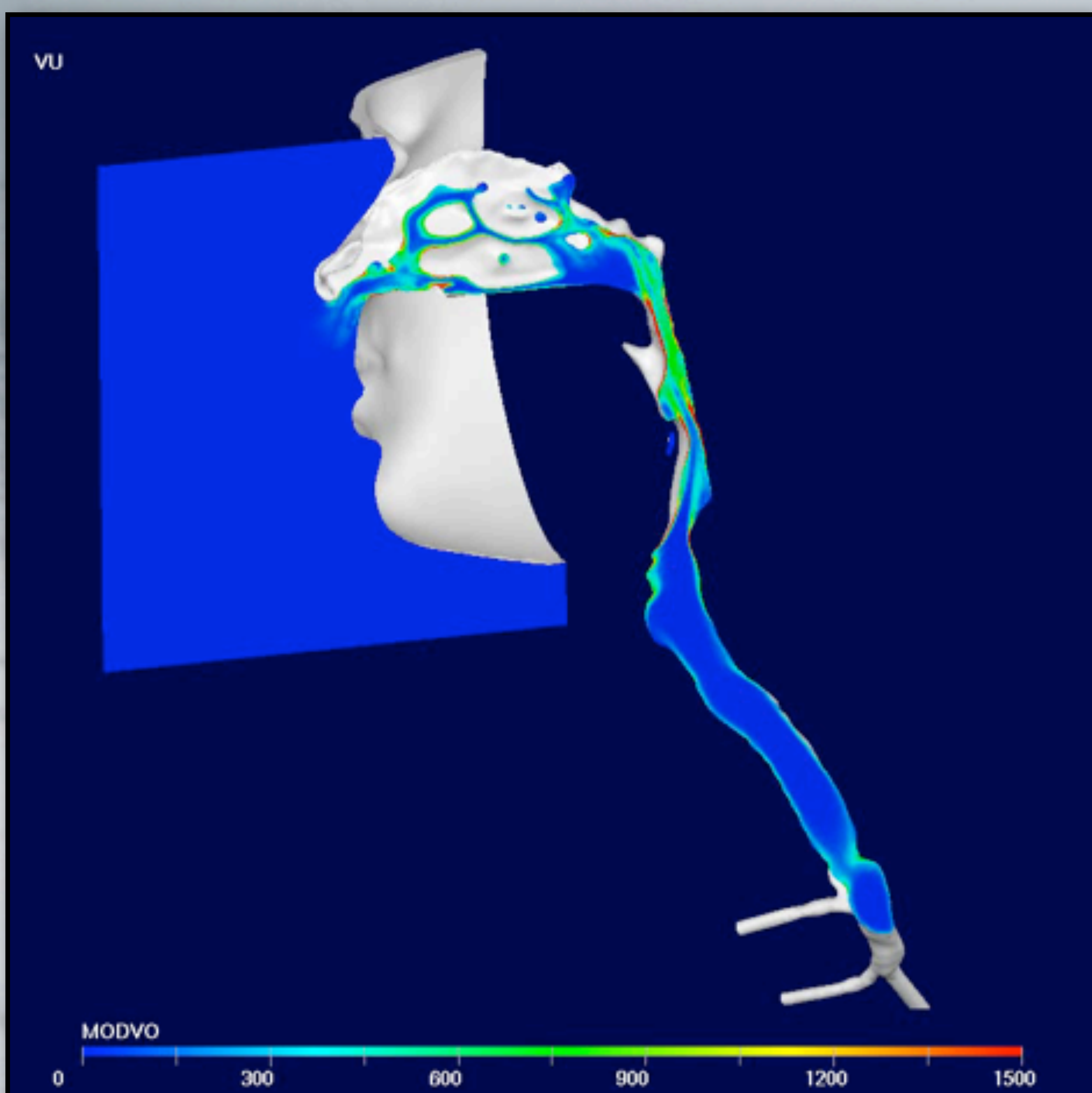
- Cardiac computational models
- **Respiratory system**
- Cerebral aneurisms rupture risk
- Long skeletal muscles
- Biomaterials and tissue engineering

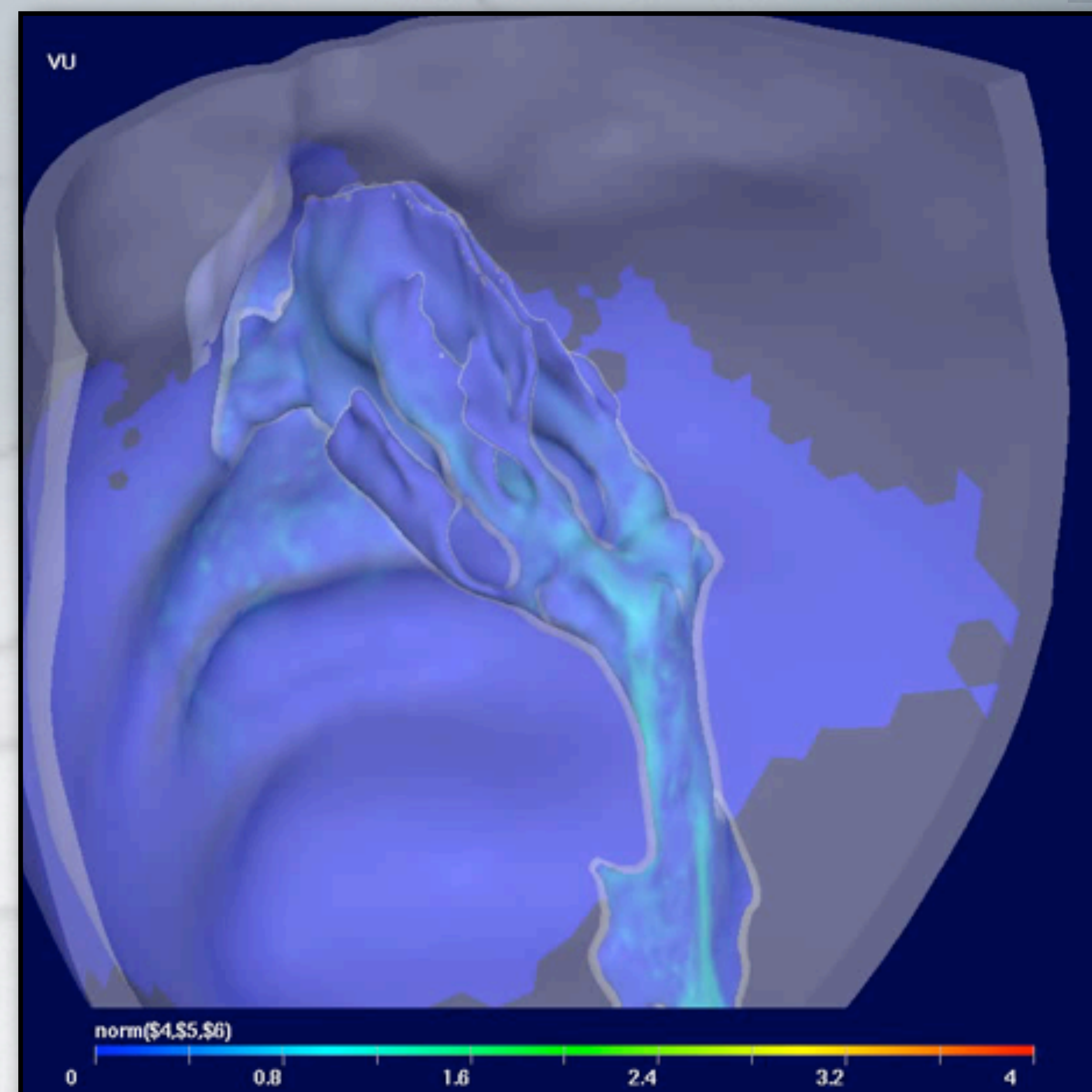
Barcelona Supercomputing Center

Respiratory system

European PRACE project: The Computational Respiratory System
In collaboration with Imperial College London - Jackson State Univ.

Transitional flow
30 million CPU hours allotted in Jugene and Curie
Heavy postprocess





The Computational Dummy

A Computational Man: the best possible "dummy" for biomedical research

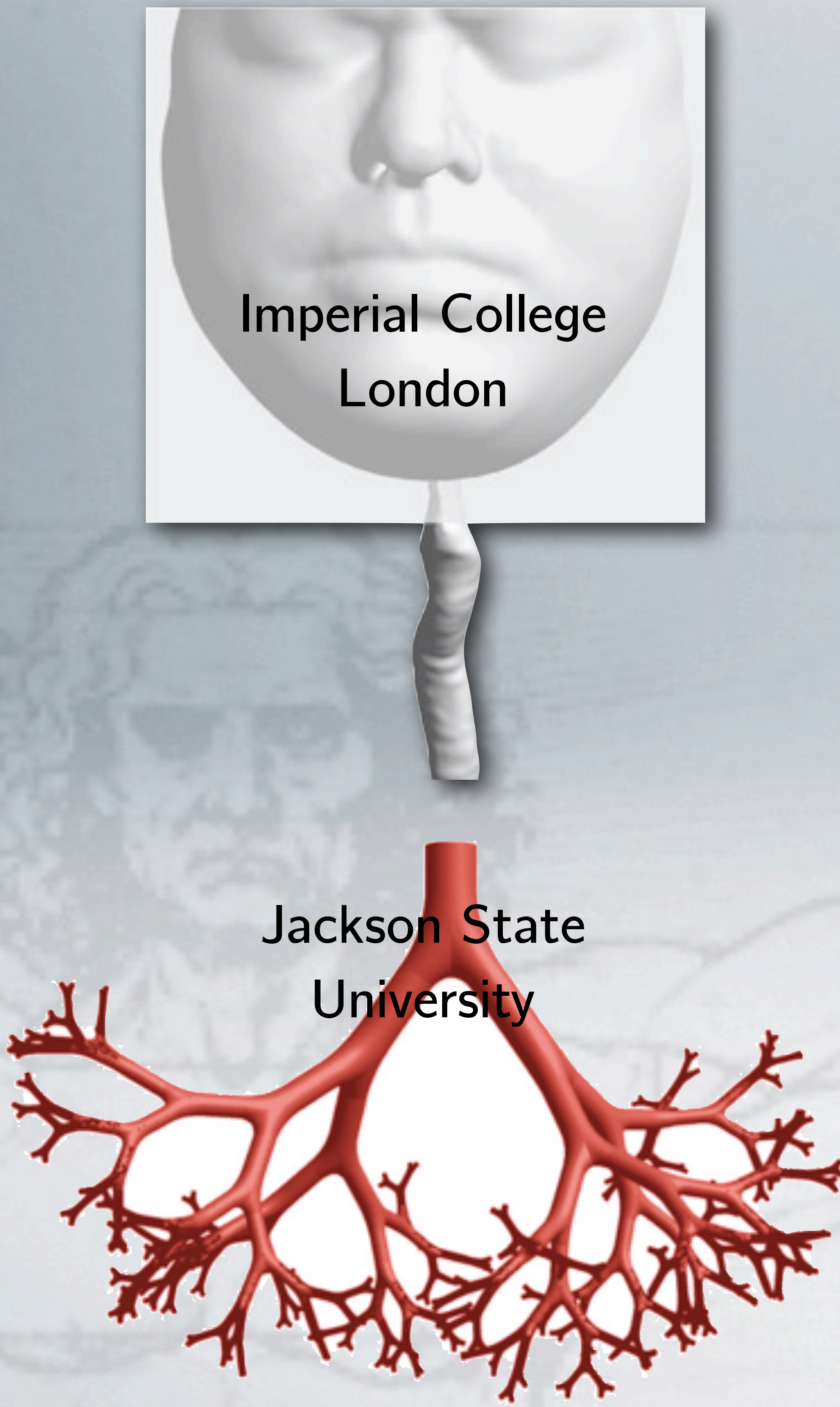
First, create the dummy. **Then**, adapt it to patients.

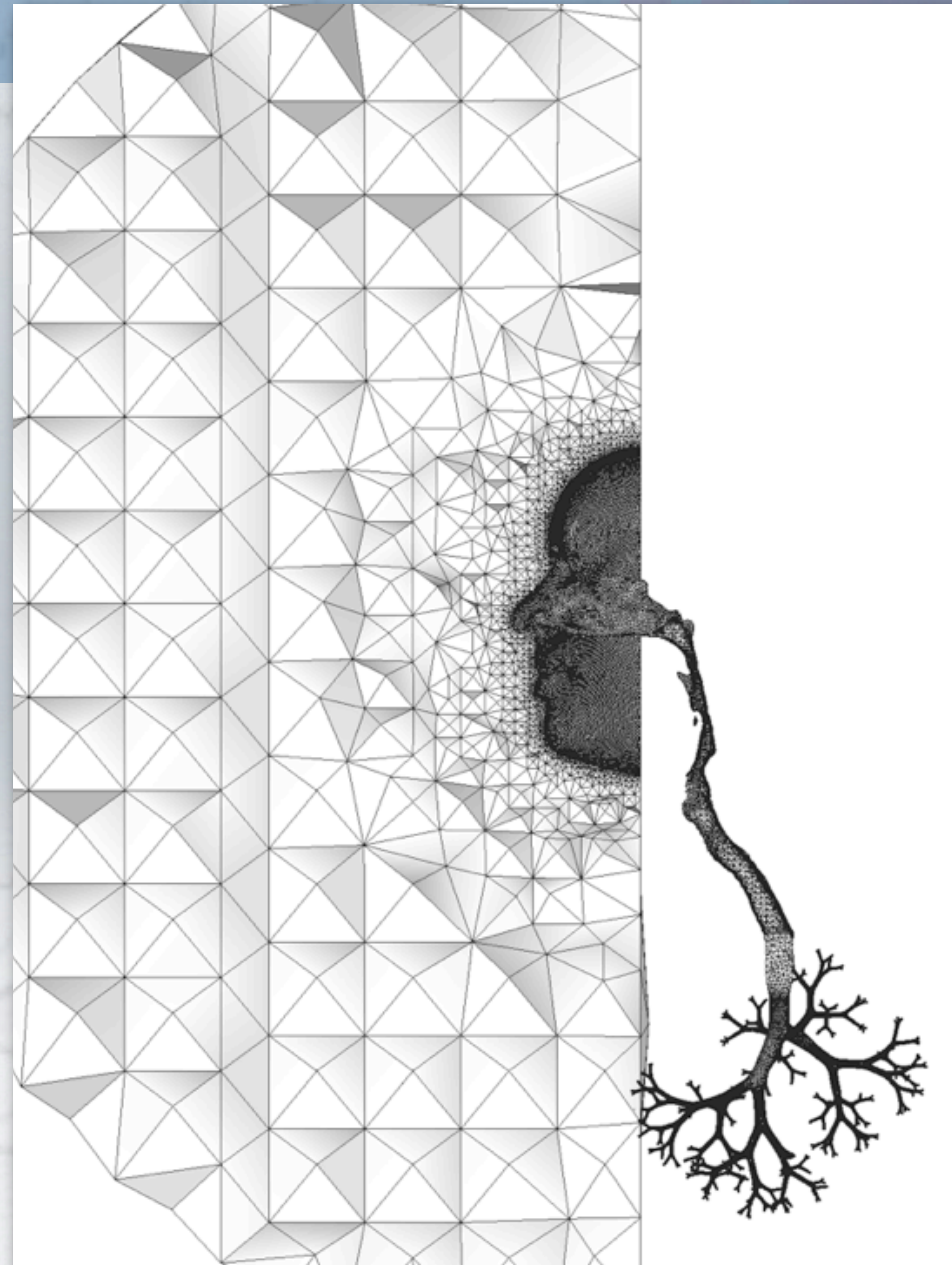
Case I: Perform simulations on the dummies and offer the data-base for analysis

Case II: Perform simulations on the dummies for biomedical design

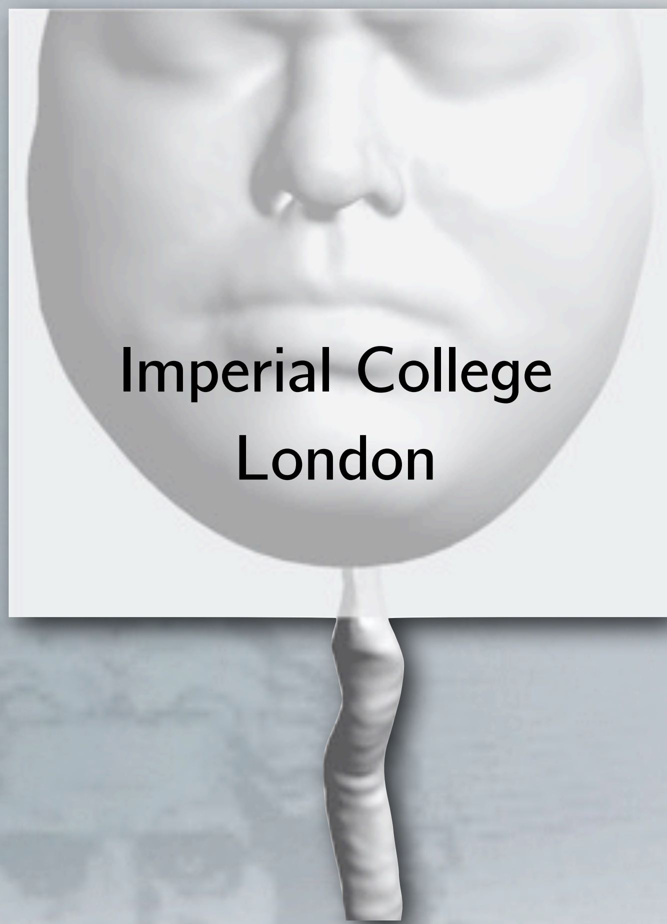
Case III: Perform personalized simulations on patients for diagnose and treatment

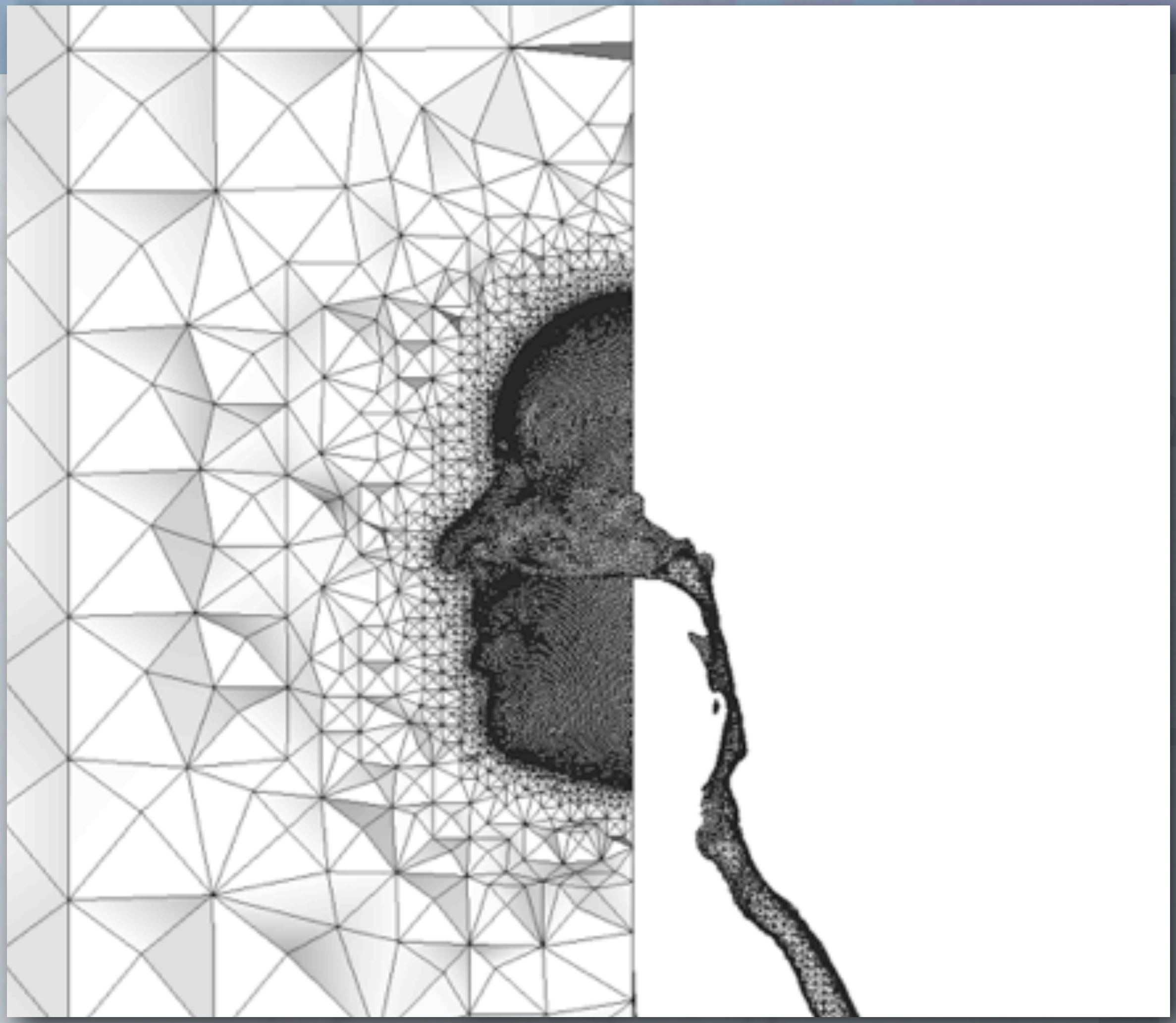
Respiratory system

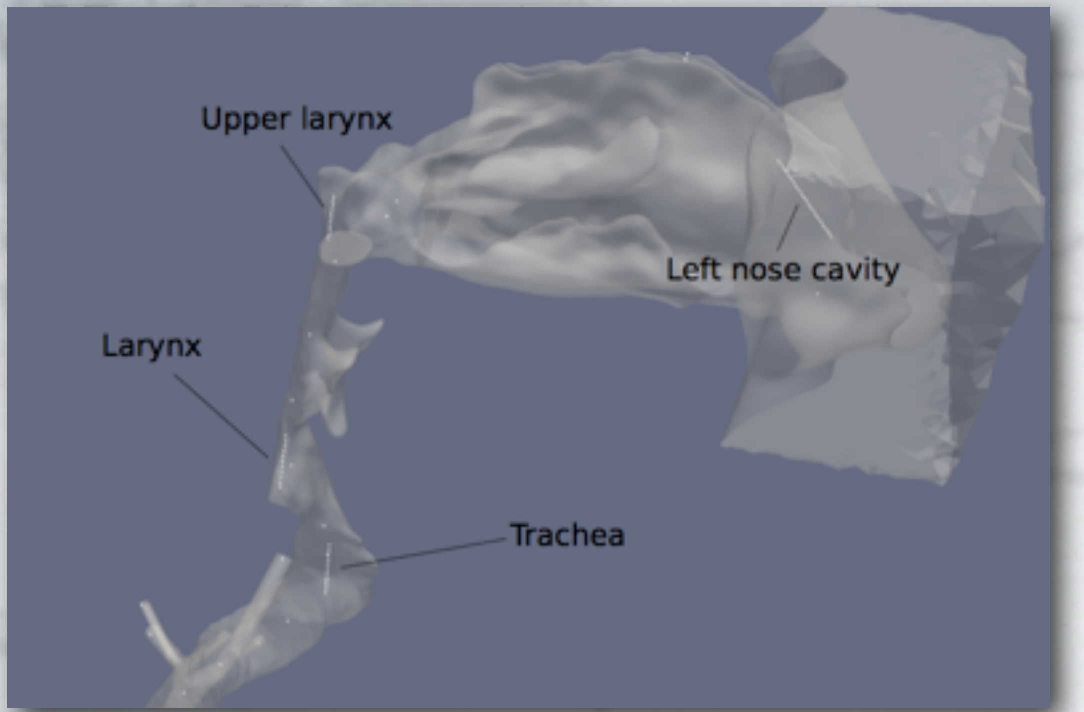


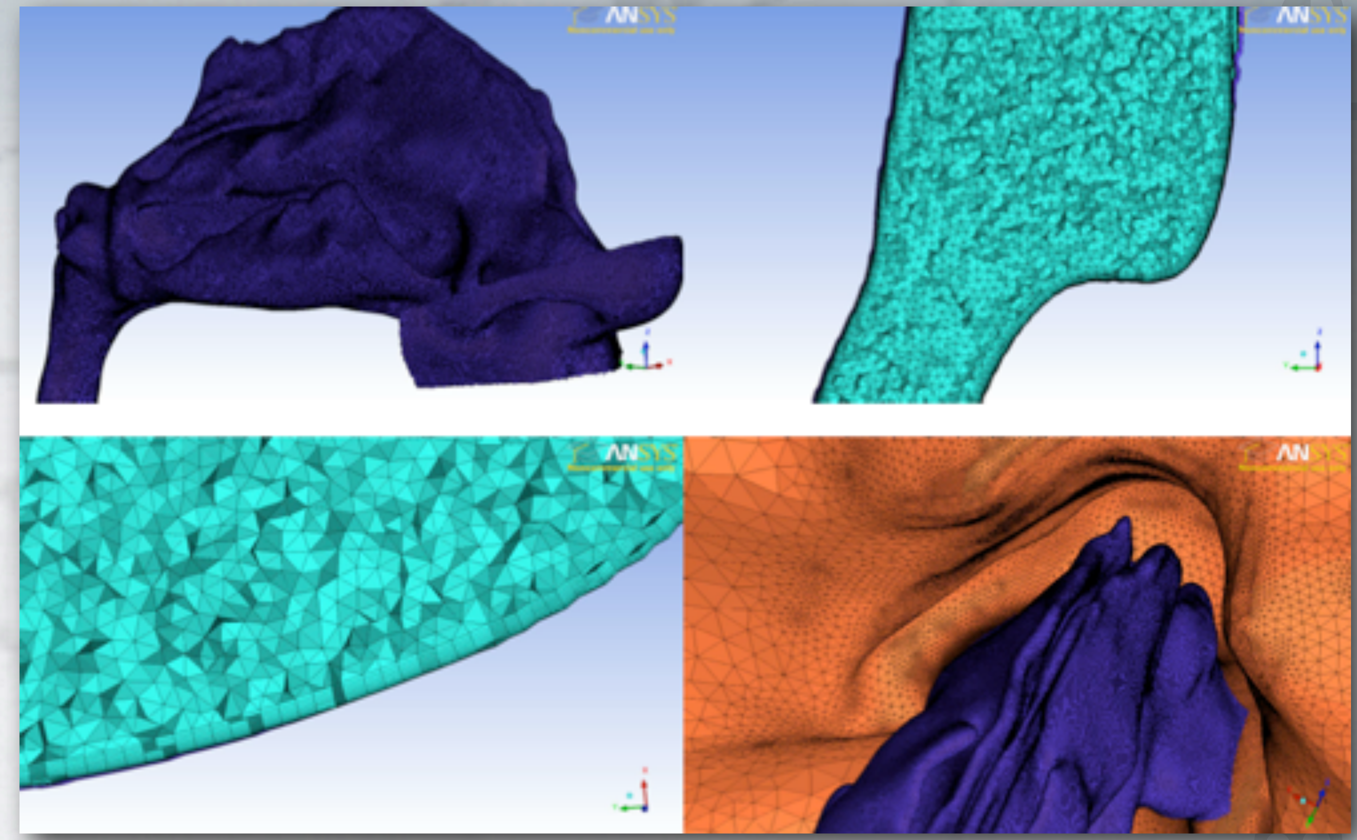


Respiratory system

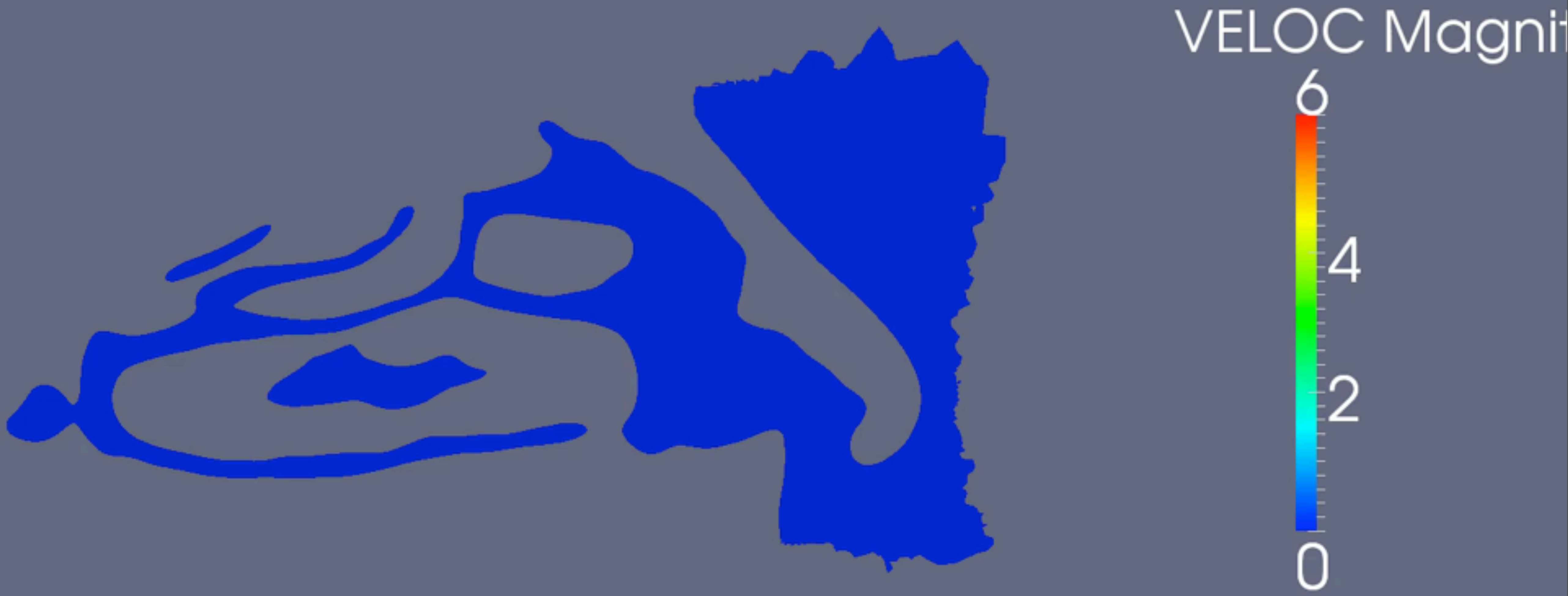








Respiratory system



Vertical section of the Nose Cavity

356 M elements (tetrahedra + prisms)

Massive particle tracking

Scenario:

High definition CFD simulations (tens to hundreds million elements)

Complex geometries, as complete and comprehensive as possible

Up to several million Lagrangian particles tracked, labelled to be identified

Trajectories computed on the fly, not as postprocess

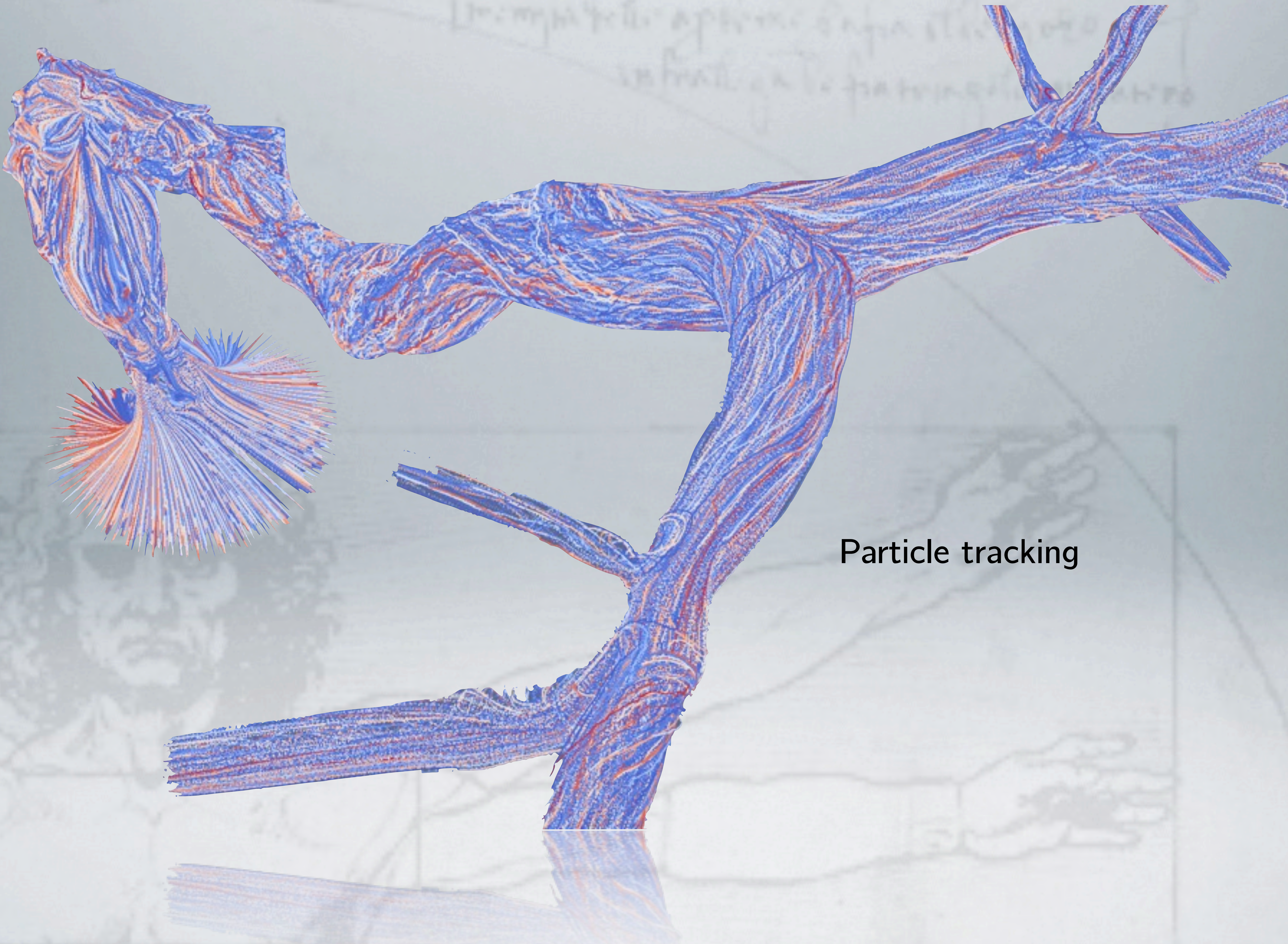
Hundreds of processors for each run

Several runs: gender, age, Physical condition; all run at different regimes

Run the simulations

Create a data base and analyze the results

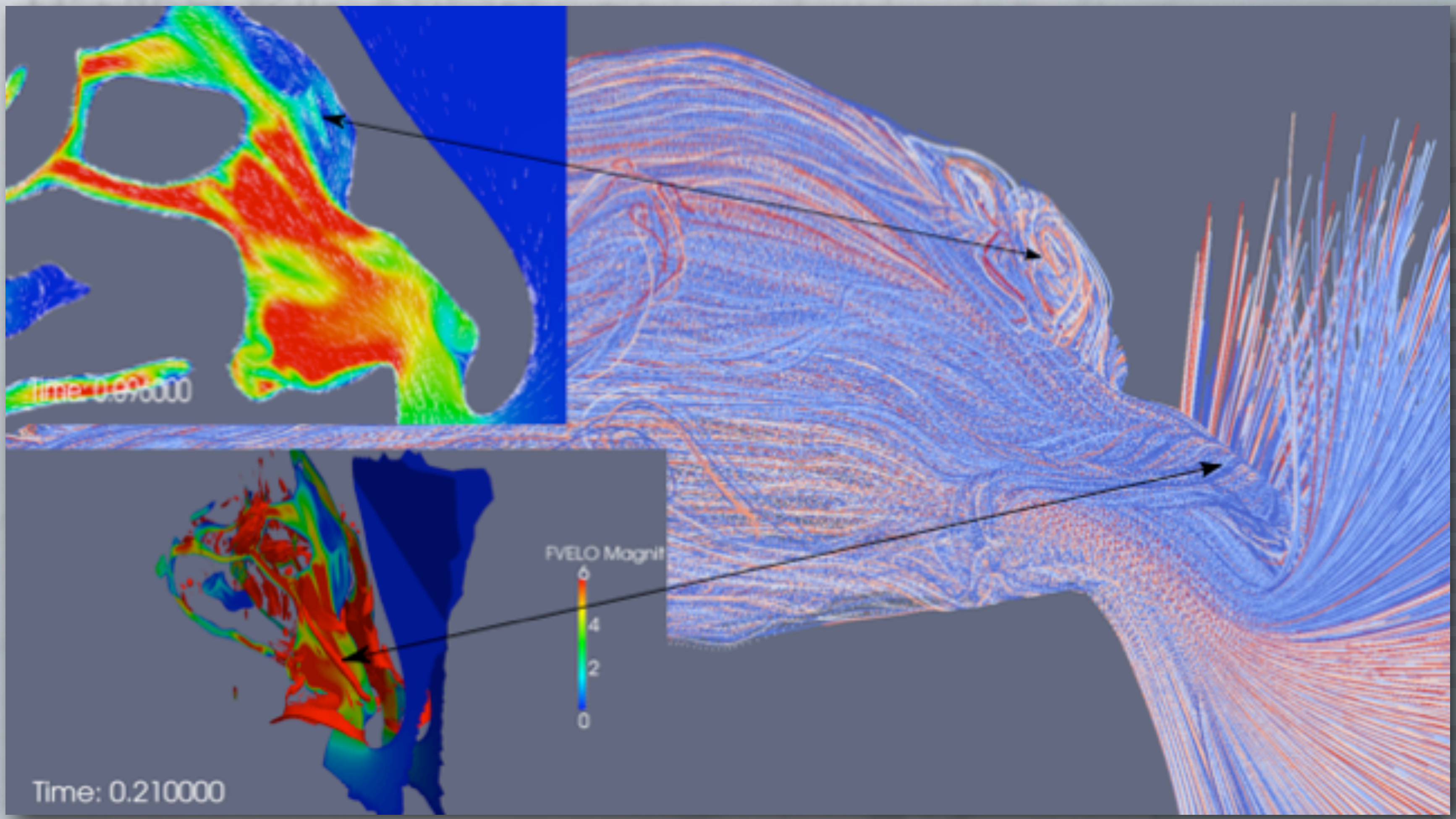
How could we identify and track the particles efficiently?

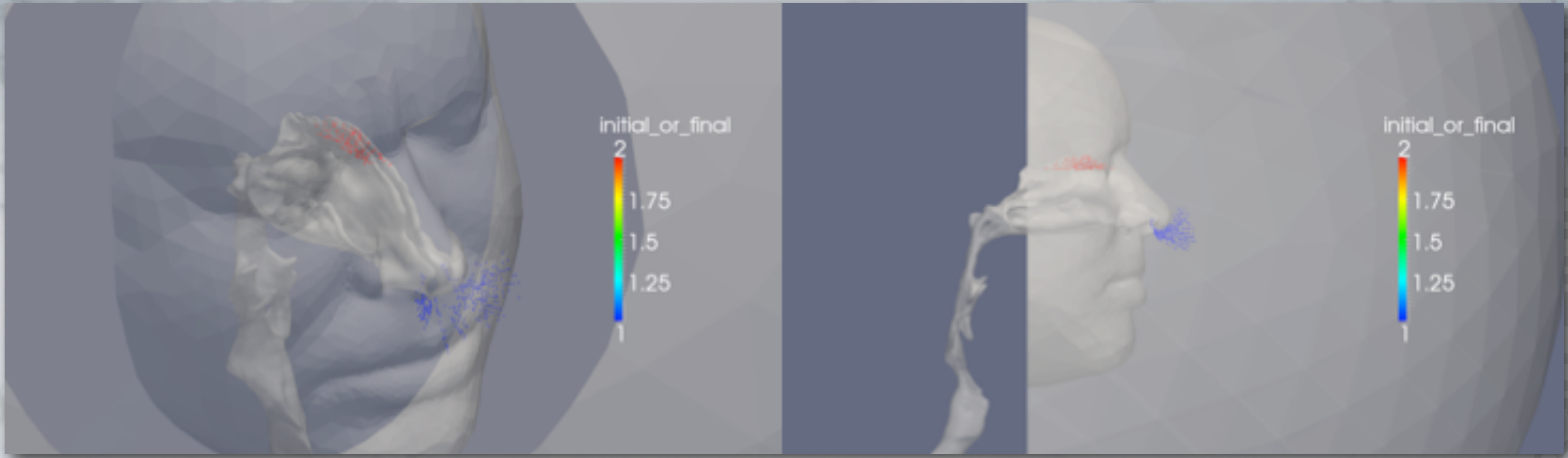


Particle tracking

Particle tracking:

Particle deposition

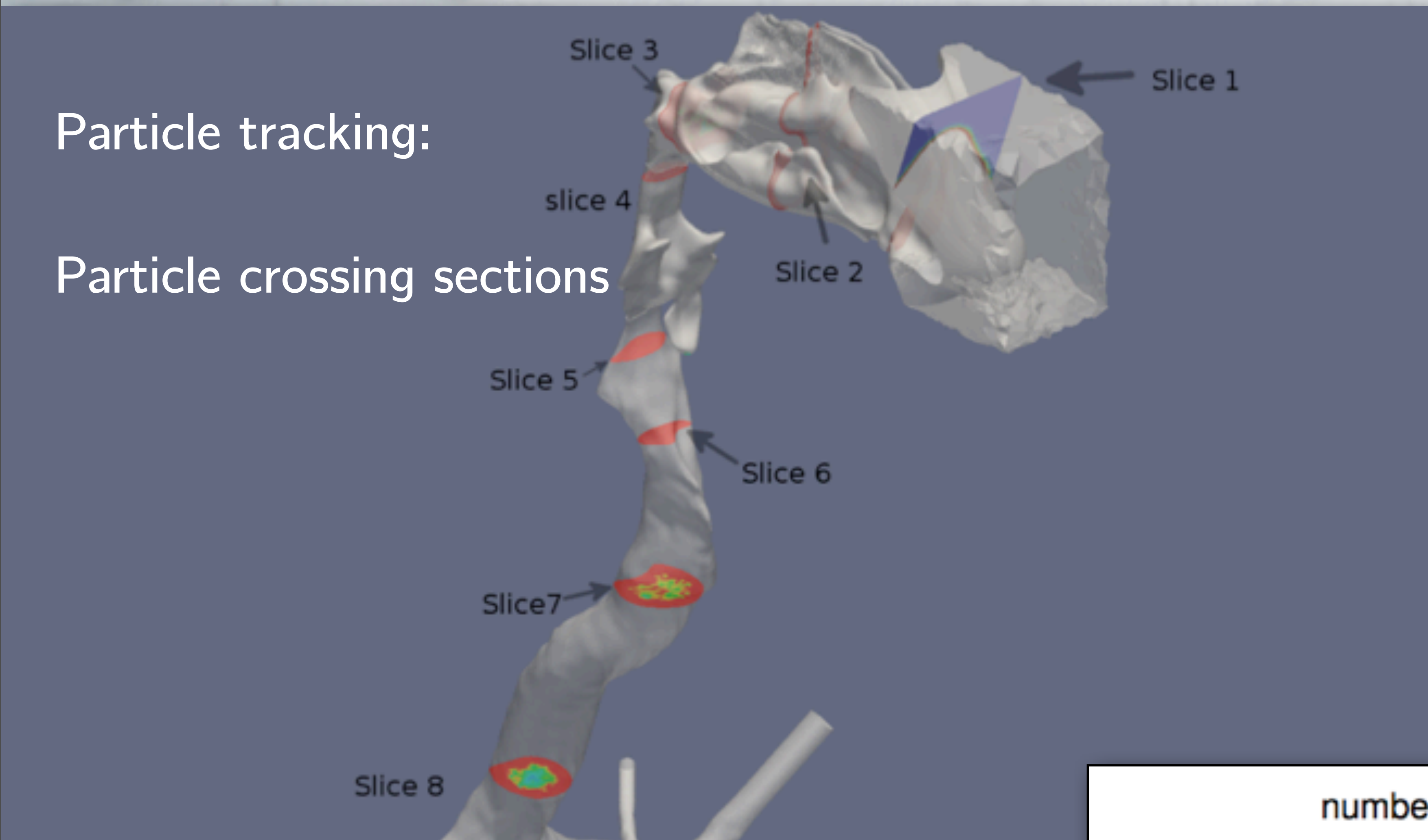


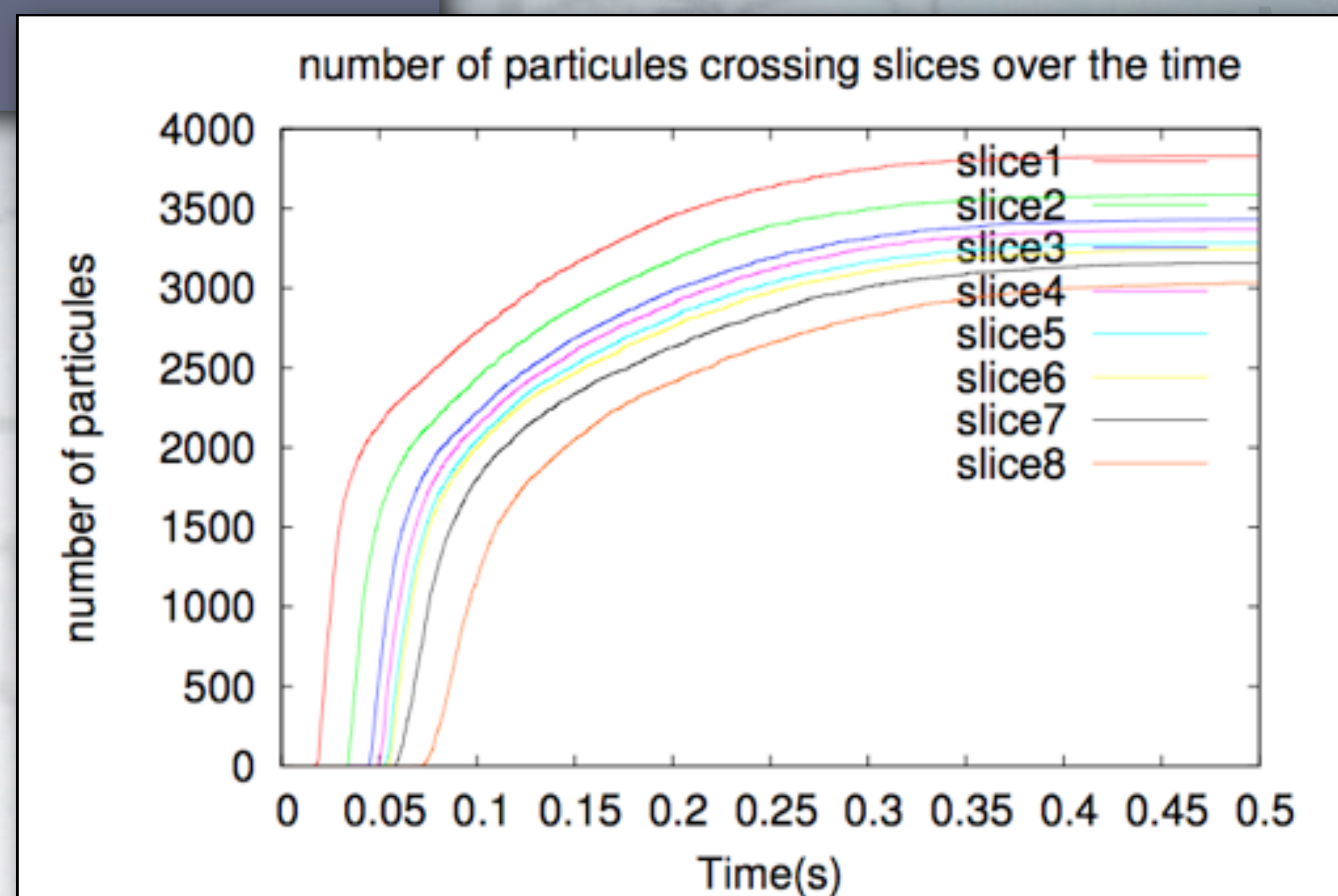


Computational Respiratory System

Particle tracking:

Particle crossing sections

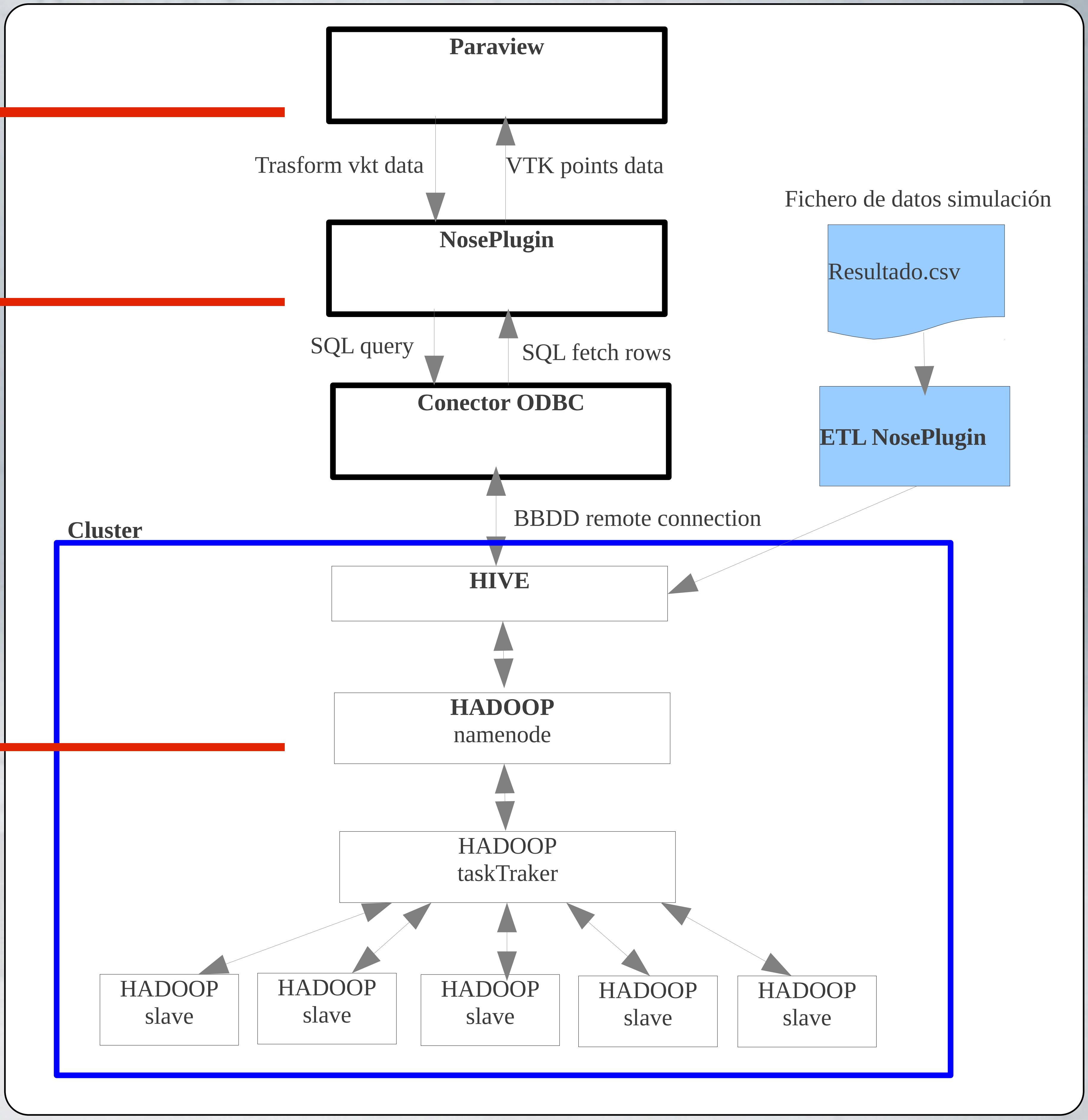


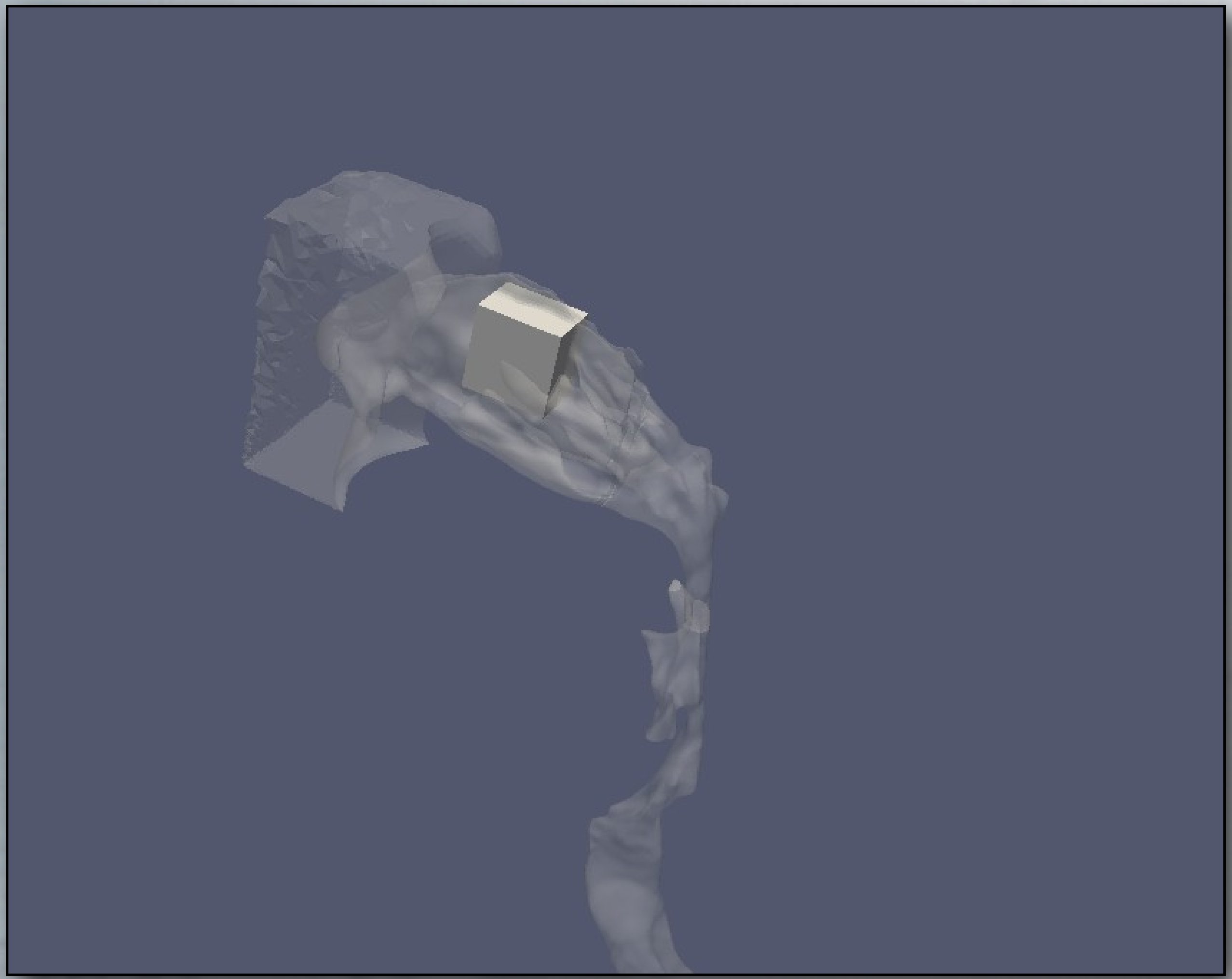


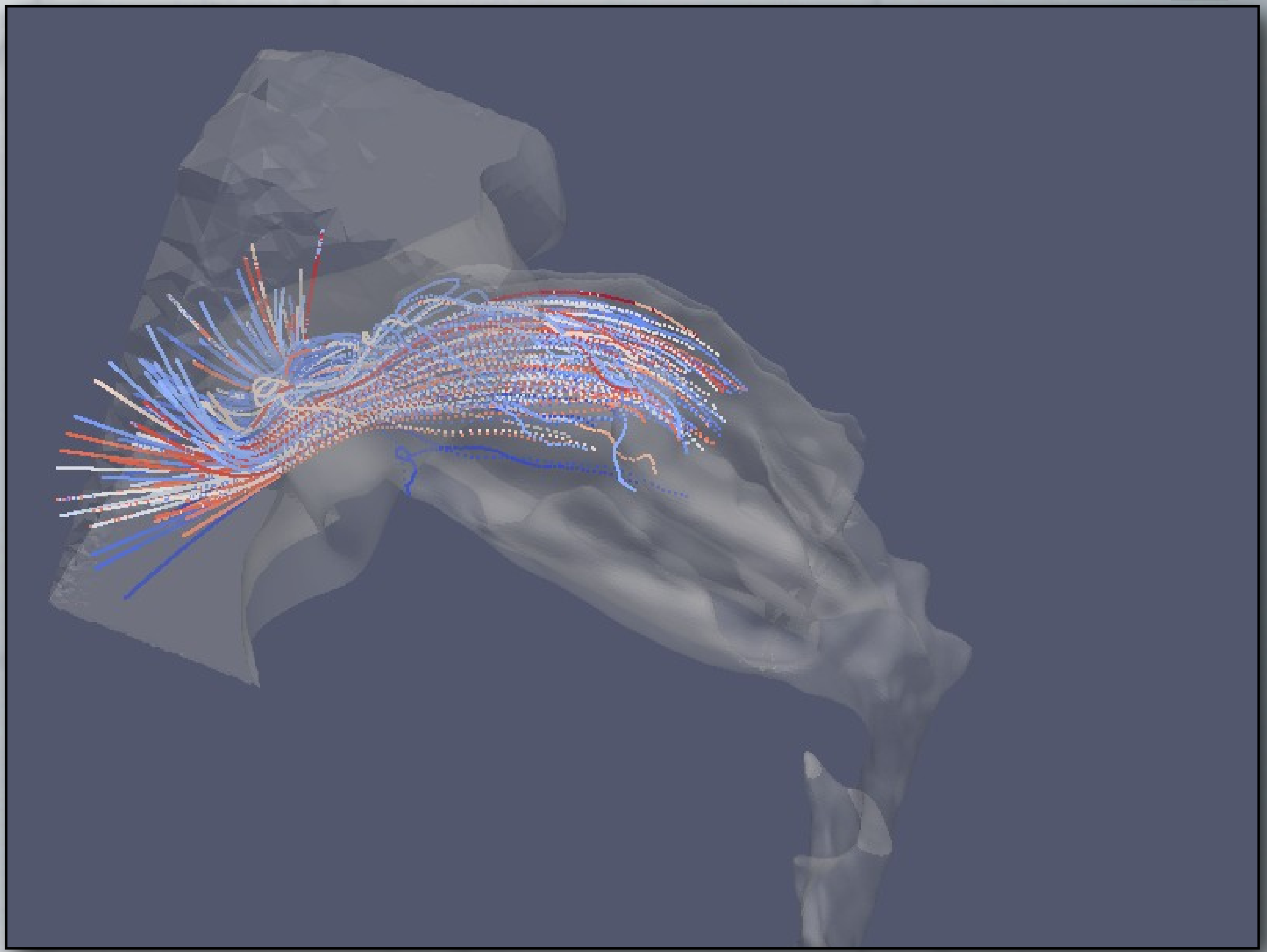
Paraview interface

Paraview plugin

Parallel Database







Example: Track back all the particles found at time t at this box

Particles can be labelled by species or initial / final situation

Database is created with files containing, at each time step, particle position, particle_id, subdomain_id (posptrocess done with HDF5), etc.

Conclusions and Future Lines

Improve the dummies:

Run the cases of the respiratory system, assessing the mesh grain

Improve the Physical models: humidity, boundary conditions, etc

Improve mesh mapping from healthy geometries to impaired ones

Improve geometries fusion

Integrate postprocess in a "doctors friendly environment"

FSI in a full heart, studying specially parallelization issues

Drug (blockers) effect

Develop an atria fiber model

Develop a mapper for fiber fields from DTI

Integrate Alya with ADAN ("*EU-Brazil CC*" project)

Contact problem for prostheses to help diastole in impaired hearts

Regenerating cardiac stem cells clustering due to stress concentration

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