High Performance Computational Biomechanics

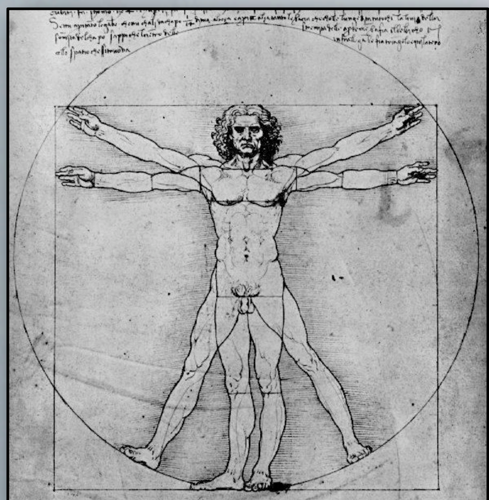
Mariano Vázquez

Barcelona Supercomputing Center
Centro Nacional de Supercomputación
Spain

HPC LatAm 2013
Mendoza - Argentina

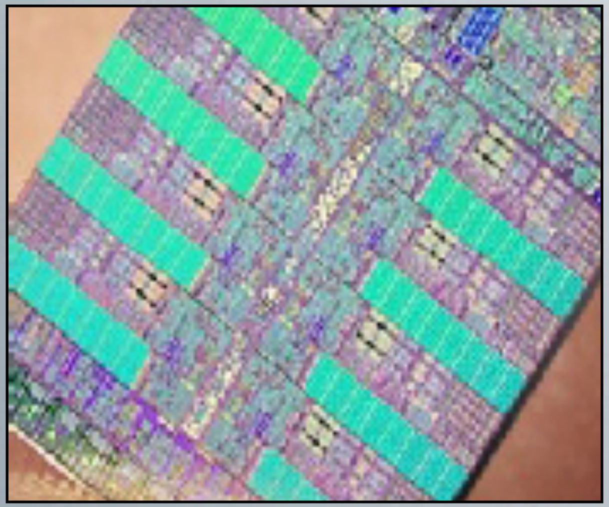
Barcelona Supercomputing Center

EXCELENCIA SEVERO OCHOA



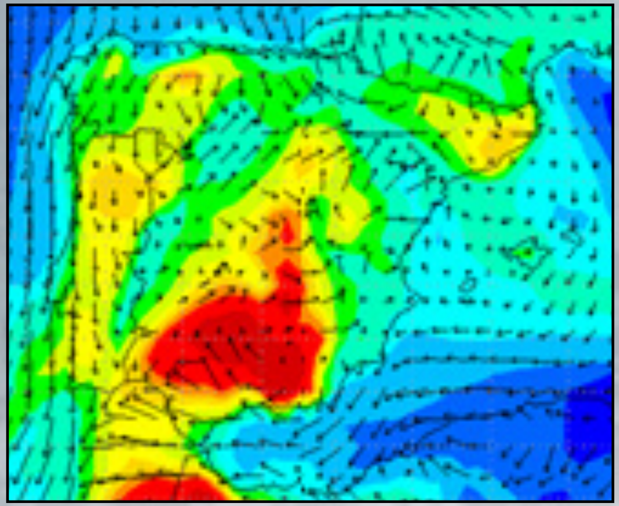
CASE Department

BSC-CNS Research Departments



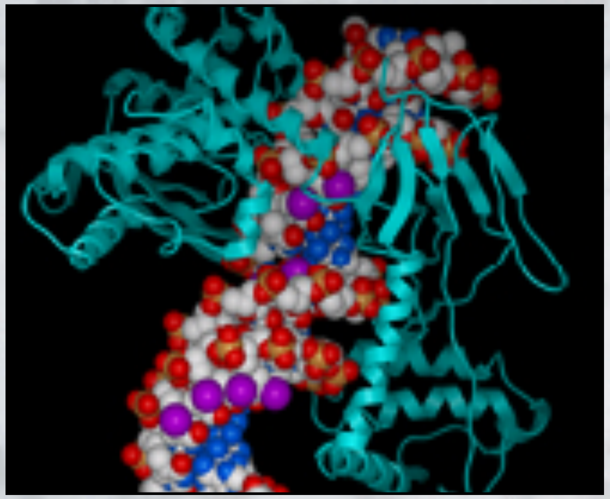
Computer Science

Performance tools
Computer architectures
Programming models



Earth Science

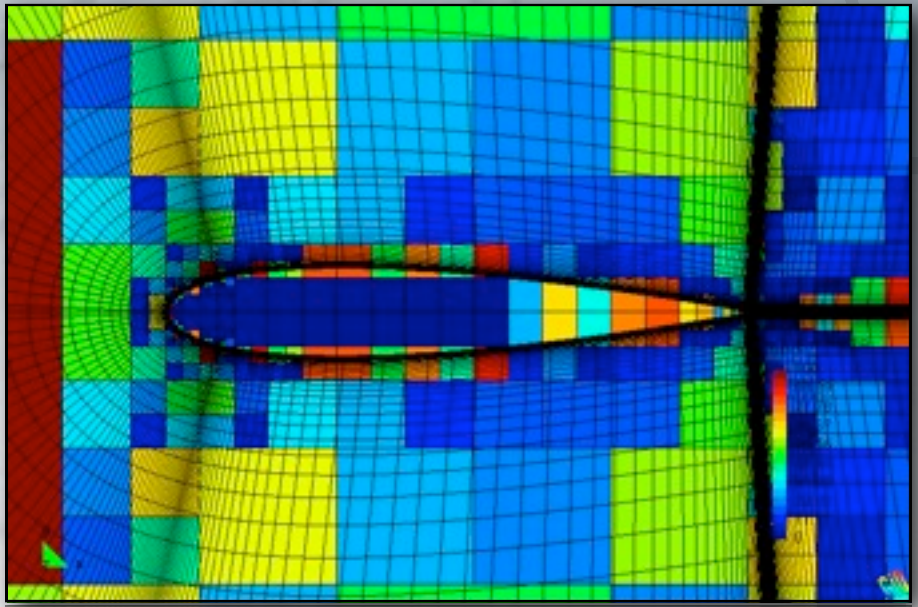
Air quality



Life Science

Genomics
Proteomics

Computer Applications in Science
and Engineering
CASE



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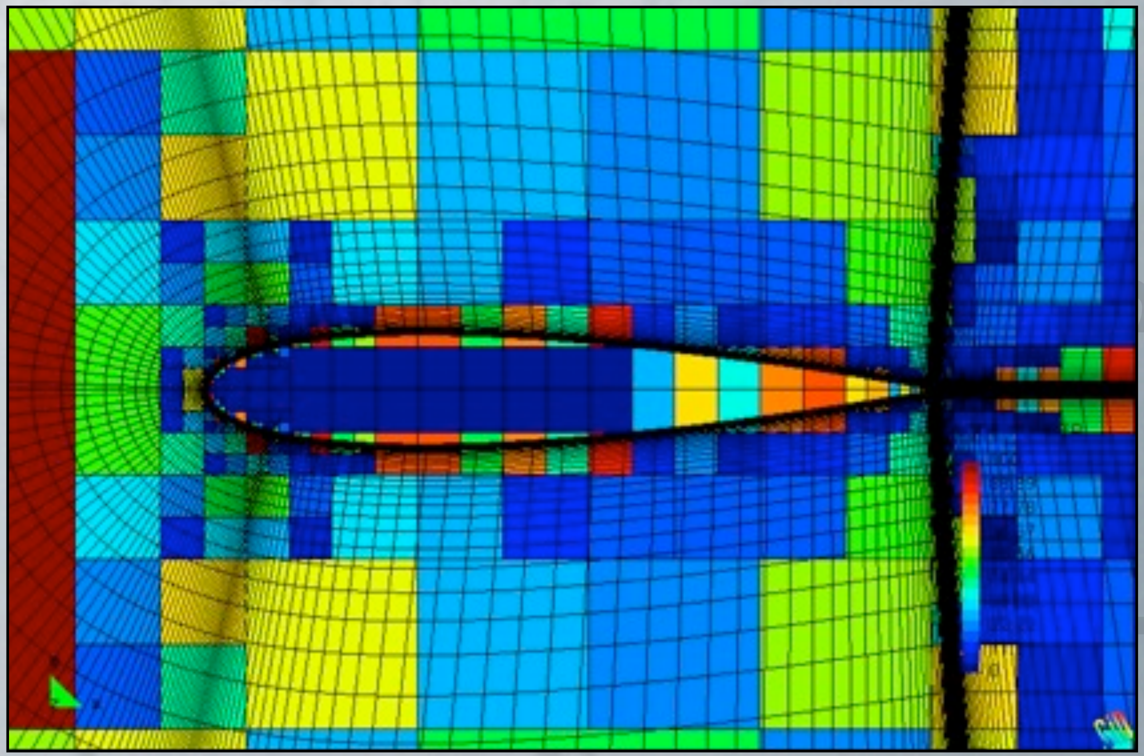


Computer Applications in Science and Engineering (CASE)

Computational Physics and Engineering

Interdisciplinary research unit of the BSC-CNS

Our mission:
To develop computational tools to simulate highly complex problems seamlessly adapted to run onto high-end parallel supercomputers

Around 40 researchers:

Post-docs, students, programmers

Computer Science, Physicists, Mathematicians, Engineers

CASE Department - Research lines

Physical and Numerical Modeling

Mesh Generation and Numerical Solution Algorithms

High Performance Computing in CM (HPCM)

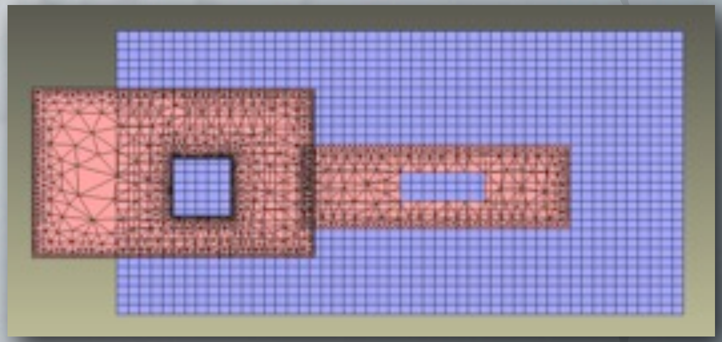
Parallelization in Distributed and Shared memory machines

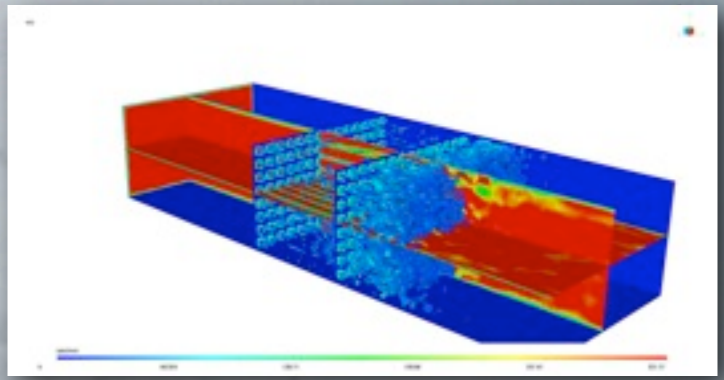
Numerical Kernels

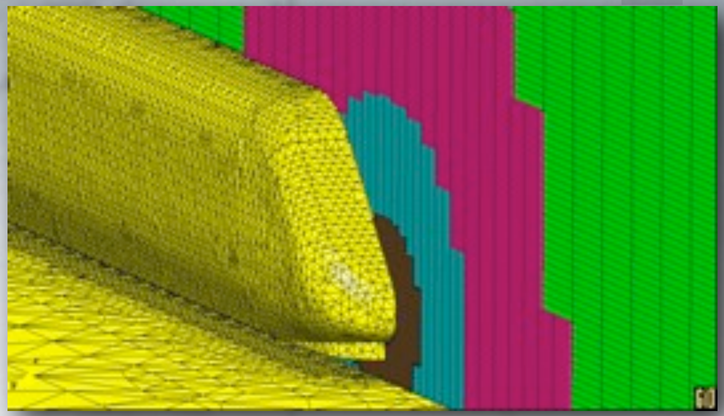
Optimization

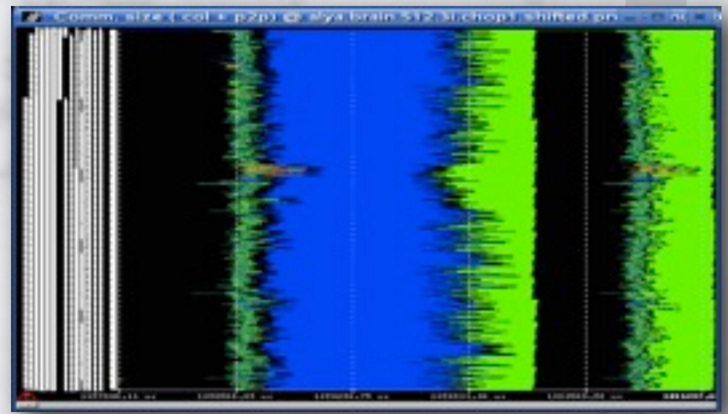
Scientific Visualization

Algebraic Solvers



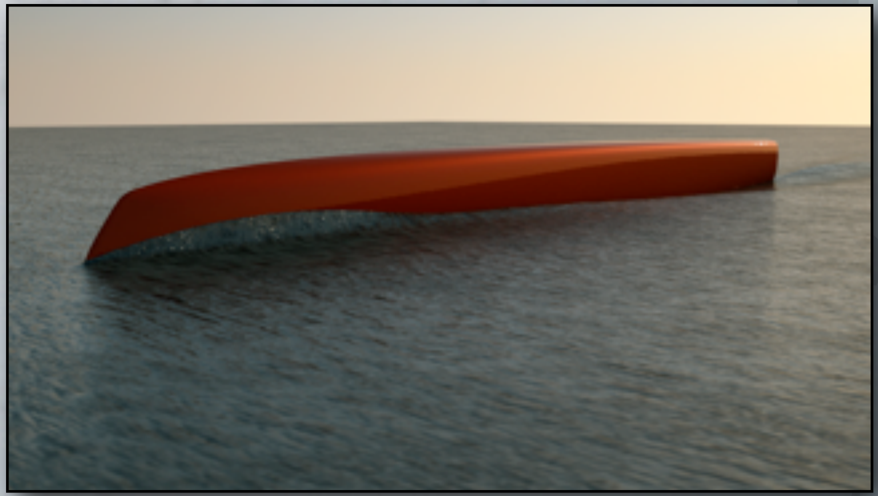
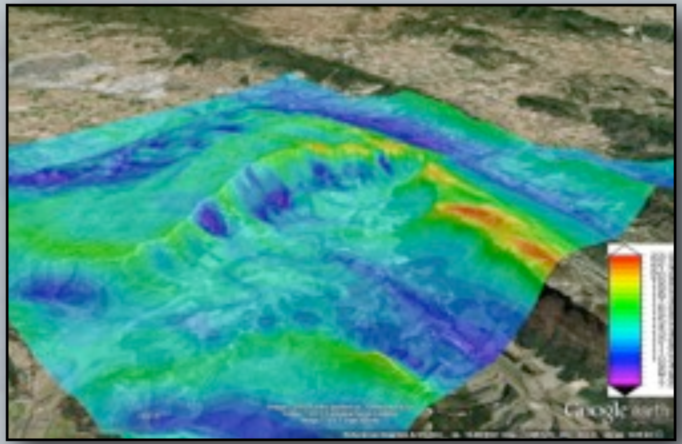
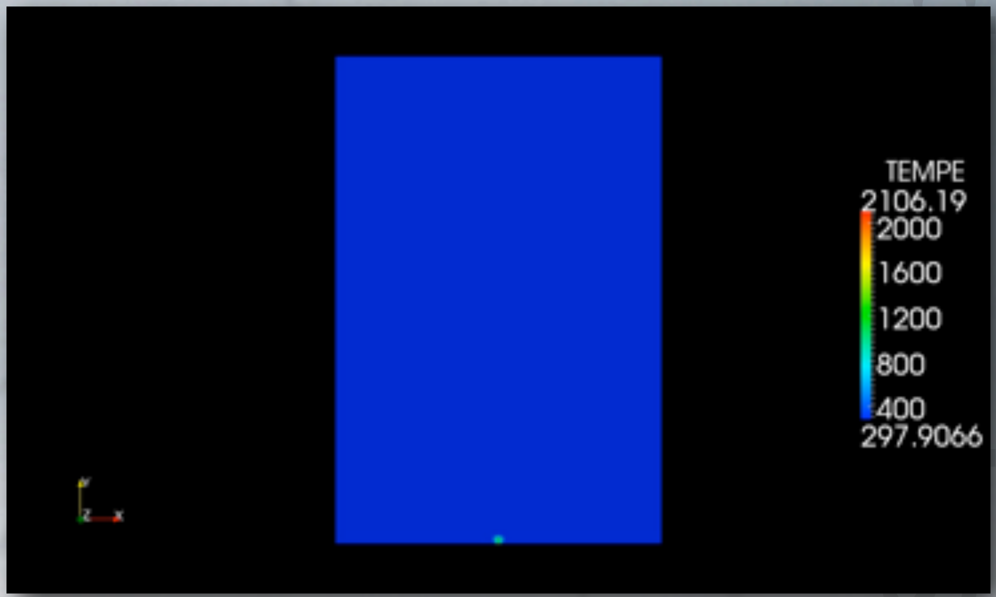


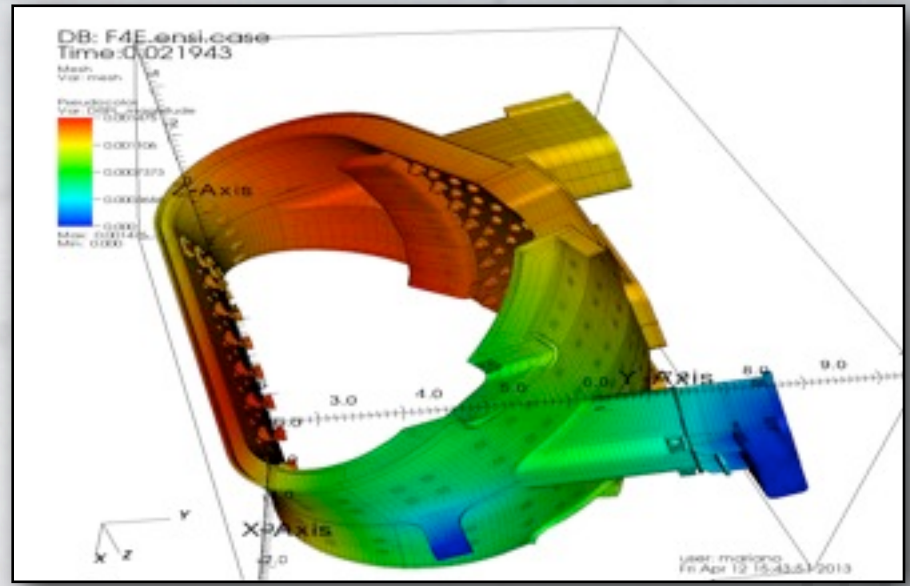




CASE Department - Application lines

- Environment
- Energy
- Aerospace
- Trains and Automotive
- Oil and Gas
- Artificial Societies
- High Energy Physics
- Materials Sciences
- Biomechanics

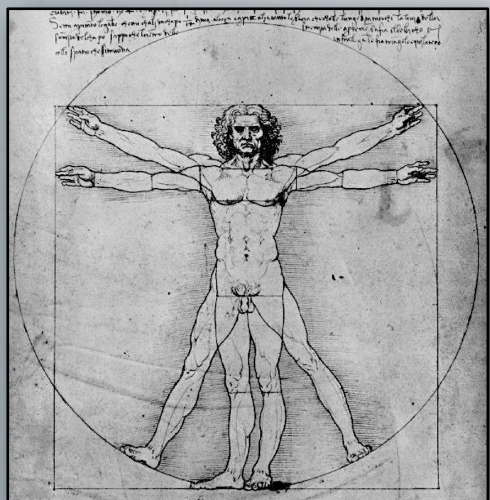





BSC & HPC in Biomedical Research

BSC-CNS is the only supercomputing center with +60 researchers devoted to Bioinformatics (45 Life Science Department) and Biomechanics (15 - 20 CASE Department)

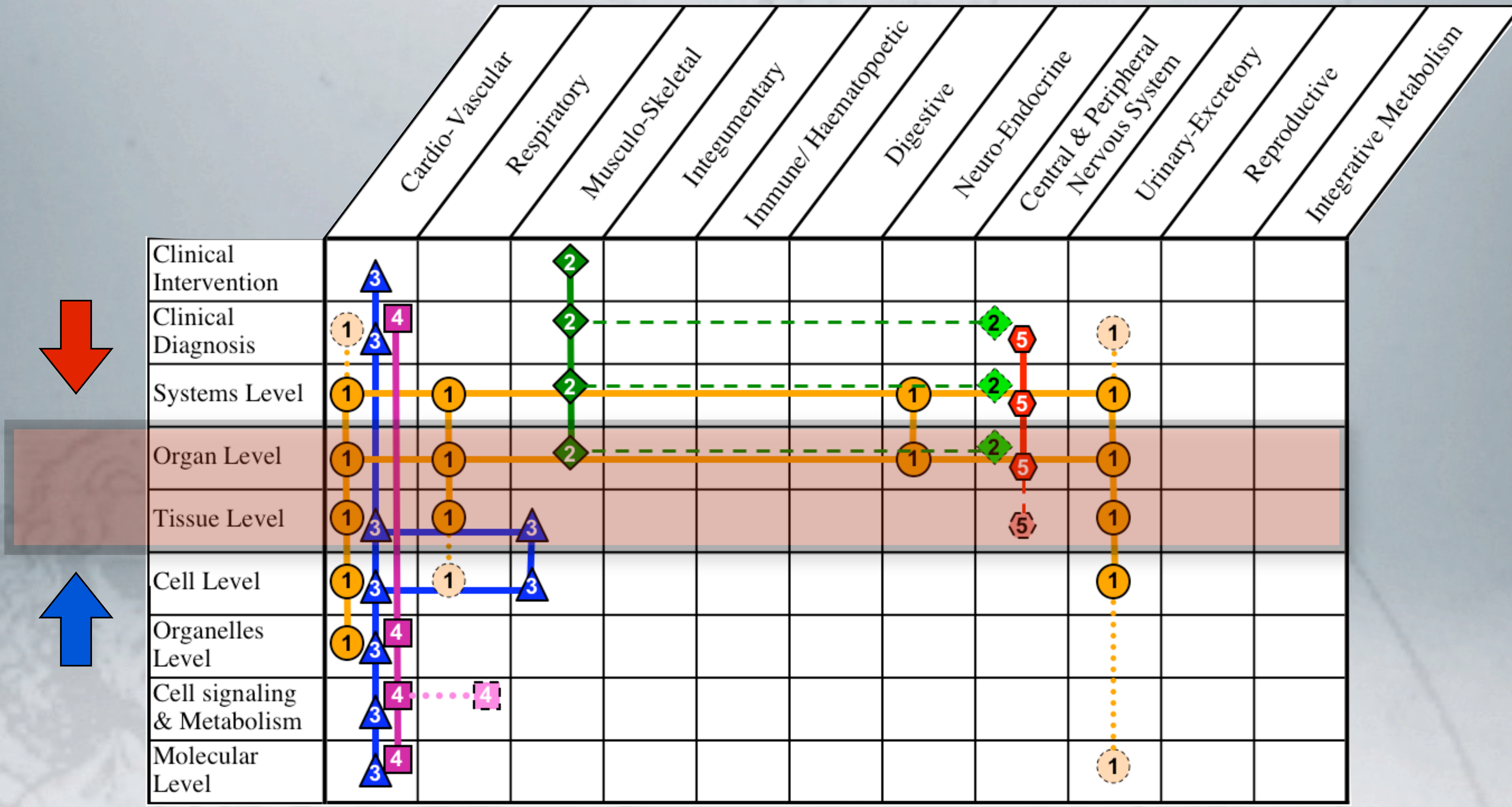
Barcelona Supercomputing Center



Computational Biomechanics

Barcelona Supercomputing Center

Biomechanics



Organ Systems vs. Levels of Organizations

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

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.

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

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

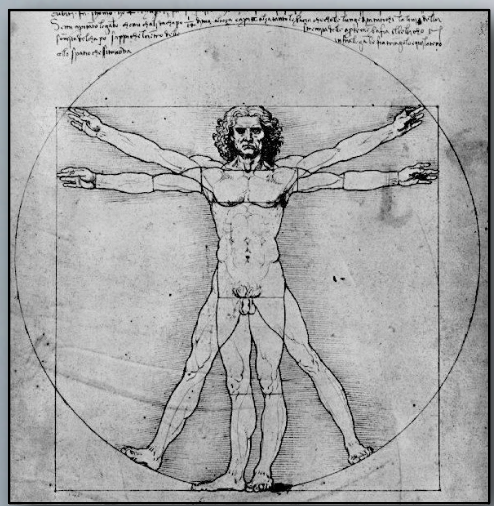
Computational scientists:

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)

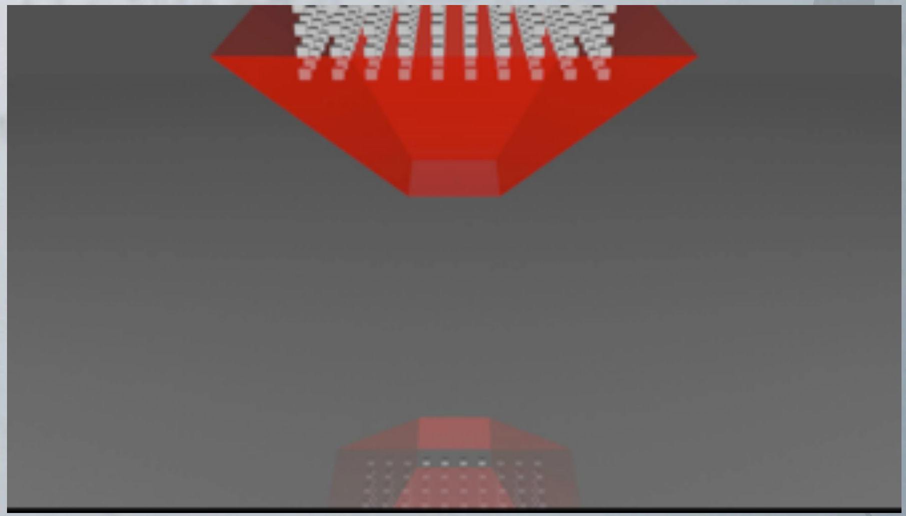
Advanced meshing issues

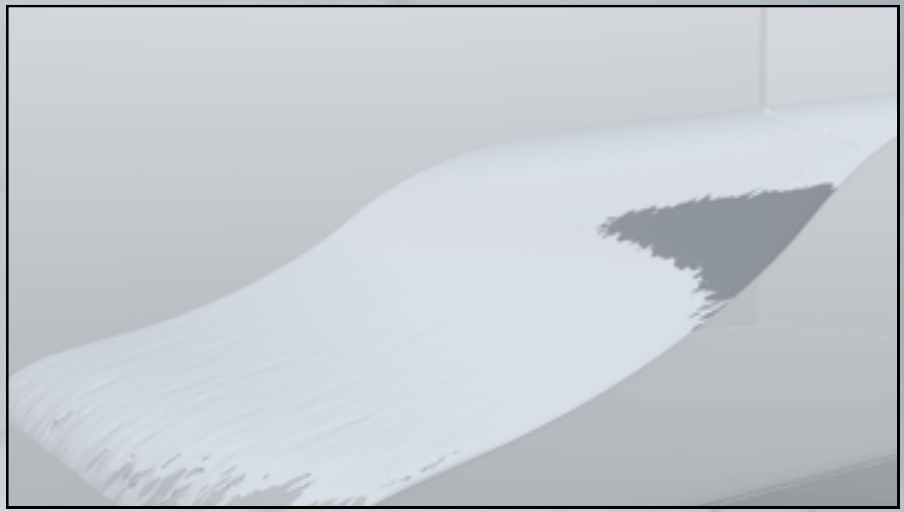
Parallelization by MPI and OpenMP

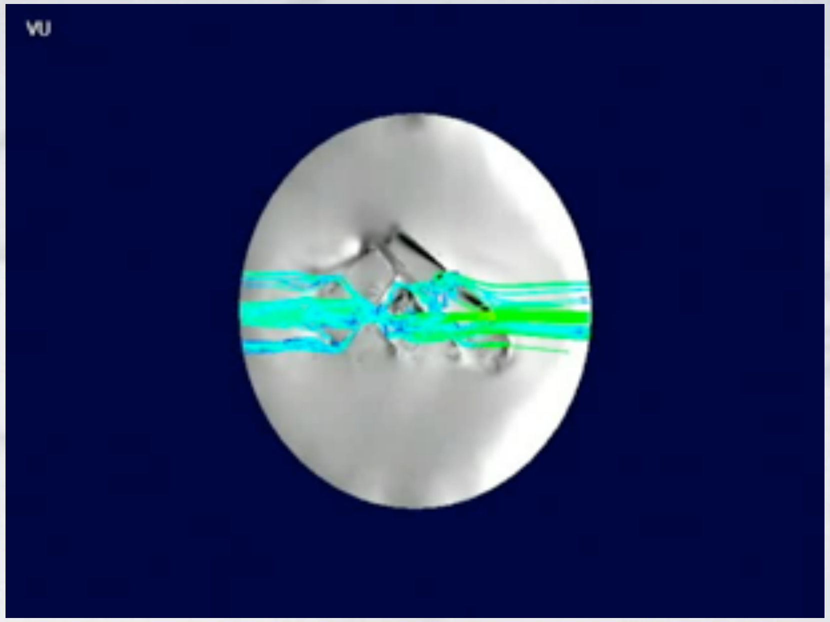
Automatic mesh partition using Metis

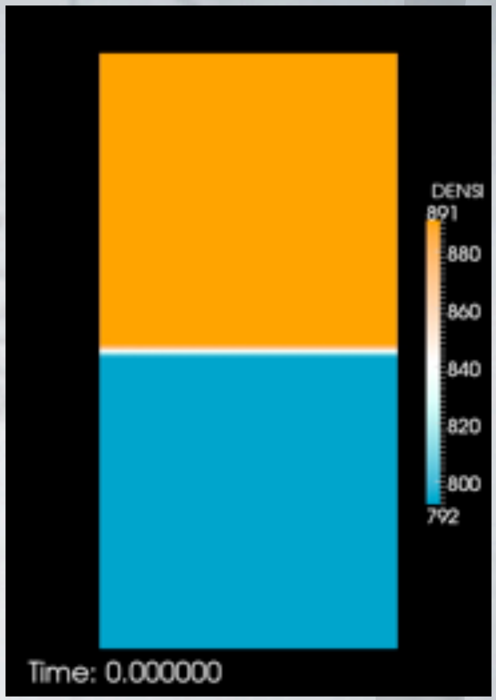
Portability is a must

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









The Alya System

Services

Kernel

Modules

- Coupled multiphysics
- Modules and services can be turned on/off
- Solvers are in-house, no external libraries
- Around 25 researchers working in it

The Alya System

Services

Kernel

Modules

Coupled multiphysics

Modules and services can be turned on/off

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Around 25 researchers working in it

Incompressible flows

Compressible flows

Turbulence

Non-linear Solid Mechanics

Embedded colliding N-bodies

Electromagnetism

Heat transport

Combustion and chemical reactions

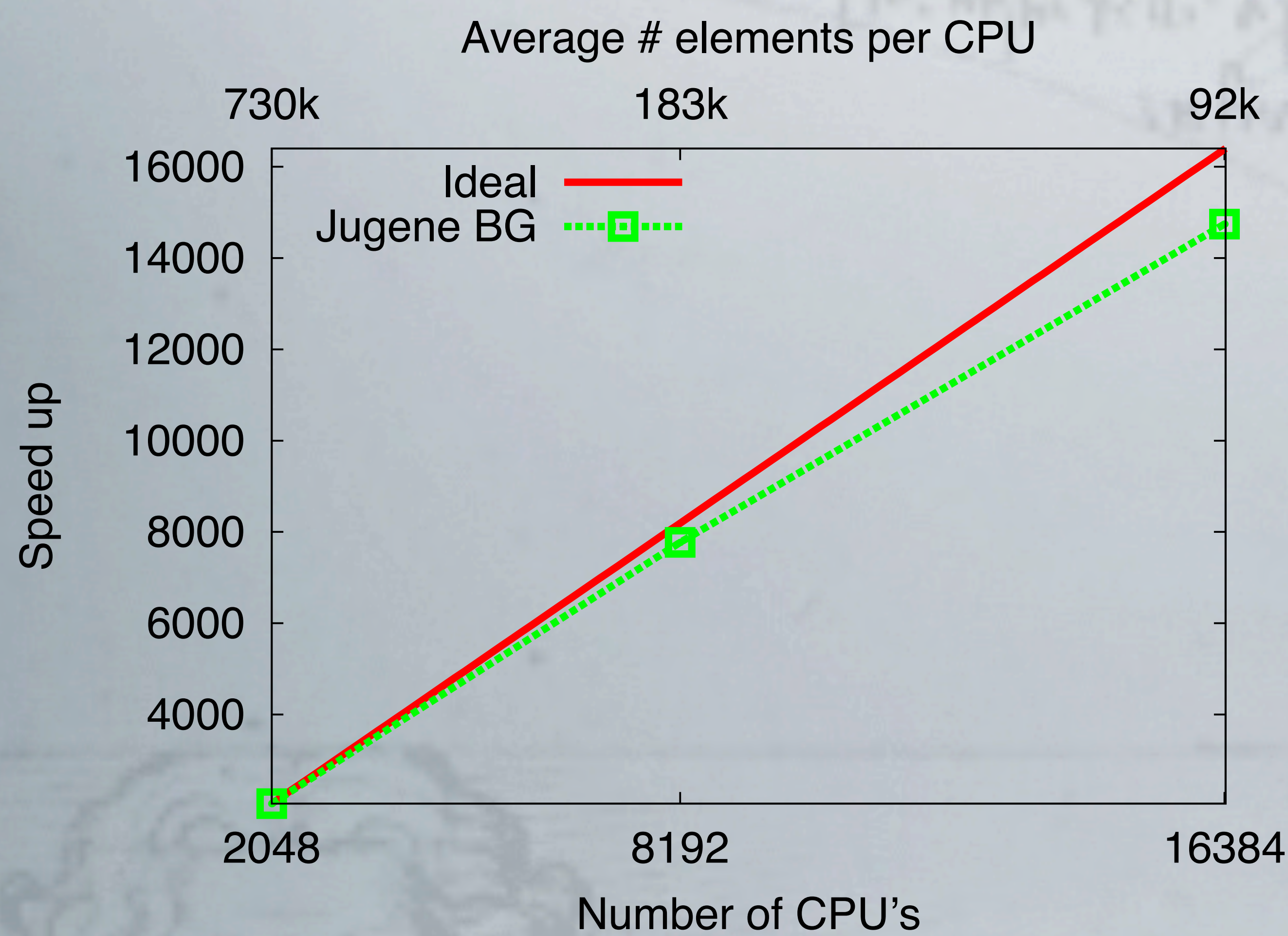
Species transport

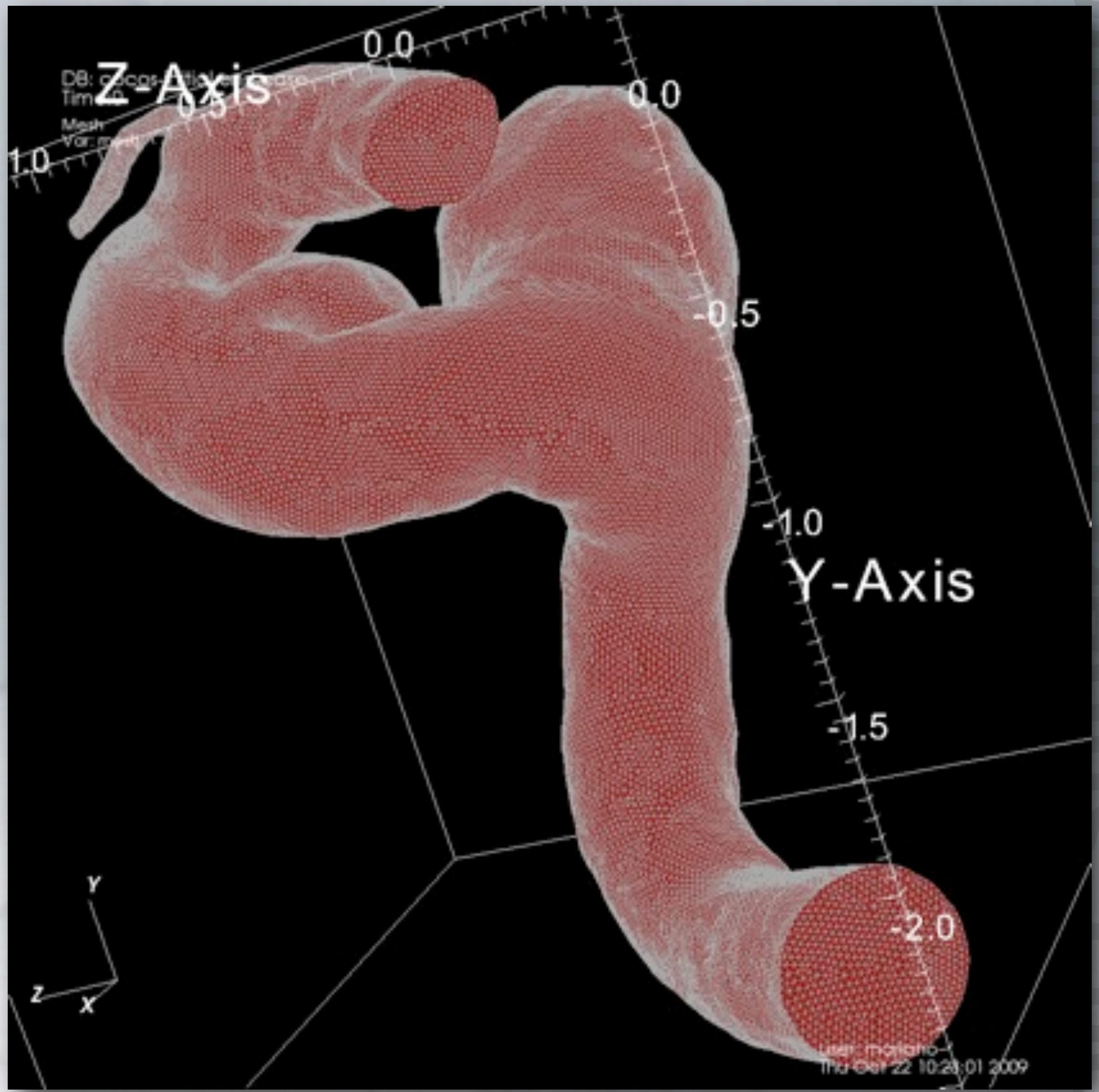
Overset meshes

Arbitrary Lagrangian-Eulerian Fluid-Structure Interaction

Adjoint-based optimization

HDF5 parallel postprocess





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 is one of the two CFD codes of the PRACE benchmark suite

respective user communities, as well the coverage of scientific a
a final list of 12 codes to form the initial version of UEABS, wh

Particle Physics:	QCD
Classical MD:	NAMD, GROMACS
Quantum MD:	Quantum Espresso, CP2K, GPAW
CFD:	Code_Saturne, ALYA
Earth Sciences:	NEMO, SPECFEM3D
Plasma Physics:	GENE
Astrophysics:	GADGET

Available online at www.prace-ri.eu

PRACE

Partnership for Advanced Computing in Europe

Selection of a Unified European Application Benchmark Suite

J. Mark Bull[a]*, Andrew Emerson[b]

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[b]CINECA, via Magnanelli 6/3, 40033 Casalecchio di Reno, Bologna, Italy.

Lindgren (Sweden), Cray XE system at PDC, incompressible flow 12288 CPU's

(collaboration with Jing Gong from PDC)

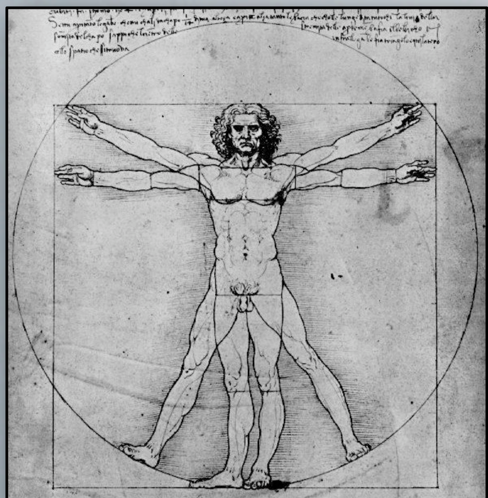
Huygens, (The Netherlands), IBM power 6, incompressible flow, 2128 CPU's

Jugene BG (Germany): 16384 CPU's, incompressible flow (Prace project for Mesh multiplication) and, running first tests of FSI in collaboration with Paolo Crosetto (Julich)

Fermi BG (Italy): 16384 CPU's, incompressible flow + species transport + Lagrangian particles (Prace project for nose)

Curie Bullx (France): 22528 CPU's, incompressible flow (collaboration with Jing Gong - PDC)

Marenostrum: 8000 CPU's compressible flow, incompressible flow, solid mechanics...



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

Francesc Carreras
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Manel Ballester
Univ. de Lleida (Spain)

Rafael Rodríguez Lecoq
Htal. Vall d'Hebron (Spain)

Rio Aguilar Torres
Hospital Univ. Bellvitge (Spain)

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)

Thomas Franz, University of Cape Town (South Africa)

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

Muscle pumping action of the heart

Multiphysics - multiscale

Complex geometries

Very expensive computational modelling

Uncertainties:

- Geometrical
- Physiological models
- Indirect validation

Cardiac Computational Model

Muscle pumping action of the heart

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Complex geometries

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- Geometrical
- Physiological models
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The goals:

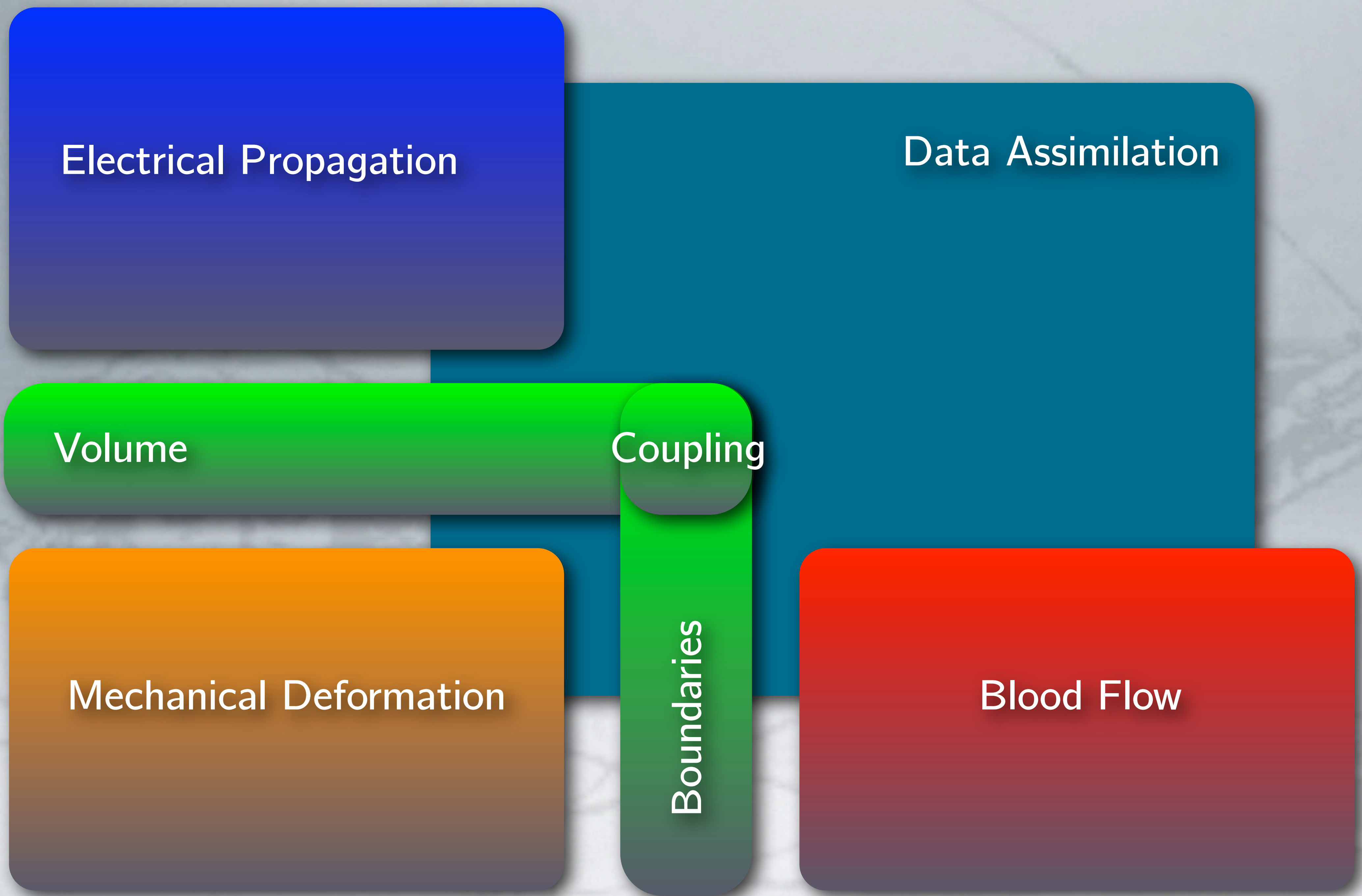
Create a CCM for a “mean” pumping heart

A computational scenario to implement new models and analyze their behavior in the coupled system

Study healthy hearts, pathologies, treatments

Adapt the mean model to patients

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

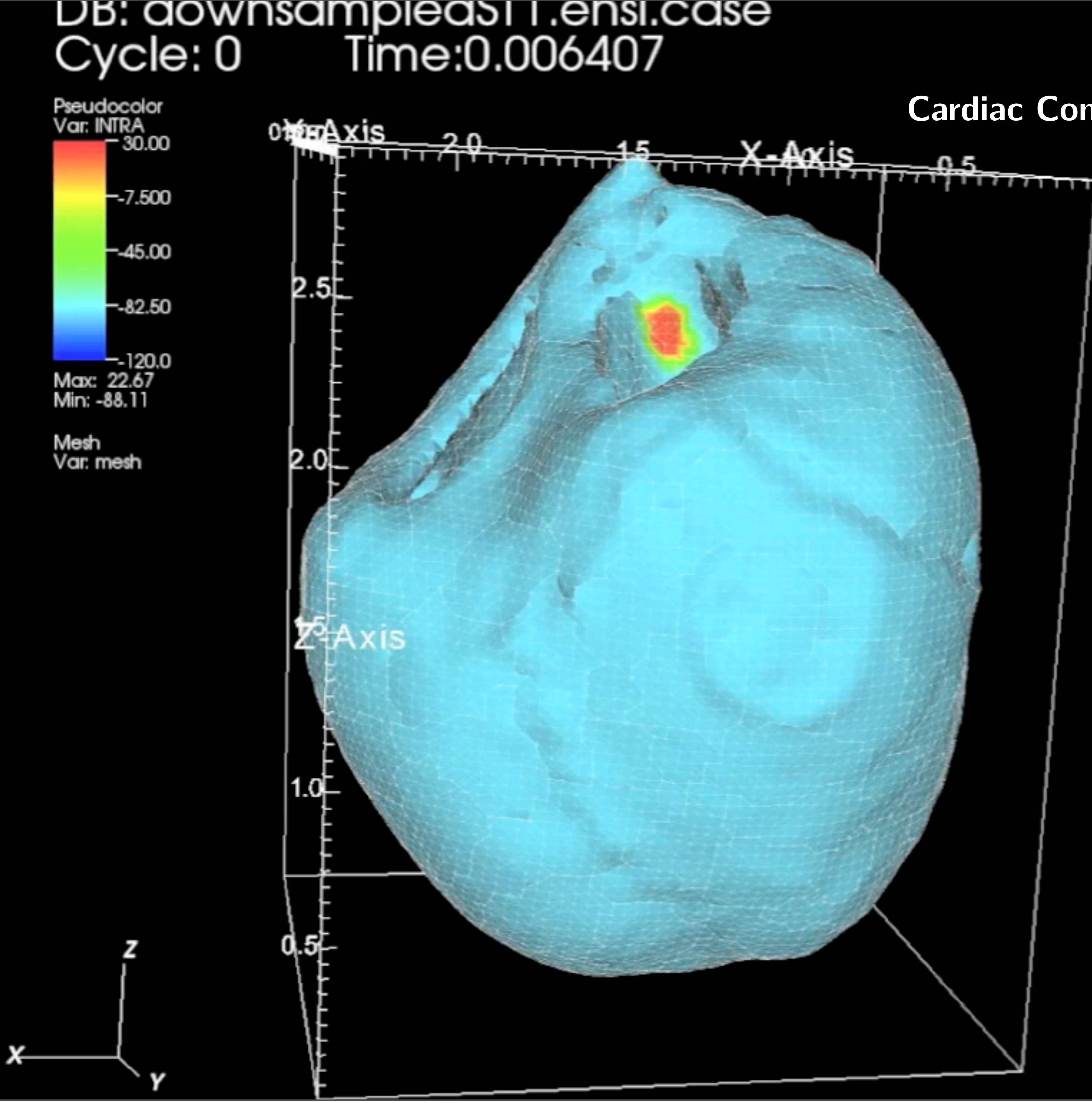
Mechanical deformation:

Large deformations + non-linear material models

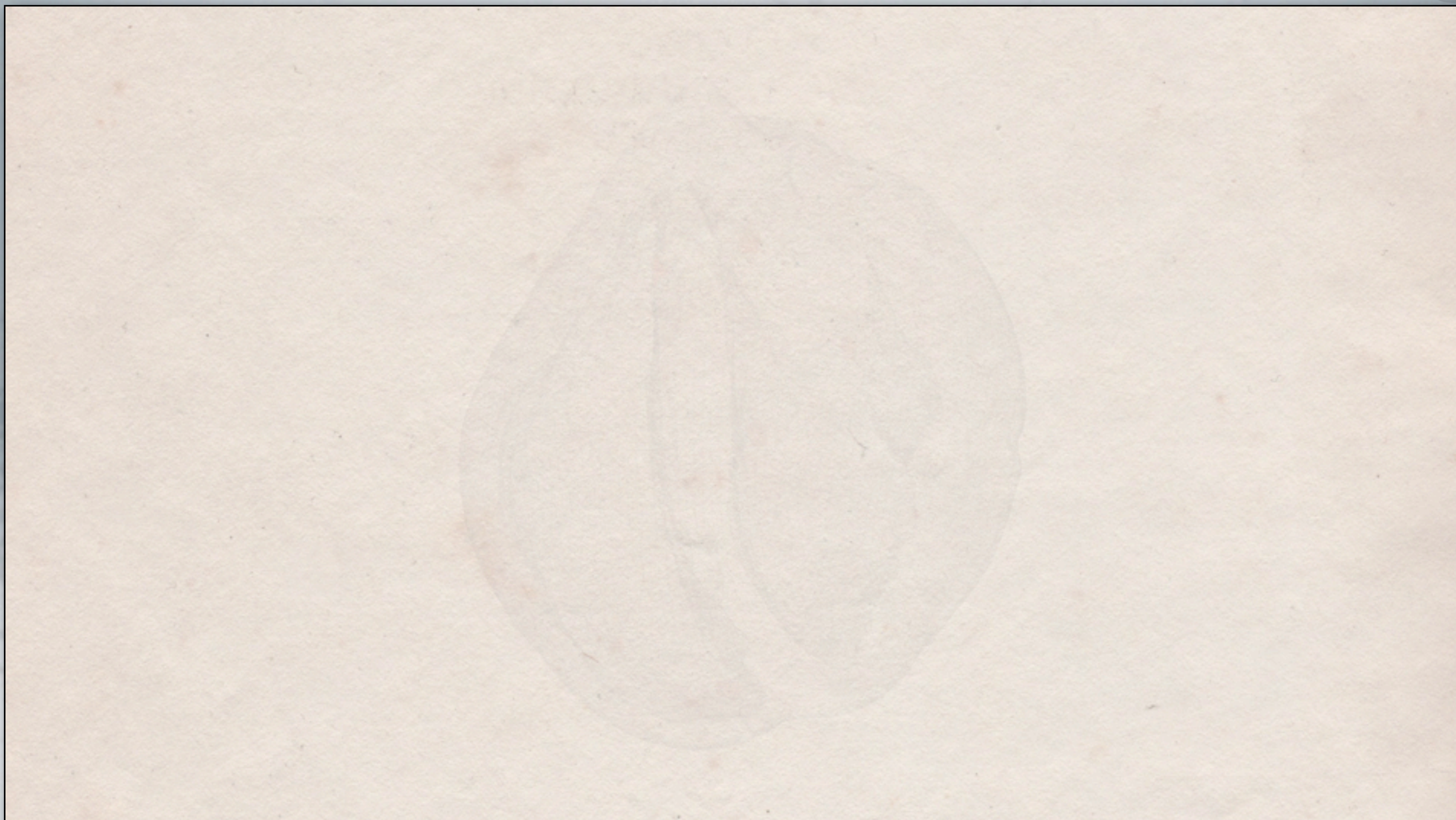
Incompressible Flow

Biomechanics

Cardiac Computational Model



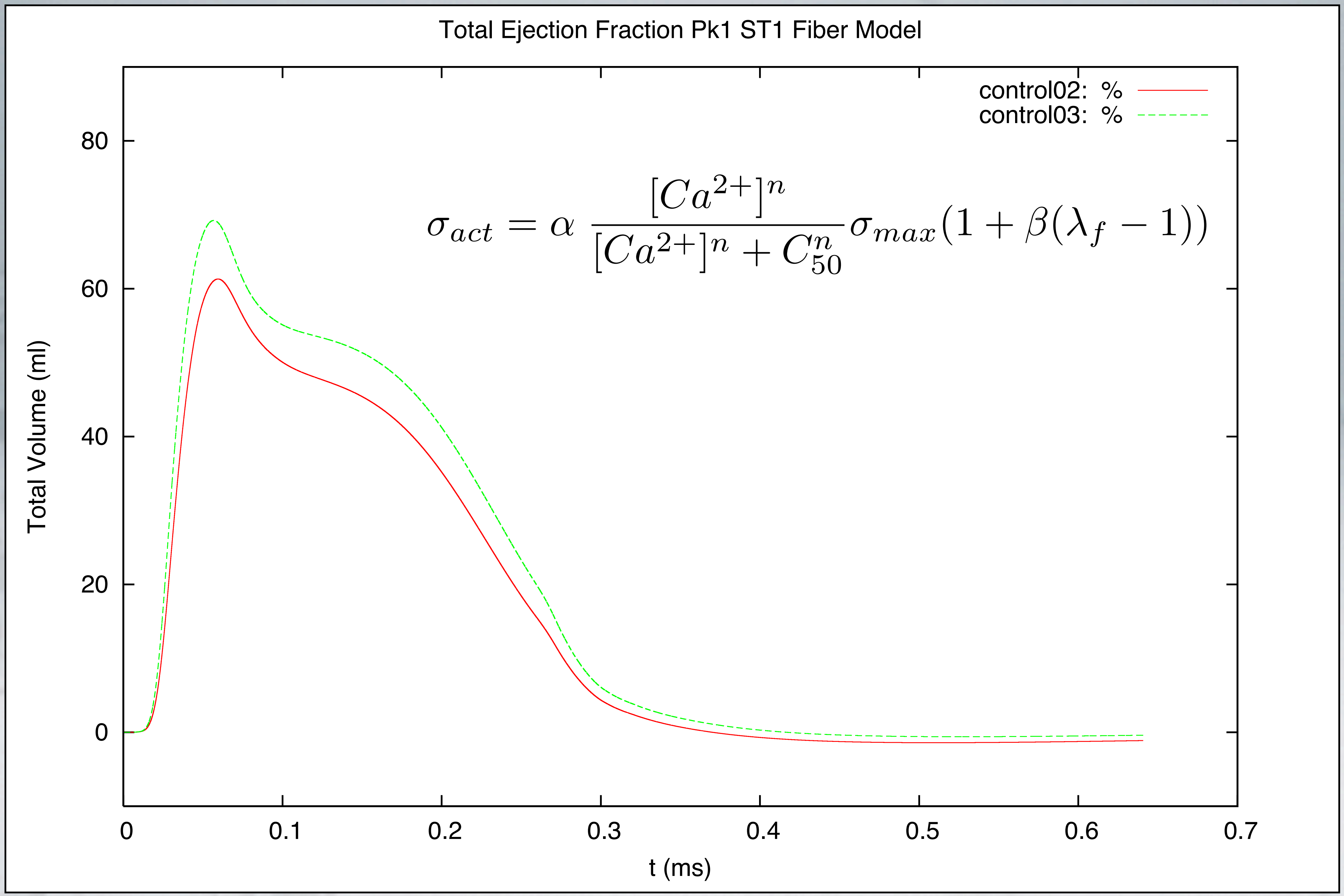
Cardiac Computational Model



Cardiac Computational Model

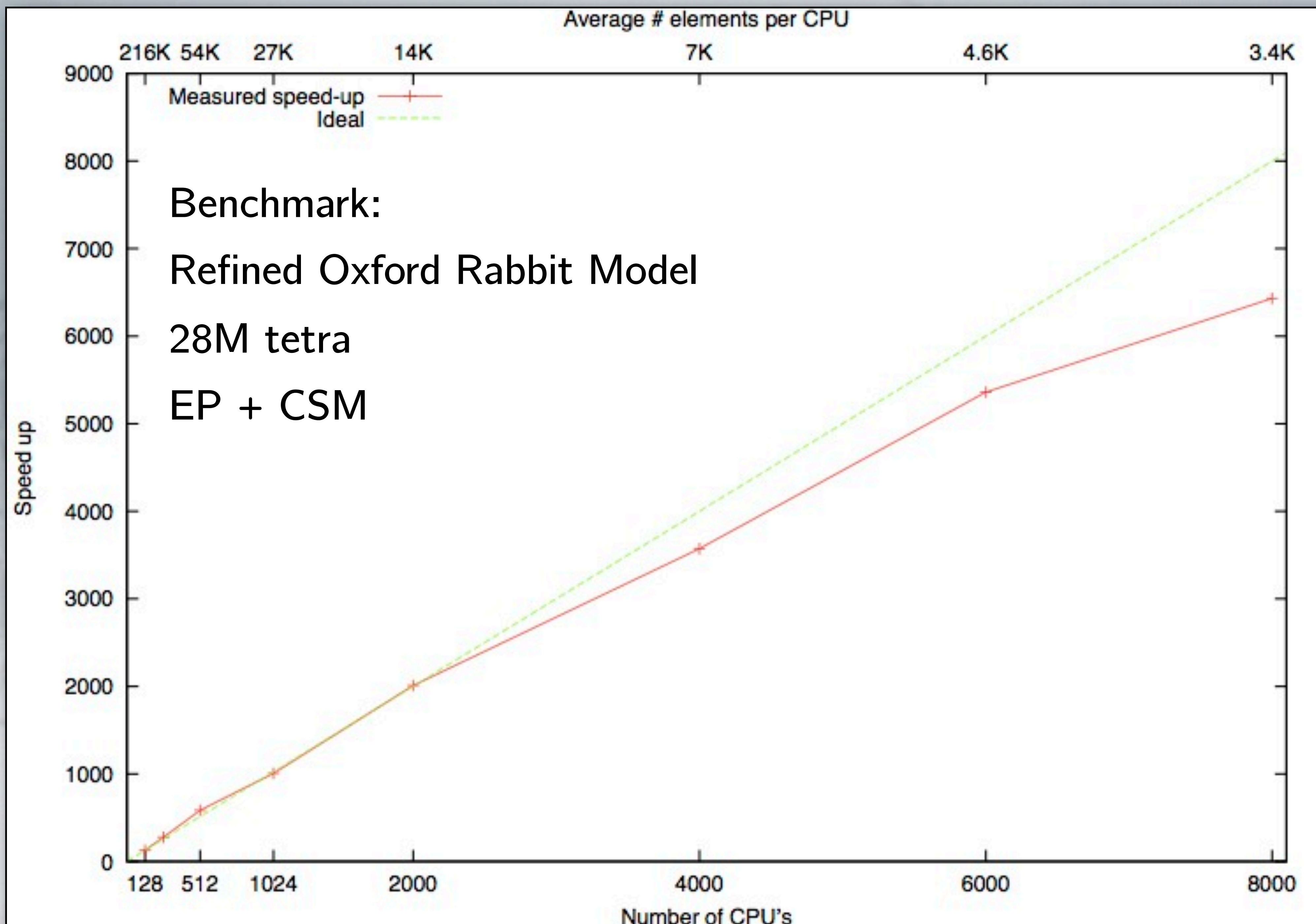
The fibers field

Sensitivity to parameter alpha: 0.2 (red) and 0.3 (green)

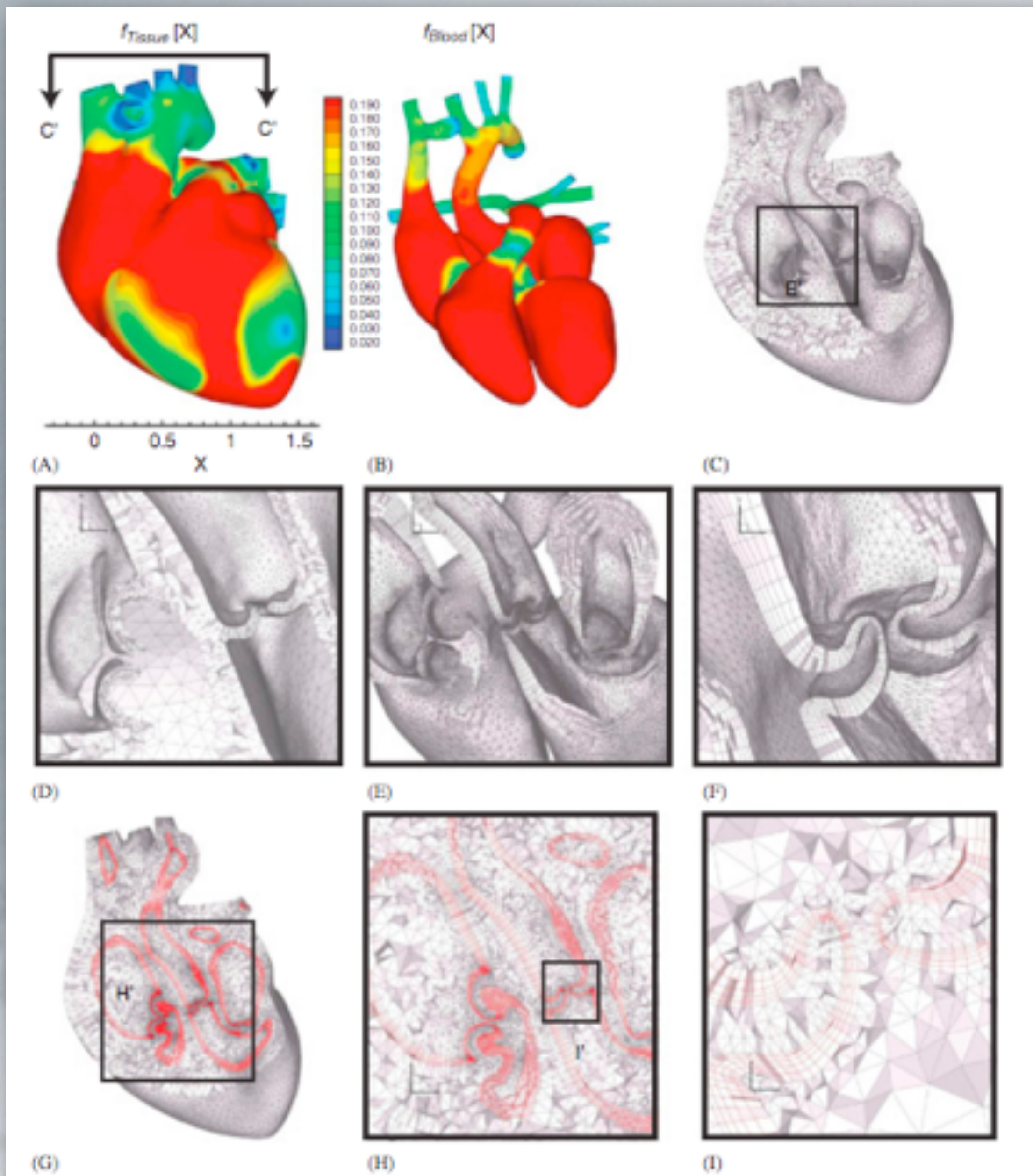


Scalability: Electro - Mechanical problem

Marenostrum III - BSC

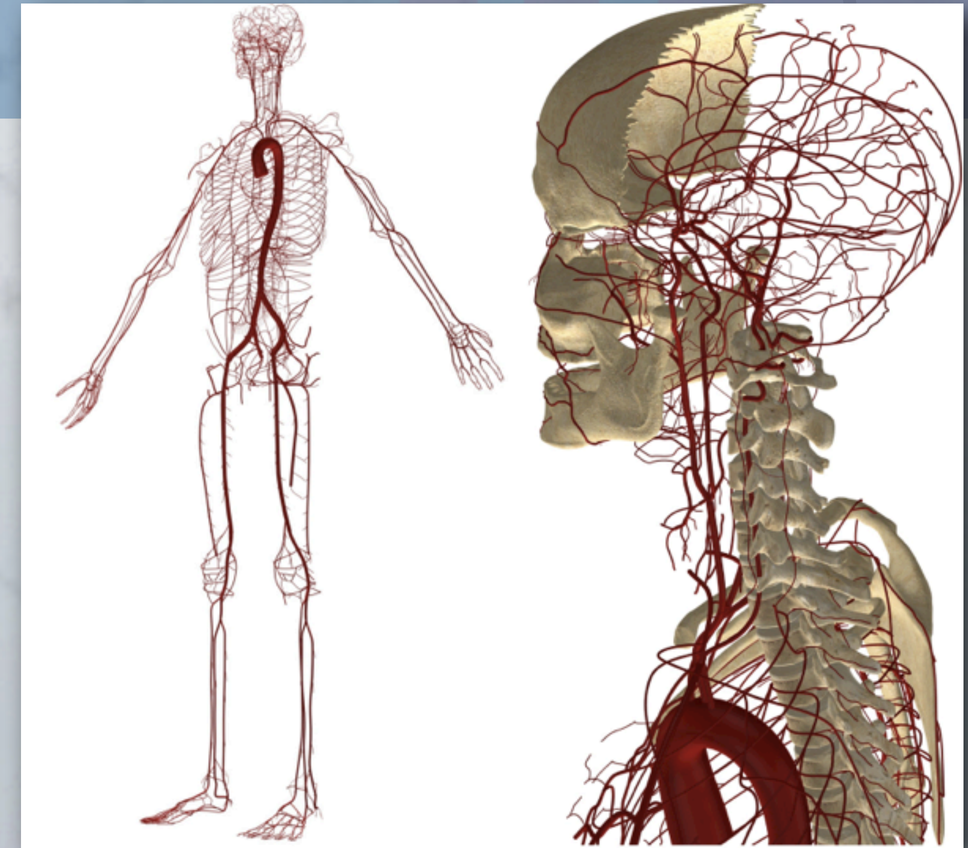


Cardiac Computational Model



Complete high-resolution cardiac geometries (D. Einstein)

Fluid-electro-mechanical model

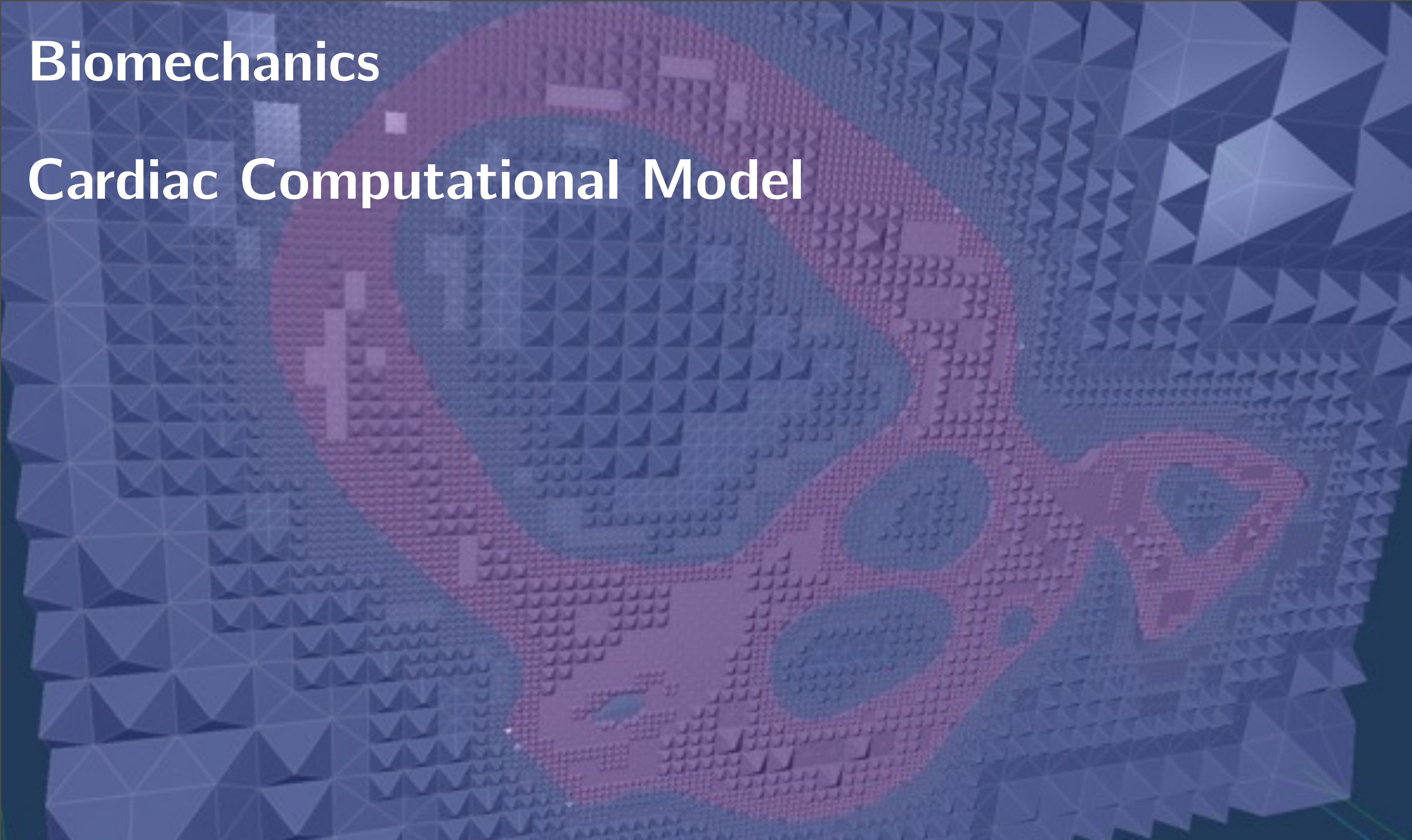


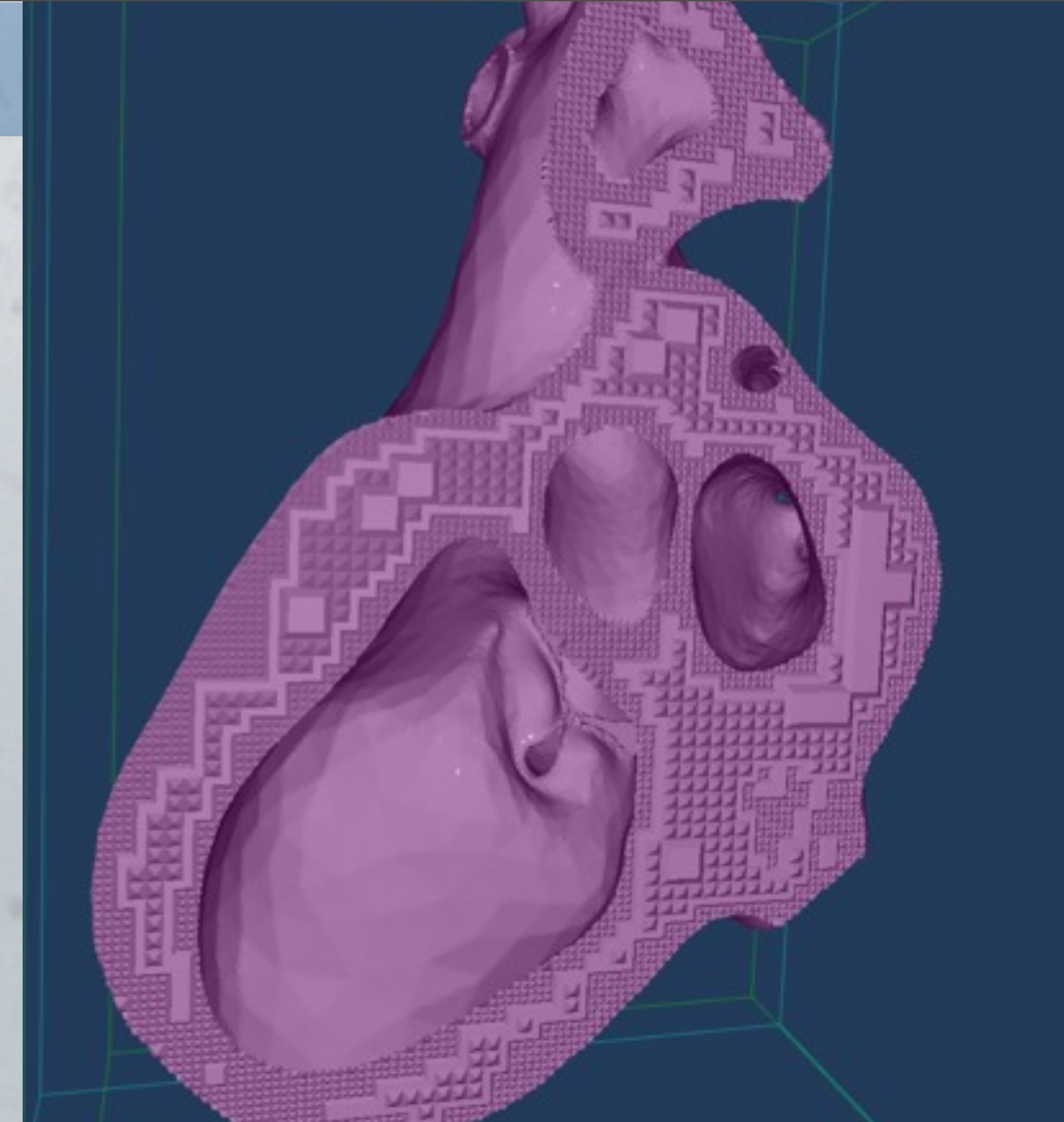
ADAN - Anatomically Detailed Arterial Network (P. Blanco)

Synthetic Purkinje system (R. Sebastian)

Biomechanics

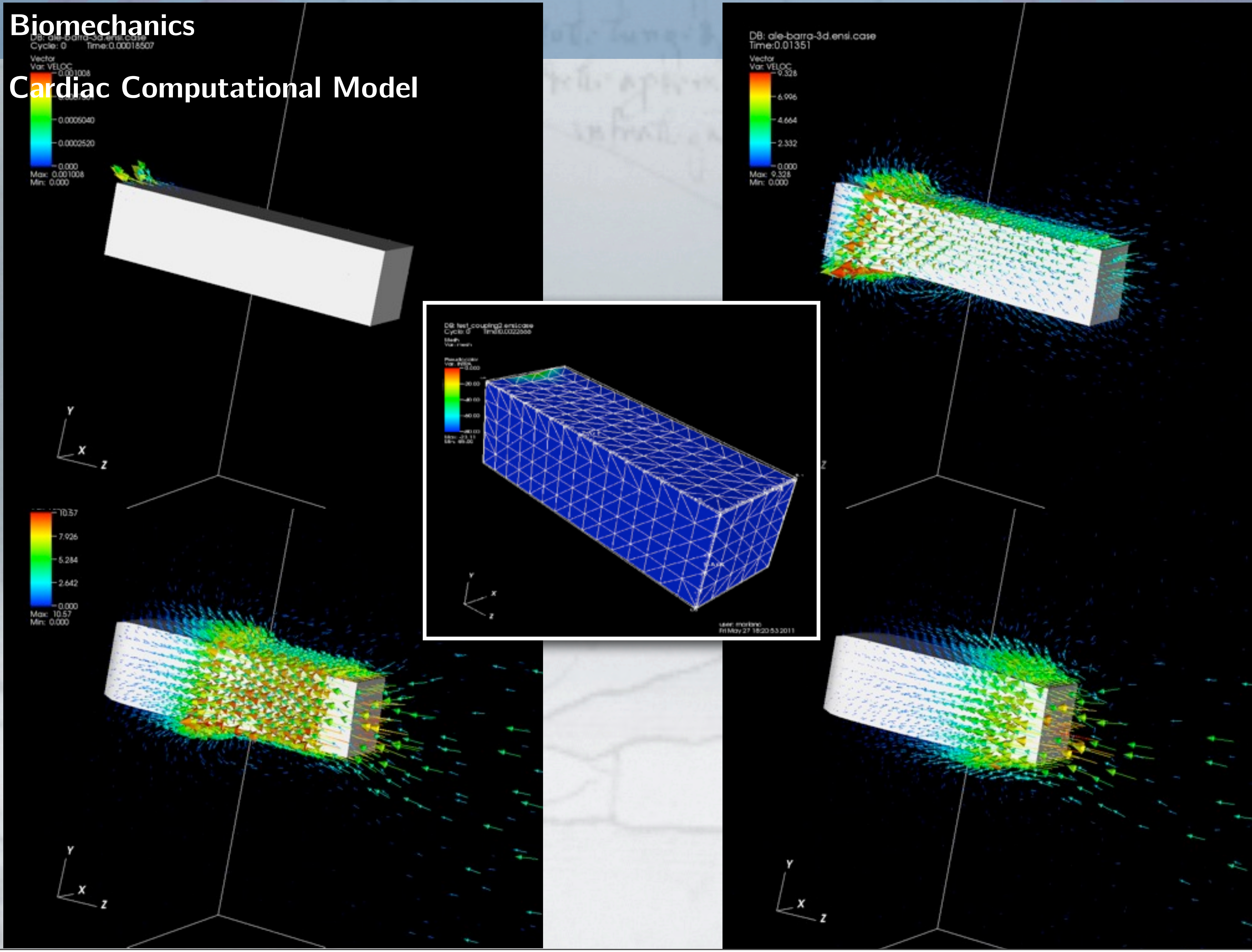
Cardiac Computational Model

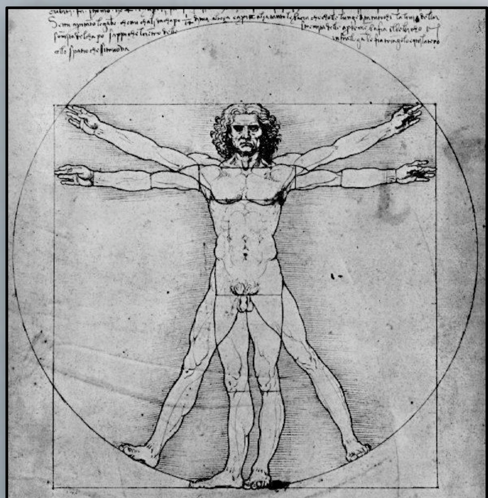




Biomechanics

Cardiac Computational Model





Alya Red

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Barcelona Supercomputing Center

Respiratory system

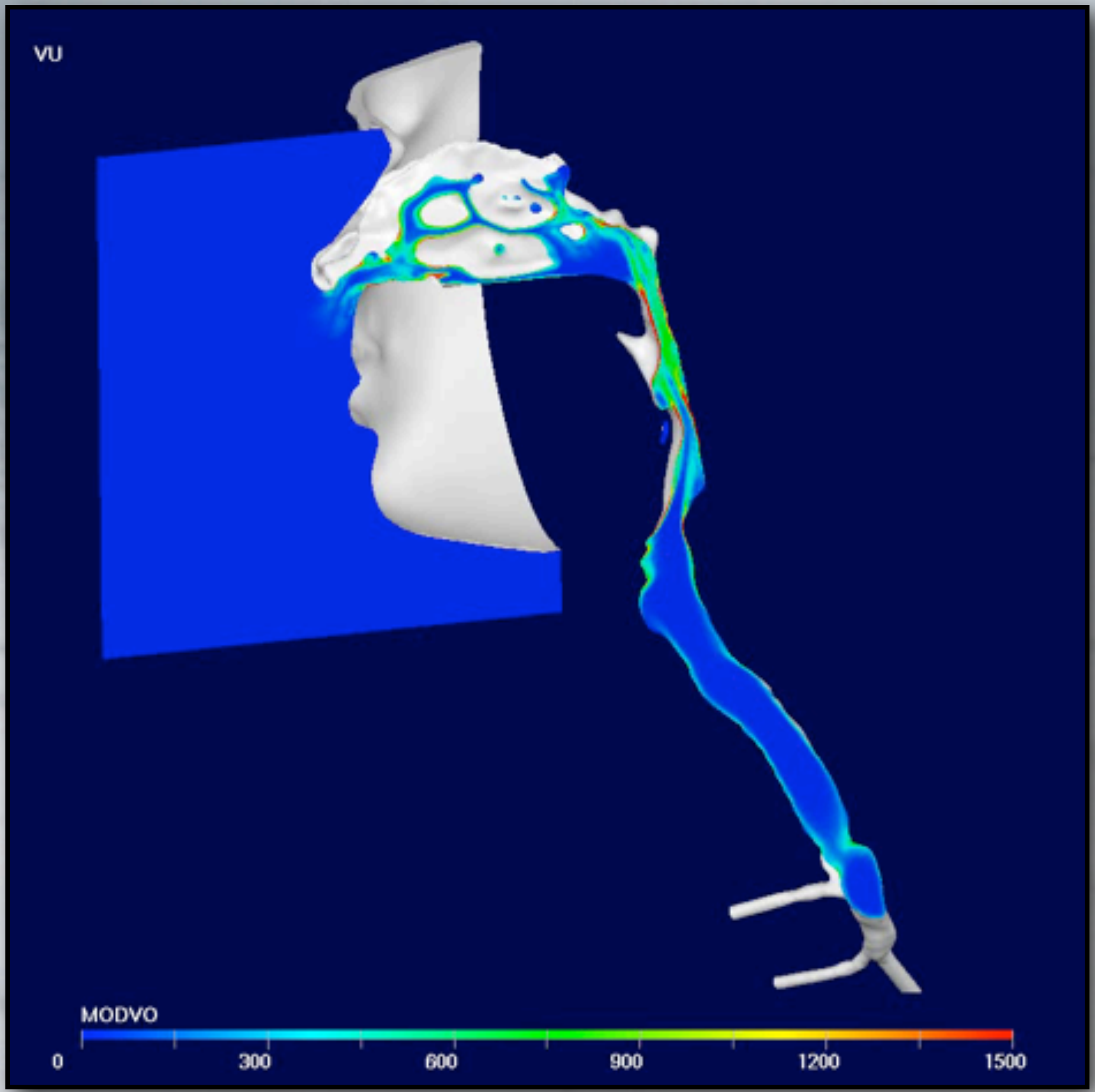
European PRACE project: The Computational Respiratory System

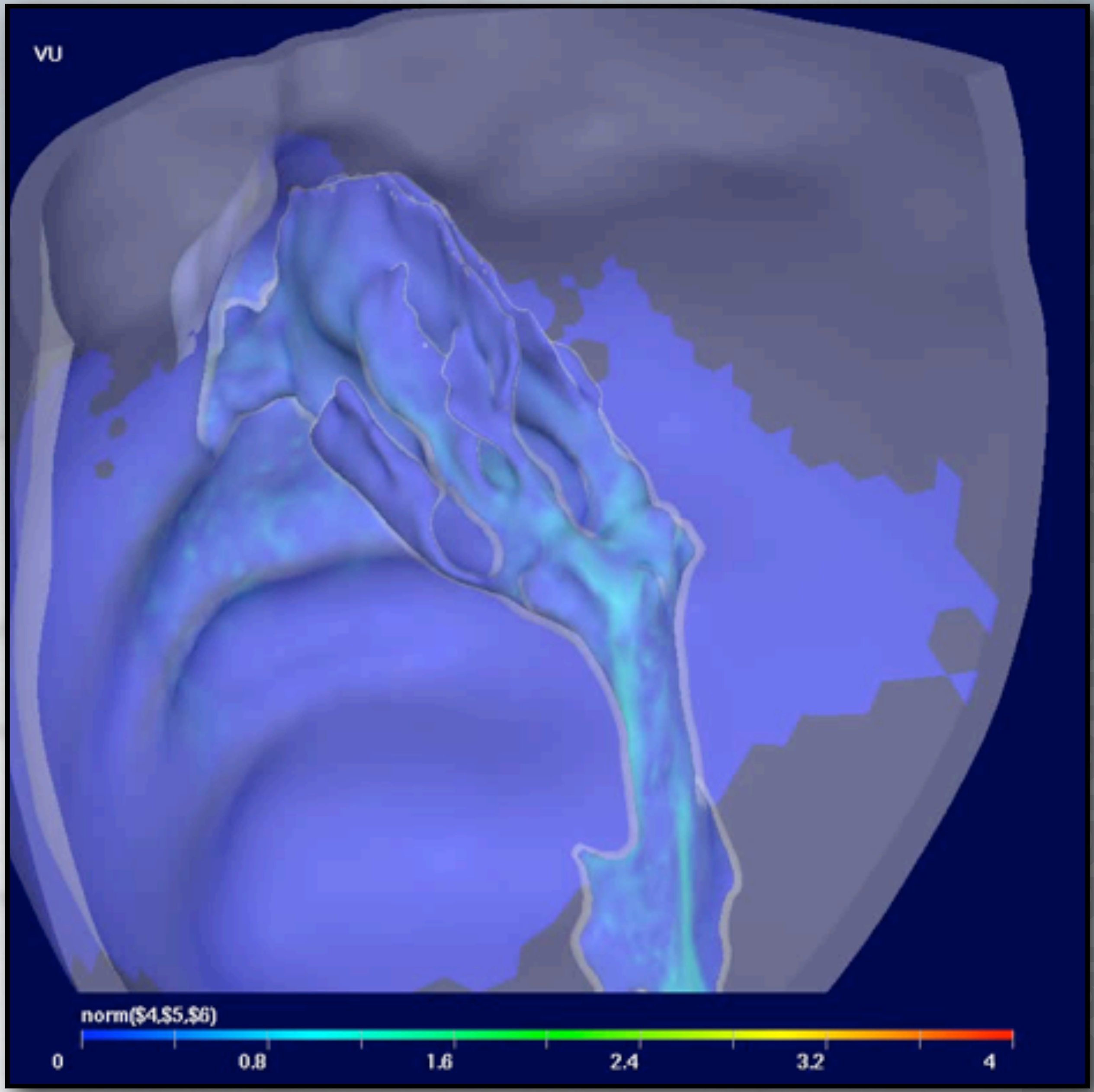
In collaboration with Imperial College London - Jackson State Univ.

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.

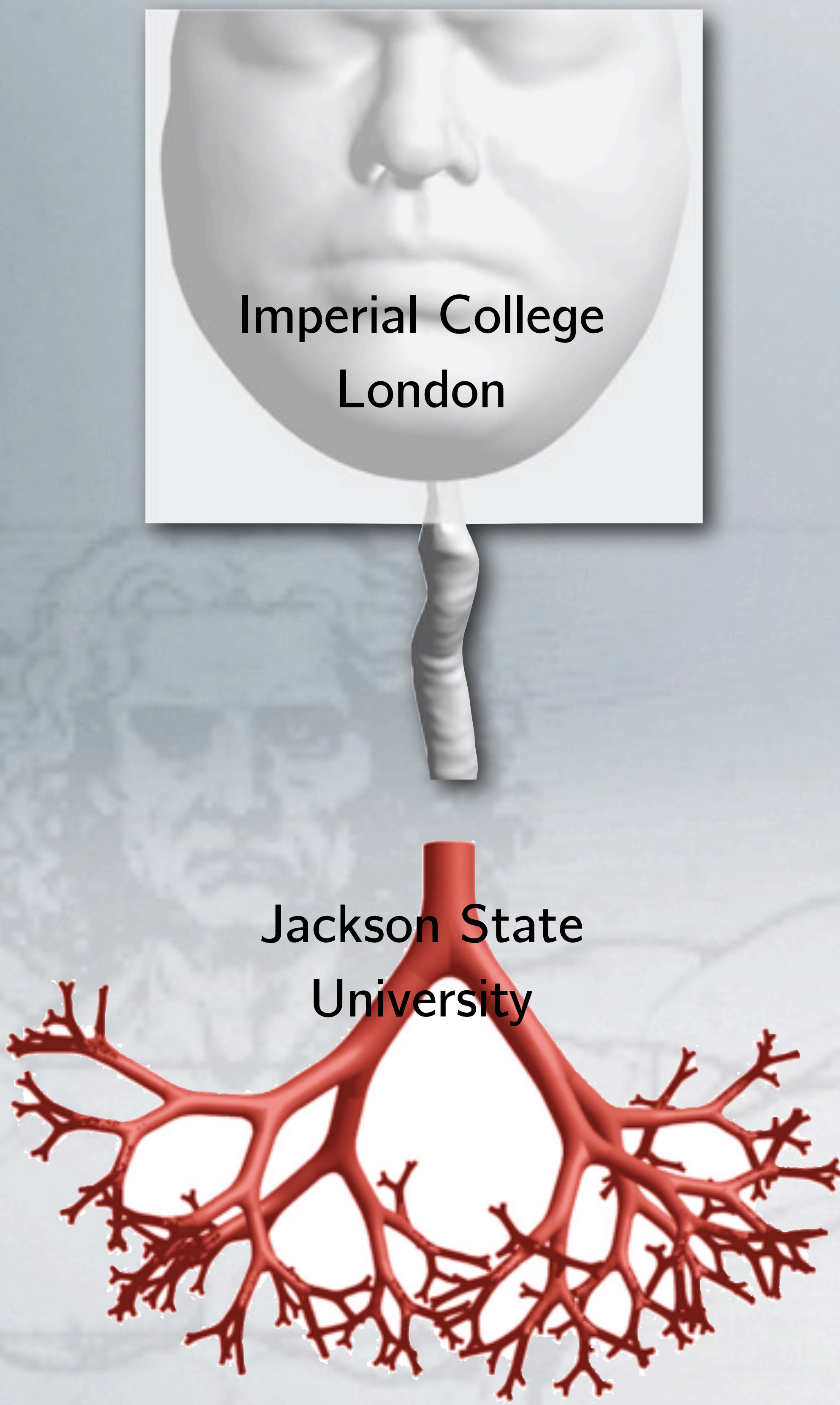
Case I: Perform simulations on the dummies and offer the data-base for analysis

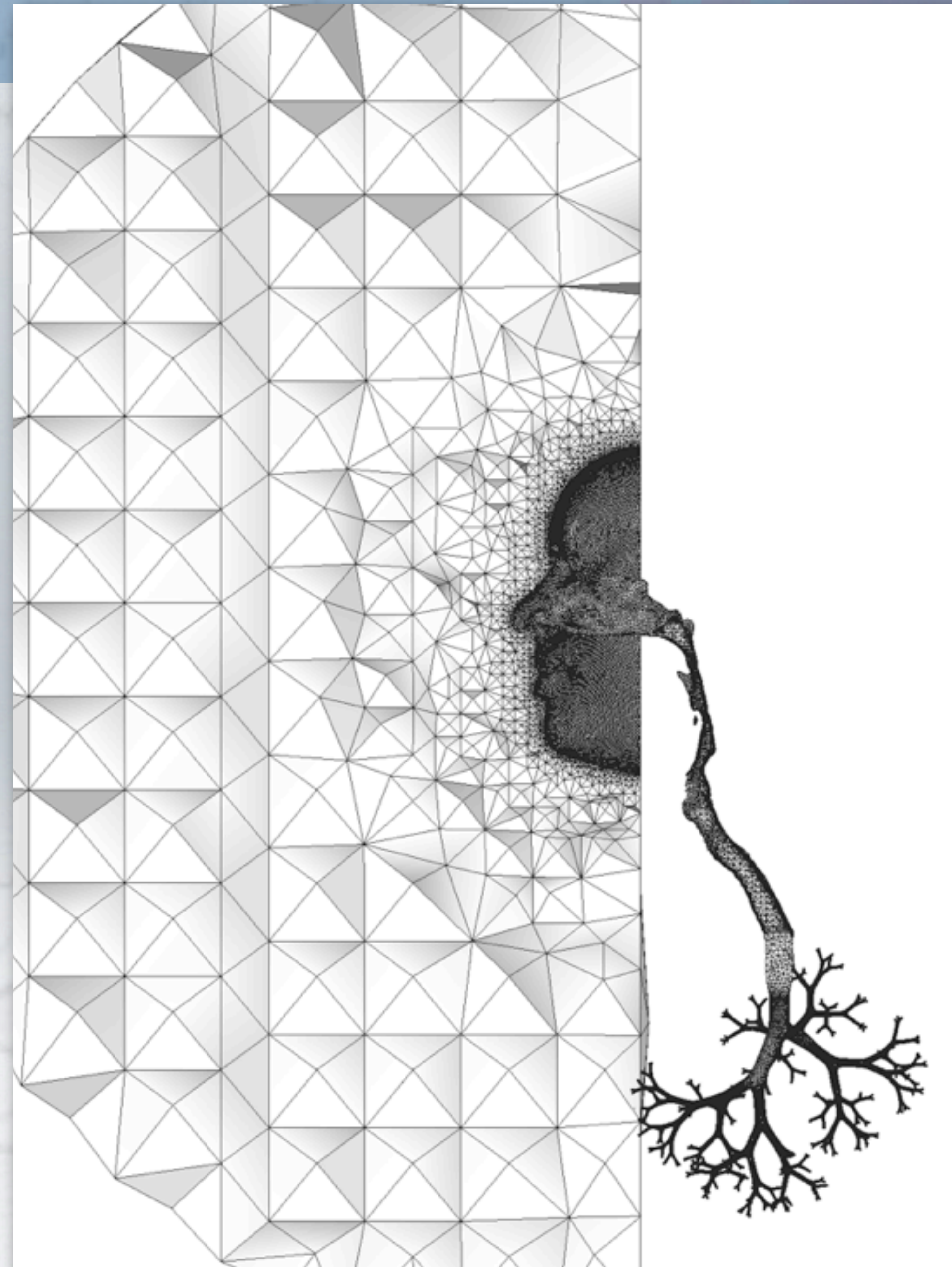
Case II: Perform simulations on the dummies for biomedical design

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

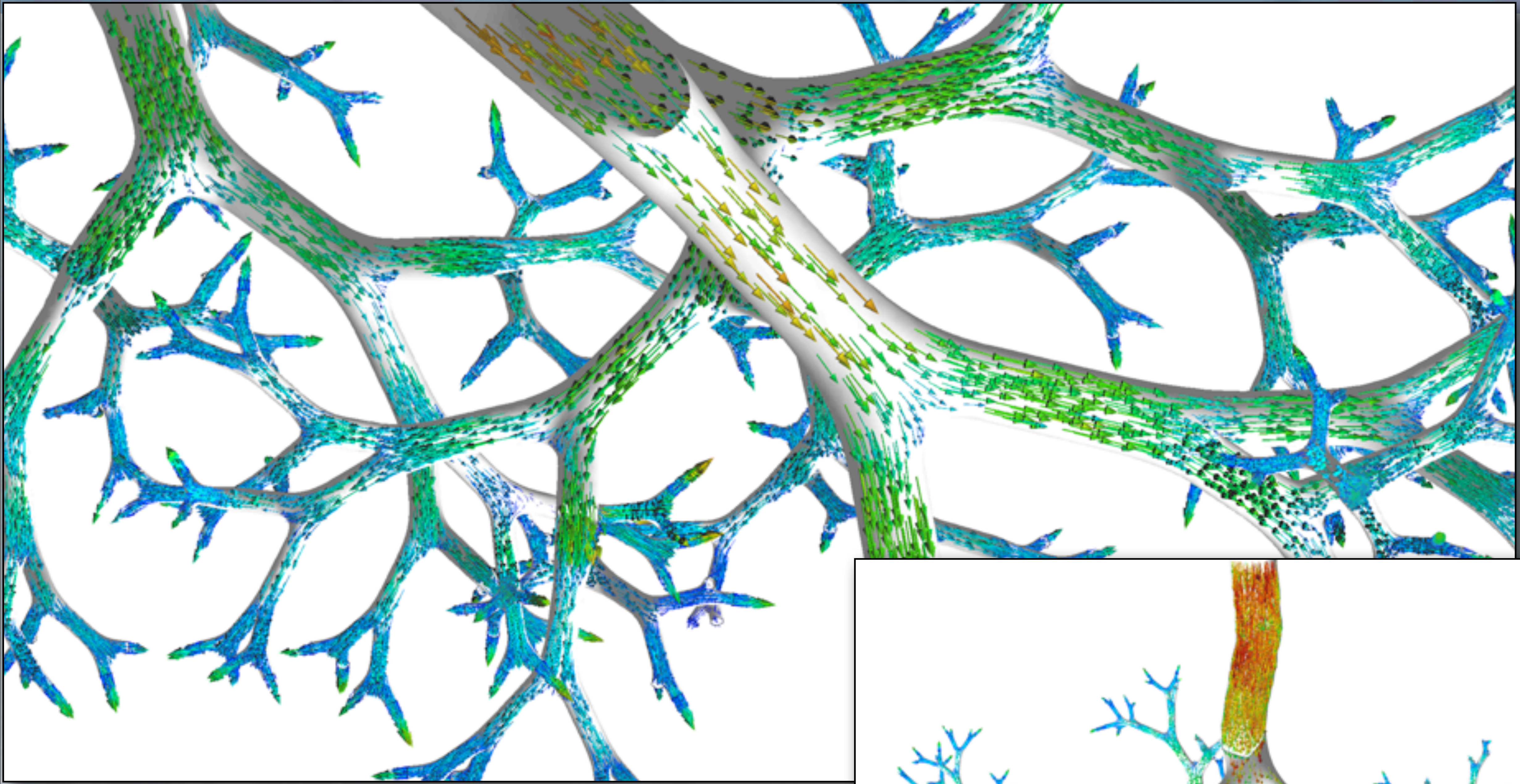
Computational Respiratory System

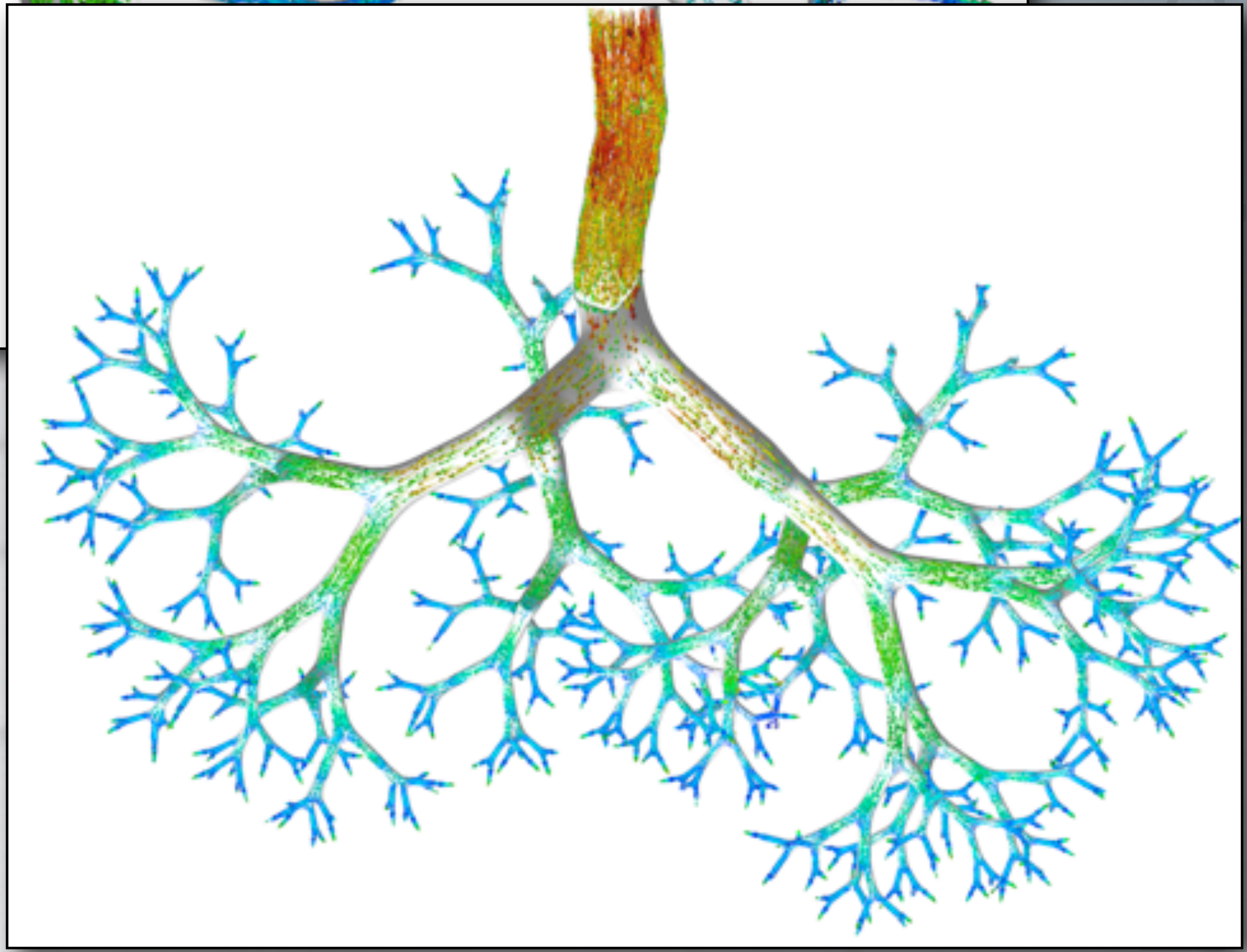
Respiratory system

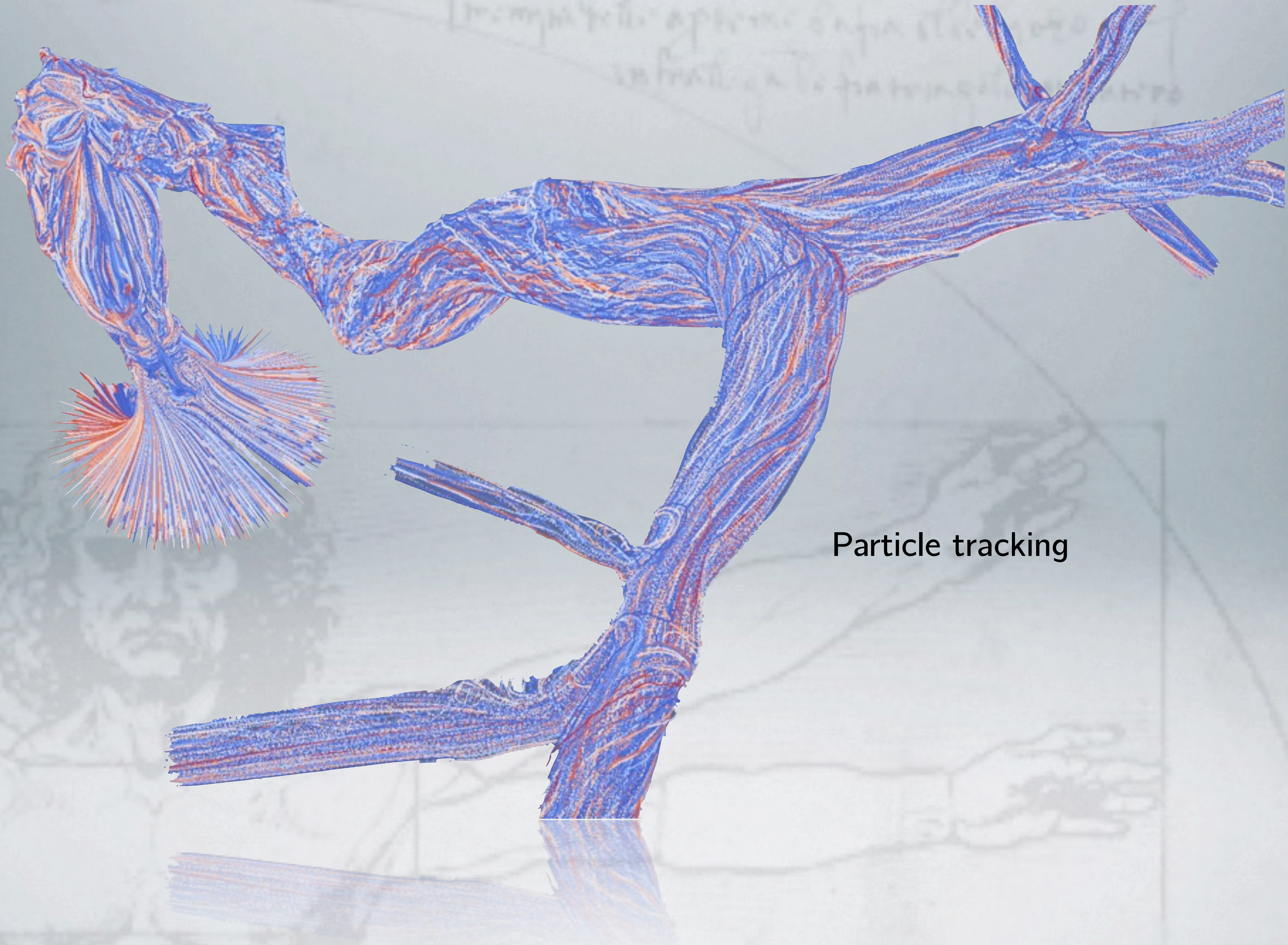




Computational Respiratory System






Particle tracking

Massive particle tracking

Scenario:

High definition CFD simulations (tens to hundreds million elements)

Complex geometries, as complete and comprehensive as possible

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

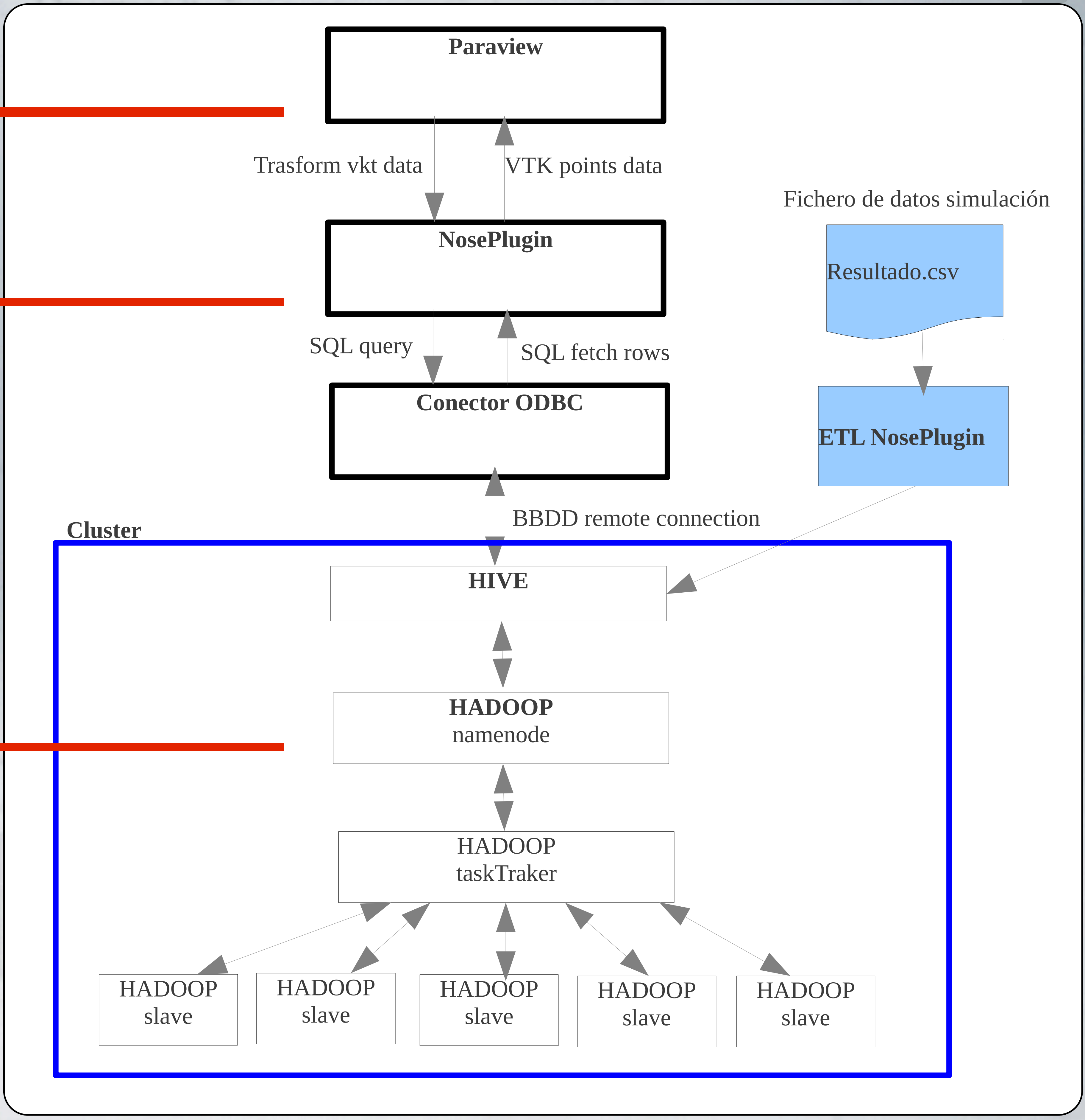
Create a data base and analyze the results

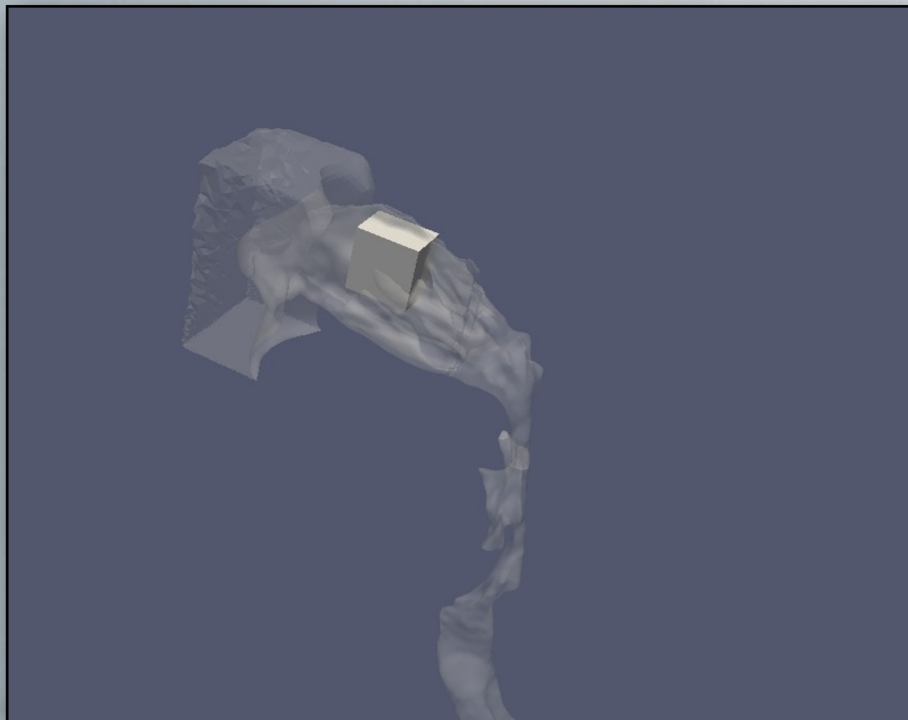
How could we identify and track the particles?

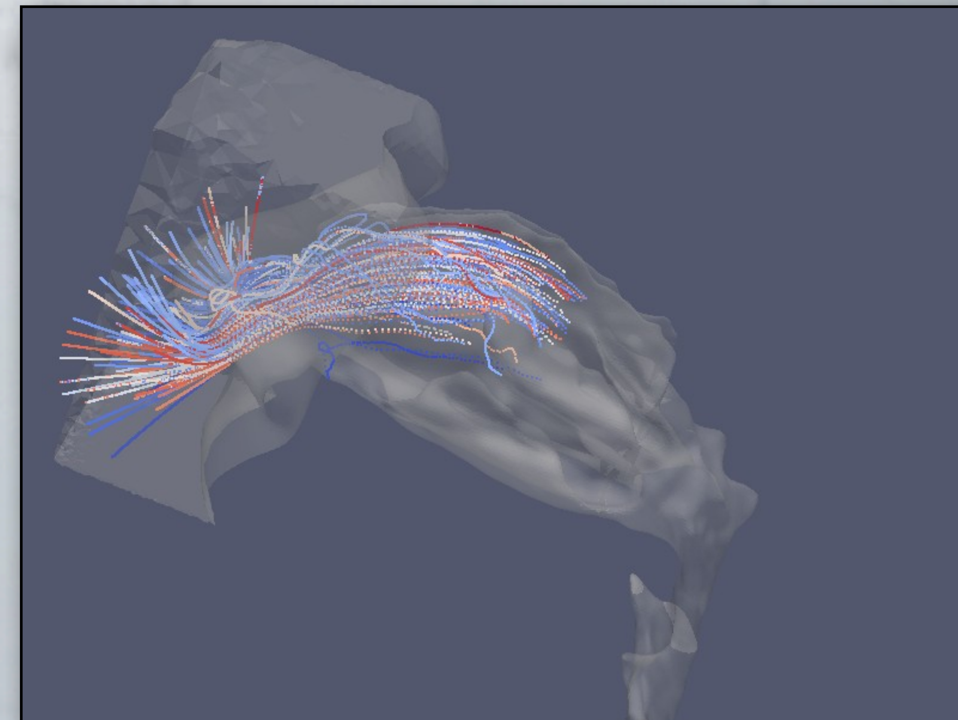
Paraview interface

Paraview plugin

Parallel Database





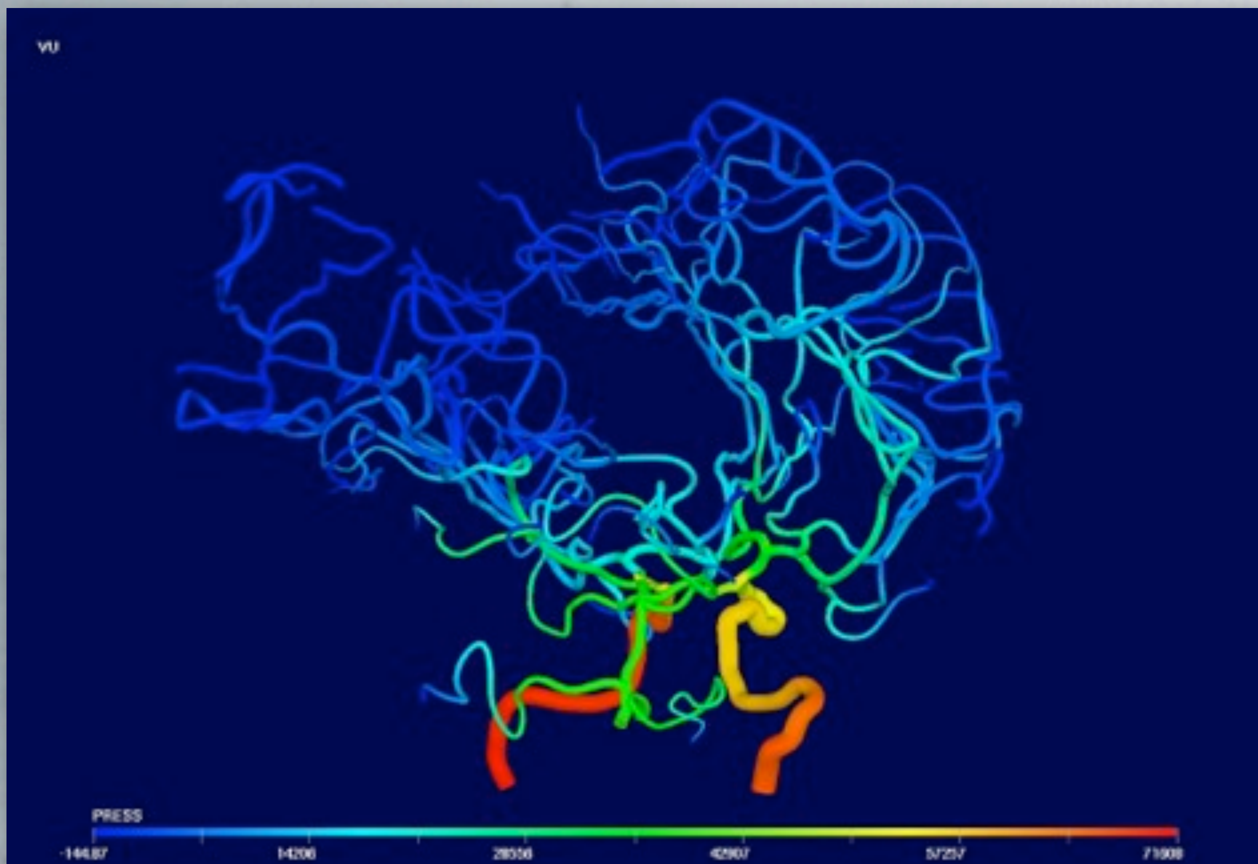


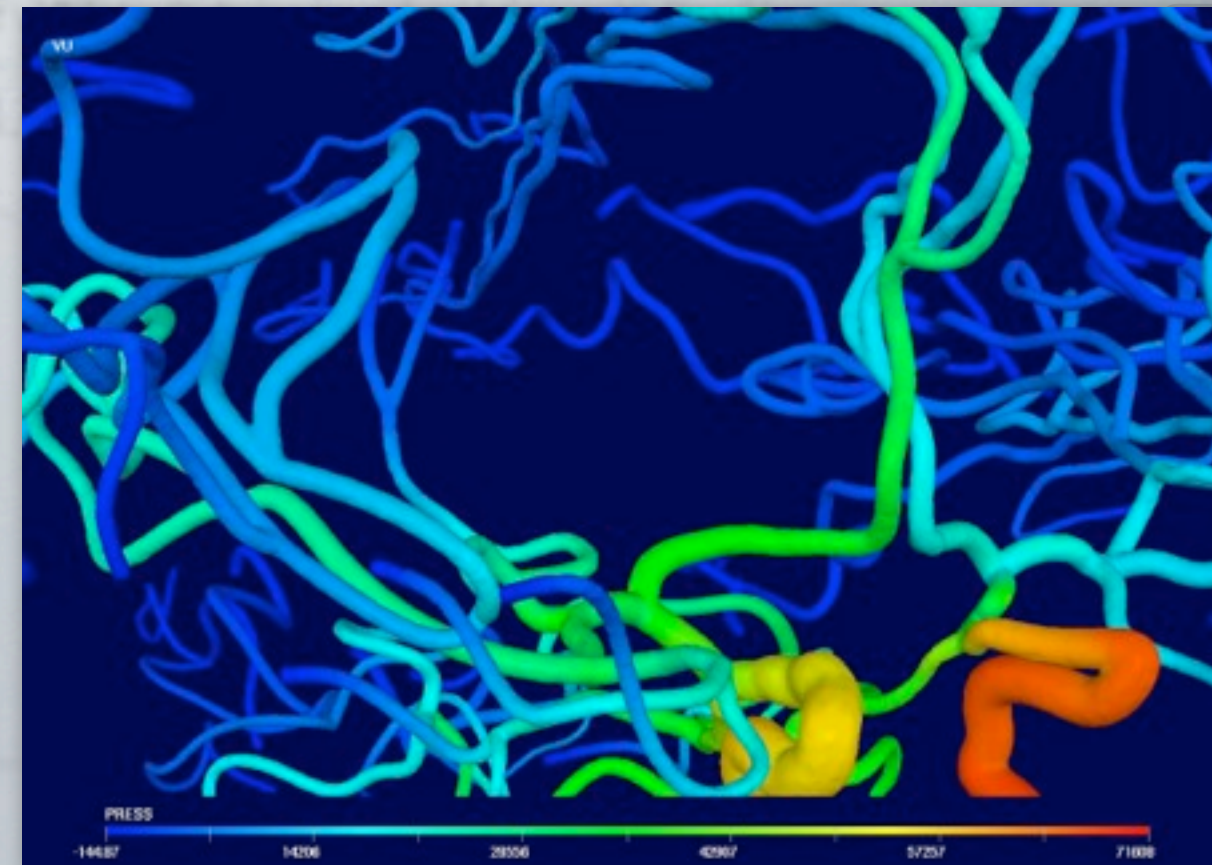
Example: Track back all the particles found at time t at this box

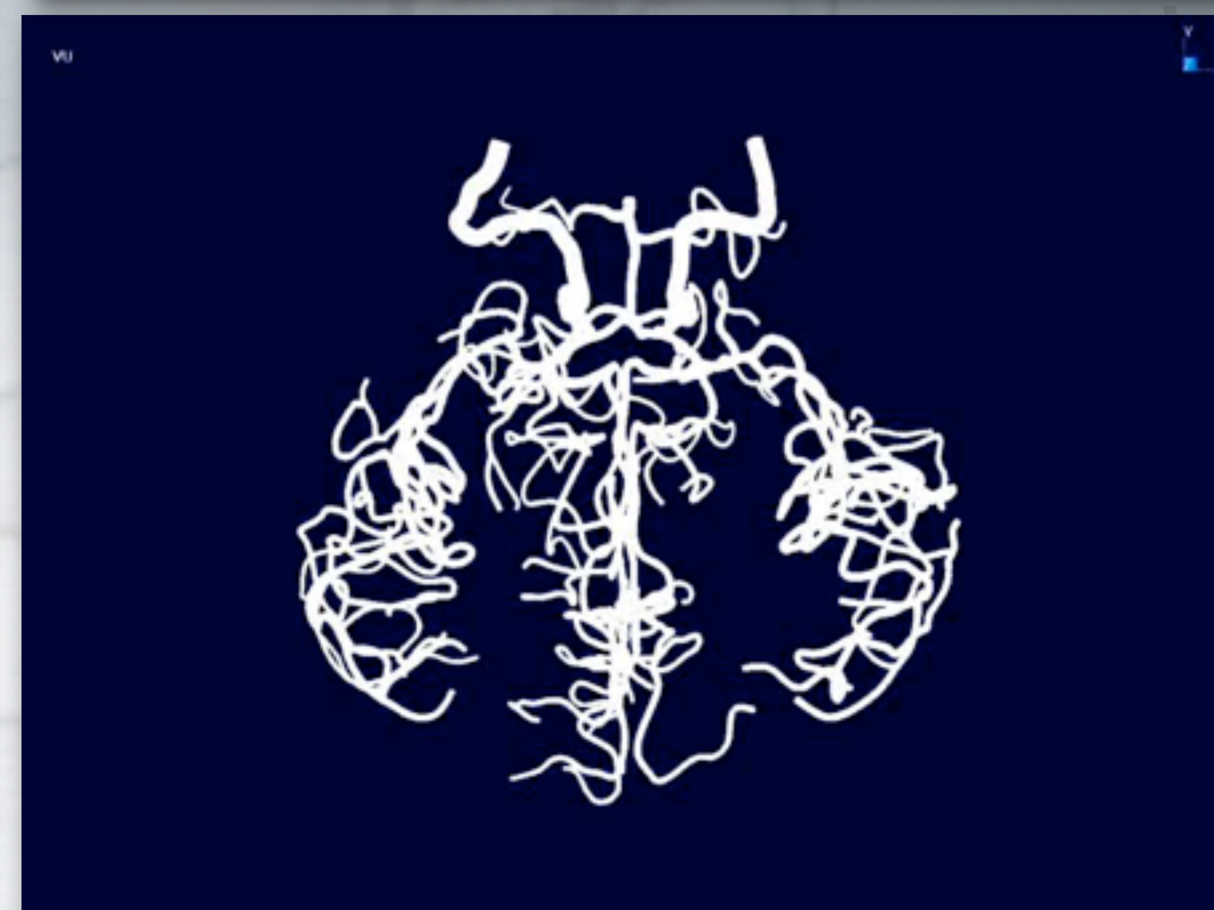
Particles can be labelled by species or initial / final situation

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

Cerebral arterial system







In collaboration with George Mason University and UCLA

Incompressible Navier-Stokes
Highly transient flow

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

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

Drug (blockers) effect

Regenerating cardiac stem cells clustering due to stress concentration

High Performance Computational Biomechanics

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Centro Nacional de Supercomputación
Spain

HPC LatAm 2013
Mendoza - Argentina