

HIGH PERFORMANCE COMPUTING FOR IN SILICO MEDICINE

COMPUTATIONAL CARDIOLOGY



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CHRIS MORTON

ELEM BIOTECH &
BARCELONA SUPERCOMPUTING CENTER

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ELEM THE VIRTUAL HUMANS
FACTORY



MARENOSTRUM IV

166.000 CORES

11.5 PFLOPS

1.3 MW / YEAR

HOSTED BY THE
BARCELONA
SUPERCOMPUTING CENTER

HARDWARE SETUP AND
MAINTENANCE
SOFTWARE DEVELOPMENT
AND EFFICIENCY
DATA MANAGEMENT



BARCELONA SUPERCOMPUTING CENTER

550 RESEARCHERS
SPANISH PUBLIC CENTER

TIER-0 EUROPEAN
SUPERCOMPUTING
NETWORK (PRACE)

APPLIED COMPUTATIONAL
SCIENCE SINCE 2005



ALYA DEV TEAM

50 RESEARCHERS
MATHEMATICIANS,
PHYSICISTS, ENGINEERS,
PROGRAMMERS...

SENIOR AND PHD
STUDENTS

BORN WITH BSC IN 2005



FLAMANG, B., MARRAS, S., ET AL. 2020. REMORAS PICK WHERE THEY STICK ON BLUE WHALES. JOURNAL OF EXPERIMENTAL BIOLOGY. TO APPEAR.

ELEM BIOTECH

BSC'S SPINOFF COMPANY

BIOMEDICAL SOFTWARE
TECHNOLOGY

INSILICO CLINICAL TRIALS

HPC-CLOUD BASED
SIMULATIONS

CELL, TISSUE AND ORGAN
LEVEL



ELEM BIOTECH & BSC

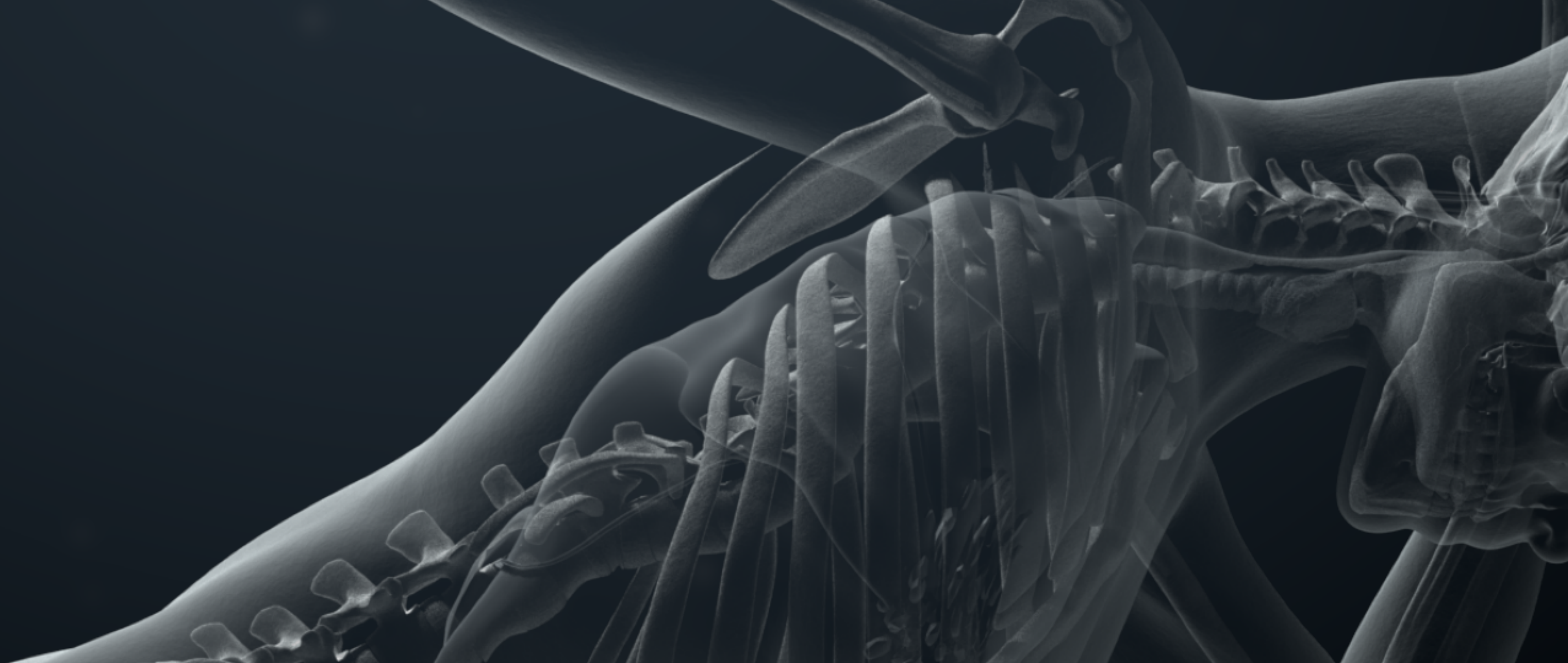
OUR GOALS

TO ENABLE BIOMEDICAL COMPANIES TO DEVELOP BETTER TREATMENTS, FASTER, AND AT REDUCED RISKS

TO PROVIDE VIRTUAL HUMAN TRIALS WHICH CAN REDUCE FROM YEARS TO MONTHS THE TIME FROM INCEPTION TO HUMAN TESTING

TO HELP MAKE MEDICAL PRODUCTS CERTIFIED AND TESTED IN SILICO BEFORE BETTING ON PATIENT'S LIFE.

BACKGROUND





ALYA

THE SIMULATION CODE

USED IN INDUSTRY RELATED PROJECTS: AEROSPACE, ENERGY,
ENVIRONMENT AND... **BIOMEDICAL**

ONLY MULTI-SCALE / MULTI-PHYSICS CODE FOR BIOMEDICAL USE AT
ORGAN LEVEL BORN AND DEVELOPED IN A SUPERCOMPUTING CENTER

VÁZQUEZ, M., HOUZEAUX, G., KORIC, S., ARTIGUES, A., AGUADO-SIERRA, J., ARÍS, R., MIRA, D., CALMET, H., CUCCHIETTI, F., OWEN, H. AND TAHA, A., 2016. ALYA: MULTIPHYSICS ENGINEERING SIMULATION TOWARD EXASCALE. *JOURNAL OF COMPUTATIONAL SCIENCE*, 14, PP.15-27.

ALYA

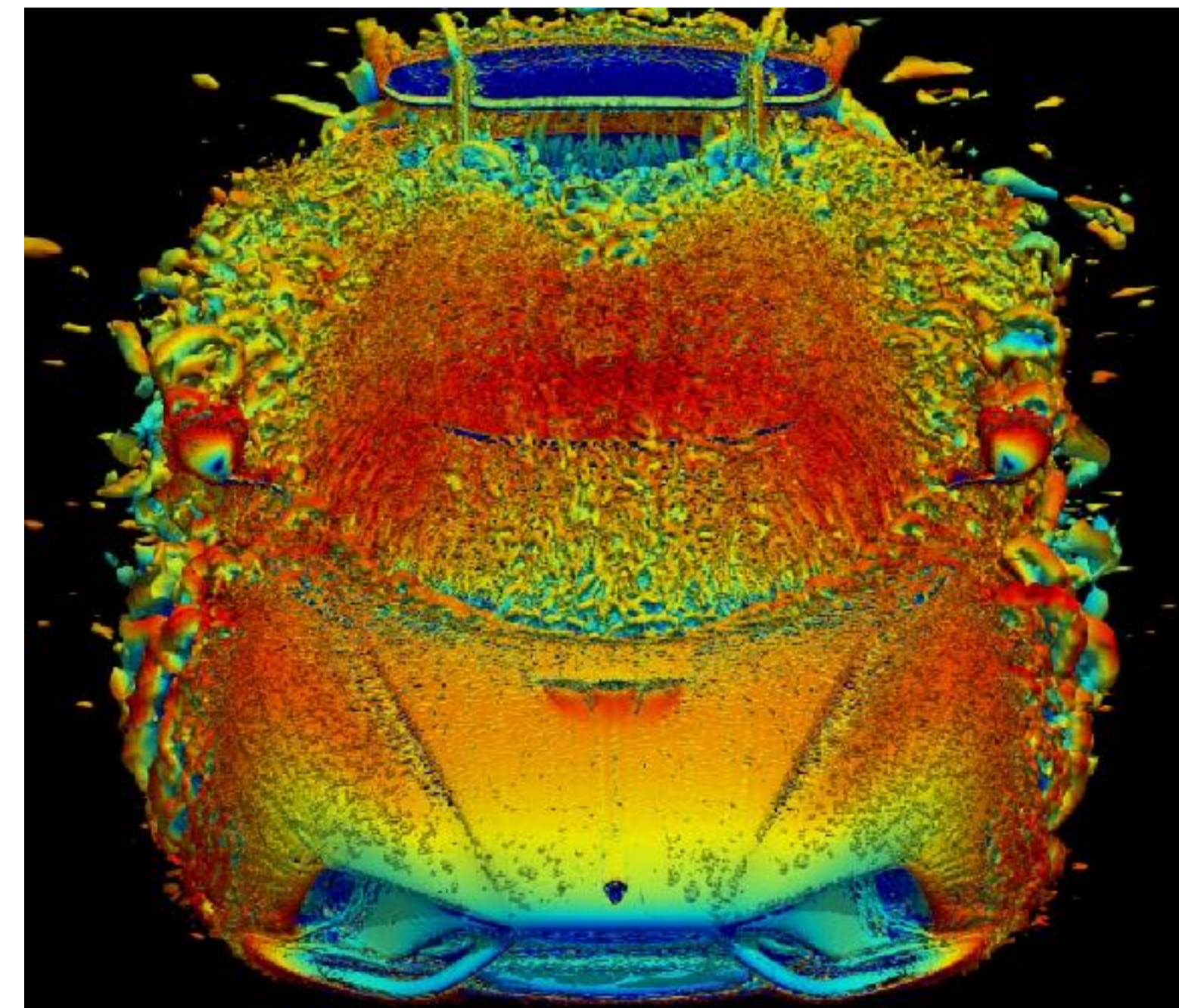
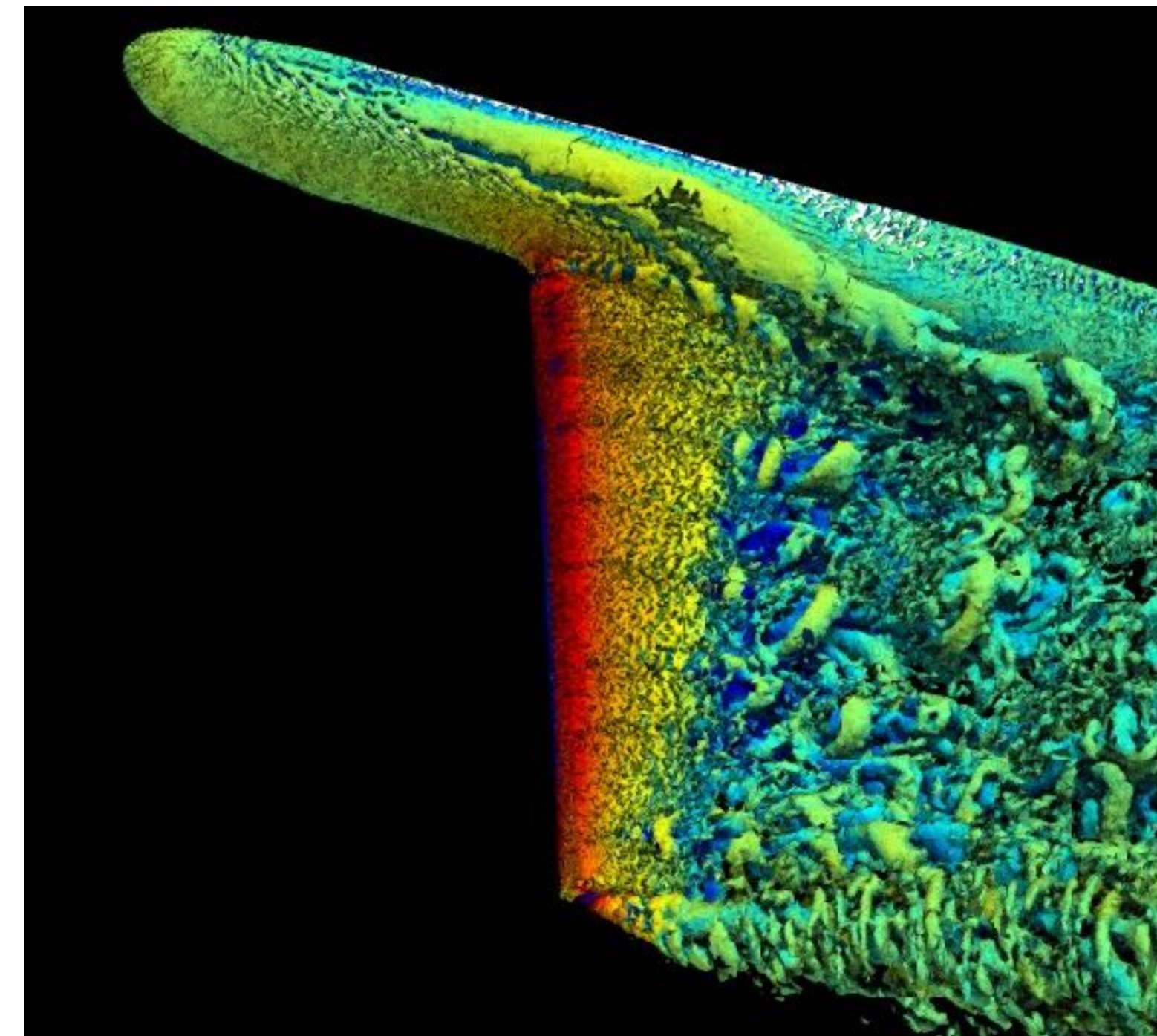
THE CONCEPT

HPC-BASED SIMULATION CODE FOR
SUPERCOMPUTERS

COUPLED MULTI-PHYSICS / MULTI-SCALE

LARGE-SCALE PROBLEMS

ANALYSE, UNDERSTAND, **PREDICT**, IMPROVE



LEHMKUHL, O., HOUZEAUX, G., OWEN, H., CHRYSOKENTIS, G. AND
RODRIGUEZ, I., 2019. A LOW-DISSIPATION FINITE ELEMENT SCHEME FOR
SCALE RESOLVING SIMULATIONS OF TURBULENT FLOWS. JOURNAL OF
COMPUTATIONAL PHYSICS, 390, PP.51-65.

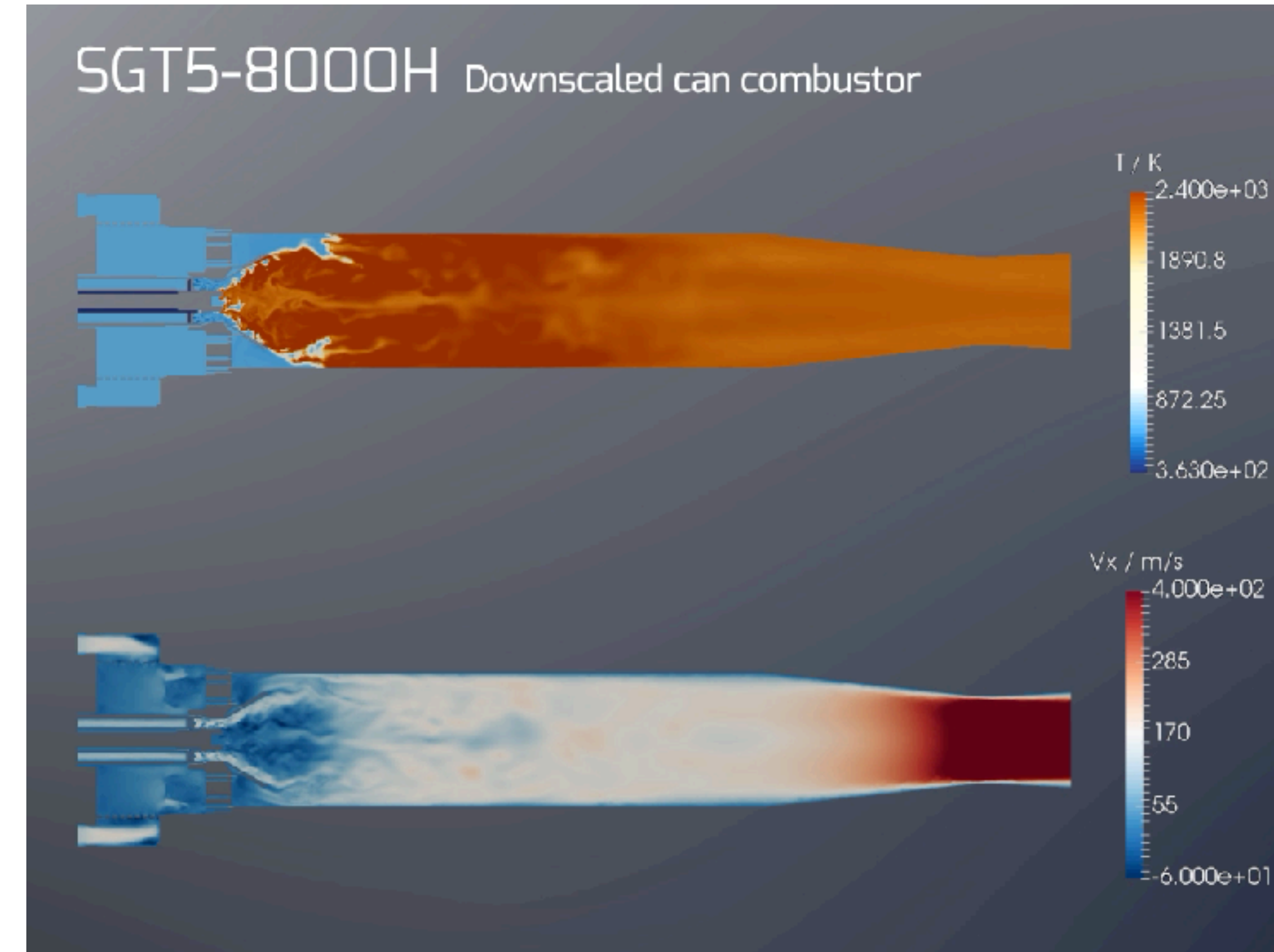
ALYA

THE KEYWORDS

COMPLEX, UNCONVENTIONAL
PHYSICAL / MATHEMATICAL MODELS

COMPLEX PRE-PROCESS (MESHING)
AND POST-PROCESS (VISUALIZATION
AND ANALYSIS)

MULTI-PHYSICS PROBLEMS
BIG DATA MANAGEMENT AND
VISUALIZATION



GÖVERT, S., MIRA, D., KOK, J.B., VÁZQUEZ, M. AND HOUZEAUX, G., 2015.
TURBULENT COMBUSTION MODELLING OF A CONFINED PREMIXED JET
FLAME INCLUDING HEAT LOSS EFFECTS USING TABULATED
CHEMISTRY. APPLIED ENERGY, 156, PP.804-815.

ALYA RED

SIMULATION TOOLS FOR
BIOMEDICAL RESEARCH

INSILICO CLINICAL TRIALS
AND DIAGNOSE



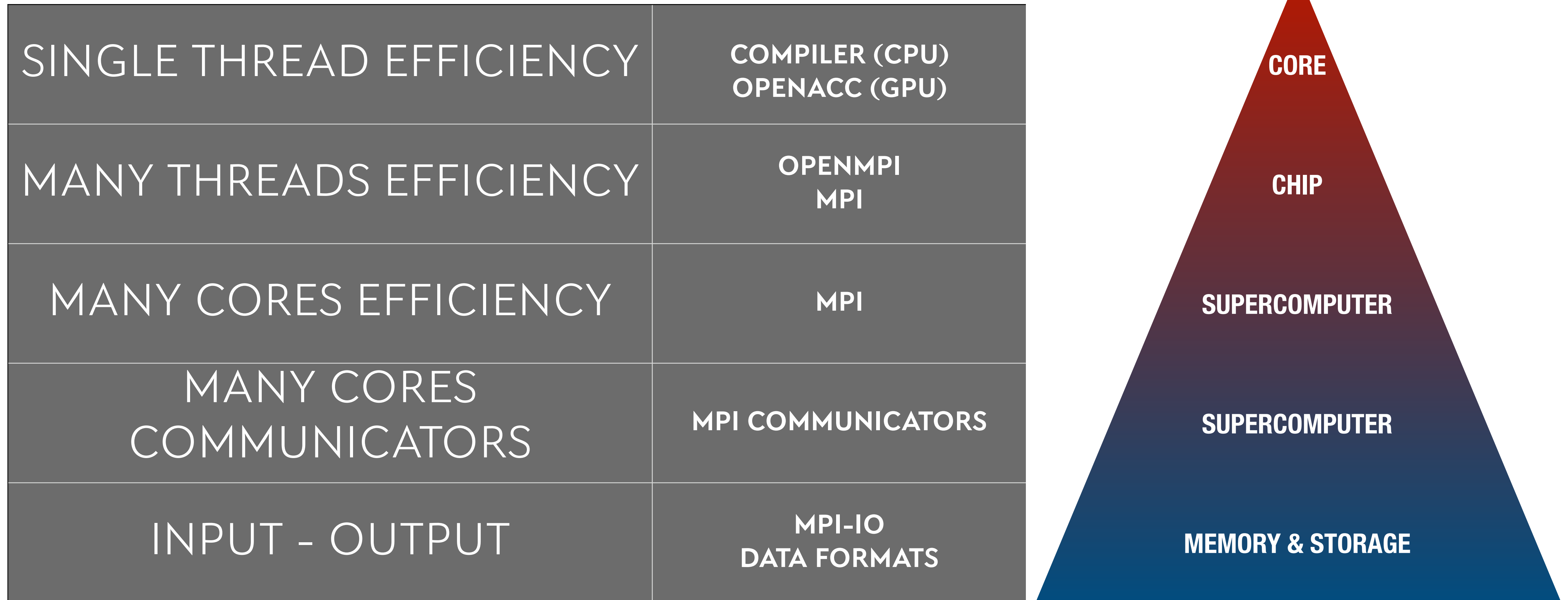
ORGAN / TISSUE LEVEL

COMPLEX PROBLEMS WHICH REQUIRE SUPERCOMPUTERS

CARDIOVASCULAR, RESPIRATORY, ...
FOR PHARMA, MEDTECH, ...

ALYA

PARALLEL PROGRAMMING: ALL LEVELS ACCOUNTABLE



HOUZEAUX, G., GARCIA-GASULLA, M., CAJAS, J.C., BORRELL, R., SANTIAGO, A., MOULINEC, C. AND VÁZQUEZ, M., 2020. PARALLEL MULTIPHYSICS COUPLING: ALGORITHMIC AND COMPUTATIONAL PERFORMANCES. INTERNATIONAL JOURNAL OF COMPUTATIONAL FLUID DYNAMICS, PP.1-22.

HOUZEAUX, G., BORRELL, R., FOURNIER, Y., GARCIA-GASULLA, M., GÖBBERT, J.H., HACHEM, E., MEHTA, V., MESRI, Y., OWEN, H. AND VÁZQUEZ, M., 2018. HIGH-PERFORMANCE COMPUTING: DOS AND DON'TS. COMPUTATIONAL FLUID DYNAMICS-BASIC INSTRUMENTS AND APPLICATIONS IN SCIENCE.



THE CARDIOVASCULAR SYSTEM

COLLABORATORS:

MEDTRONIC

THE VISIBLE HEART LAB - UNIV. OF MINNESOTA(US)

CENTRO NACIONAL DE INVESTIGACION CARDIOVASCULAR (SPAIN)

HOSPITAL DE SANT PAU (SPAIN)

UNIVERSITY OF OXFORD (UK)

UNIVERSITAT POMPEU FABRA (SPAIN)

UNIVERSITAT POLITECNICA DE VALENCIA (SPAIN)

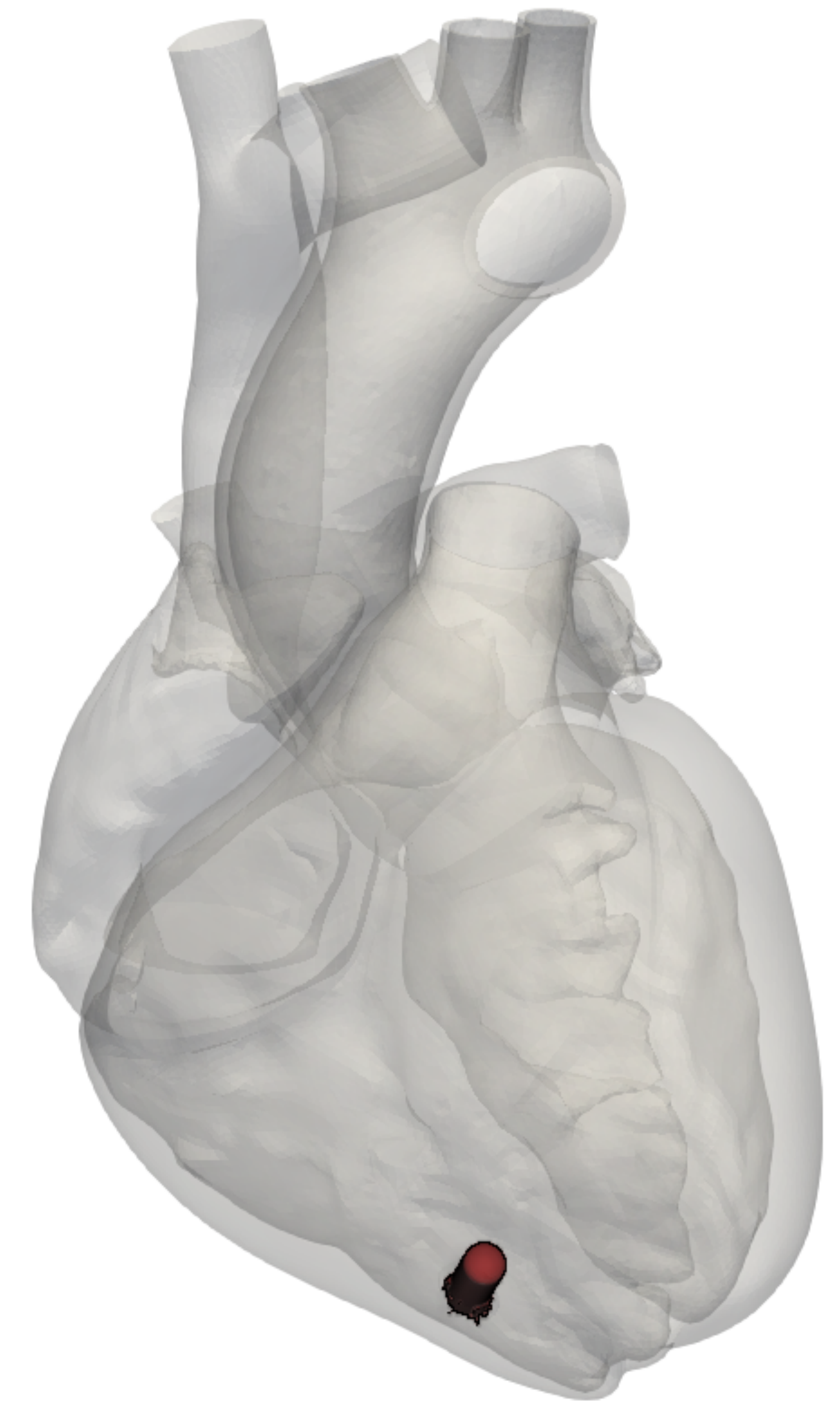
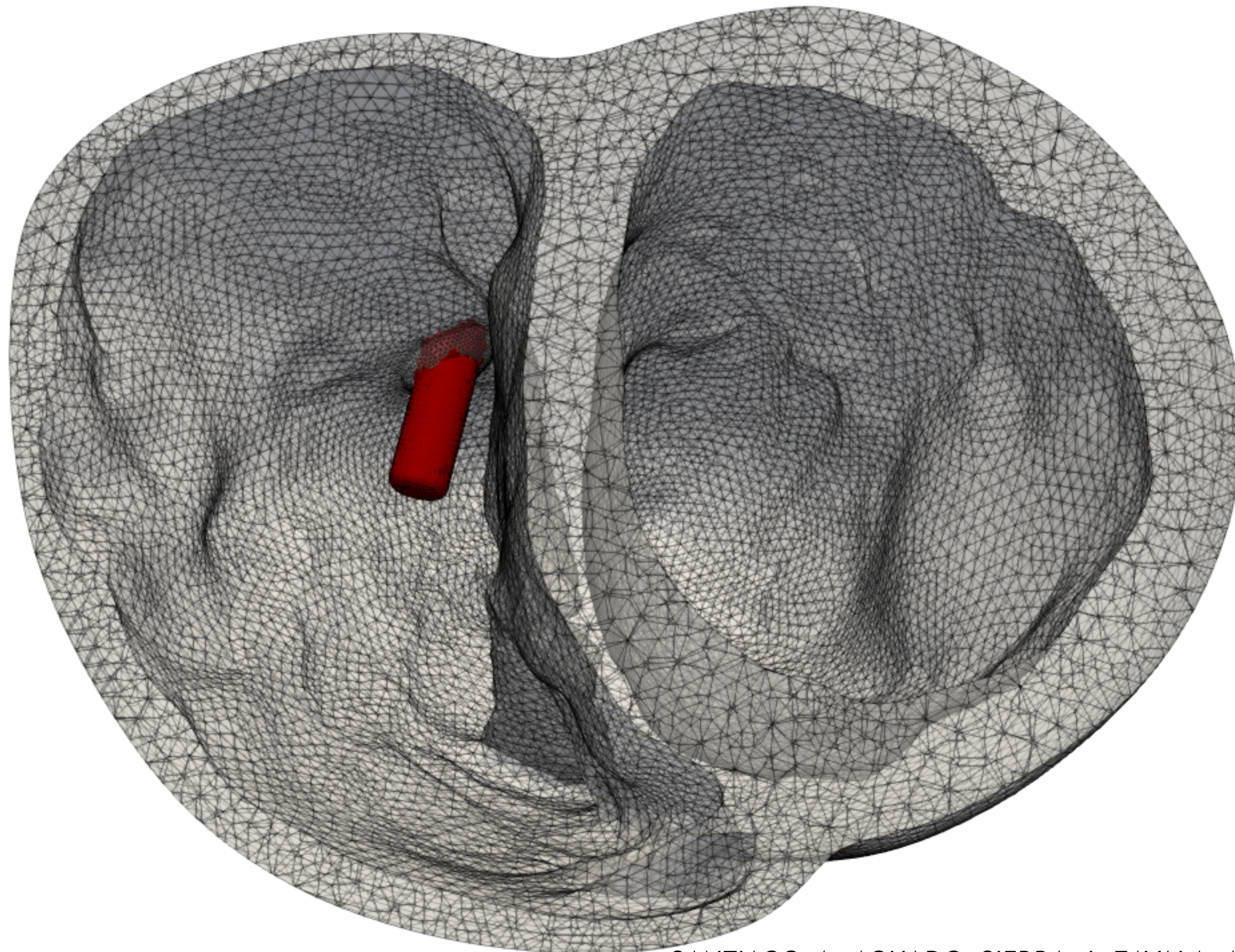
GEORGE MASON UNIVERSITY (US)

UNIVERSITY COLLEGE LONDON (UK)

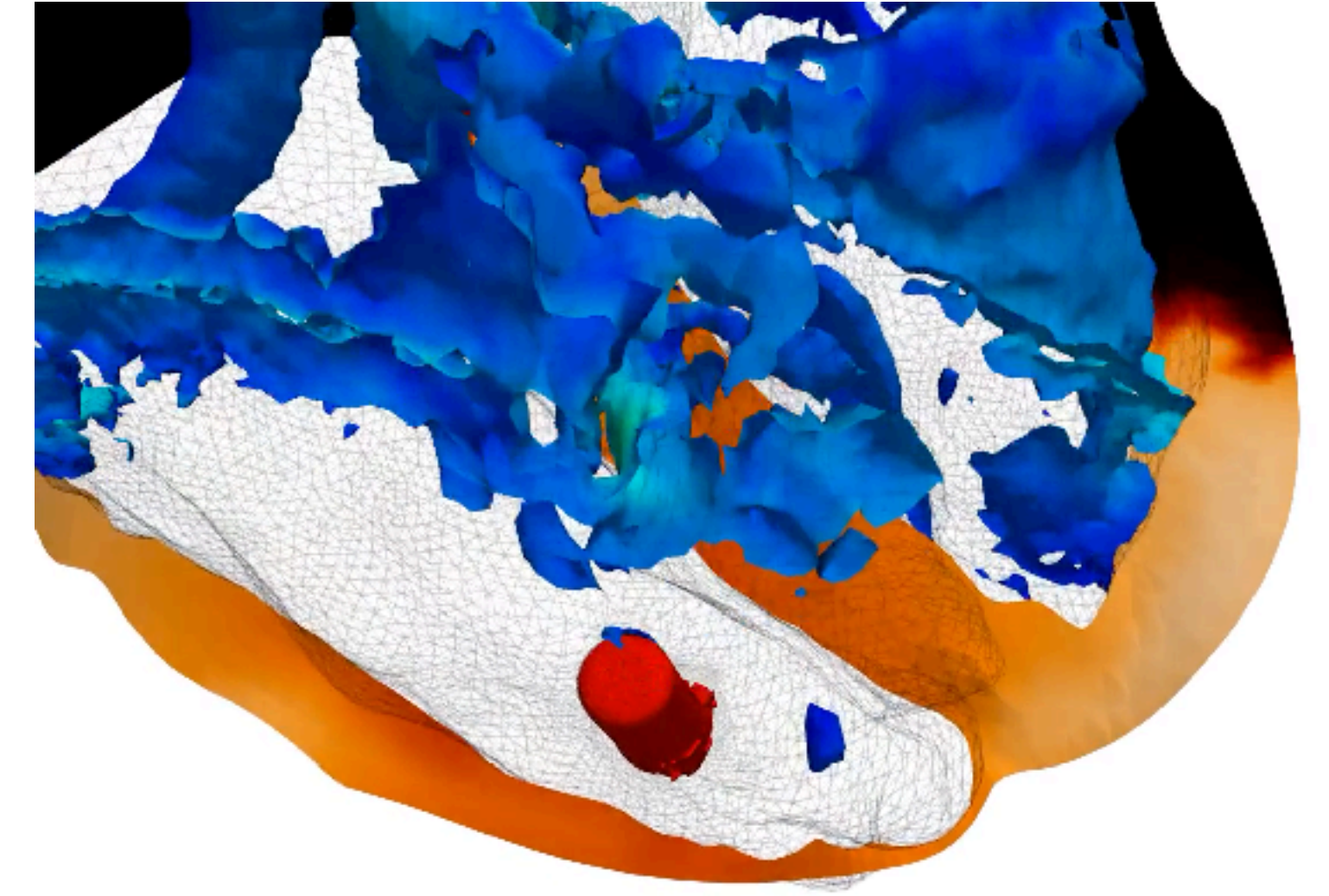
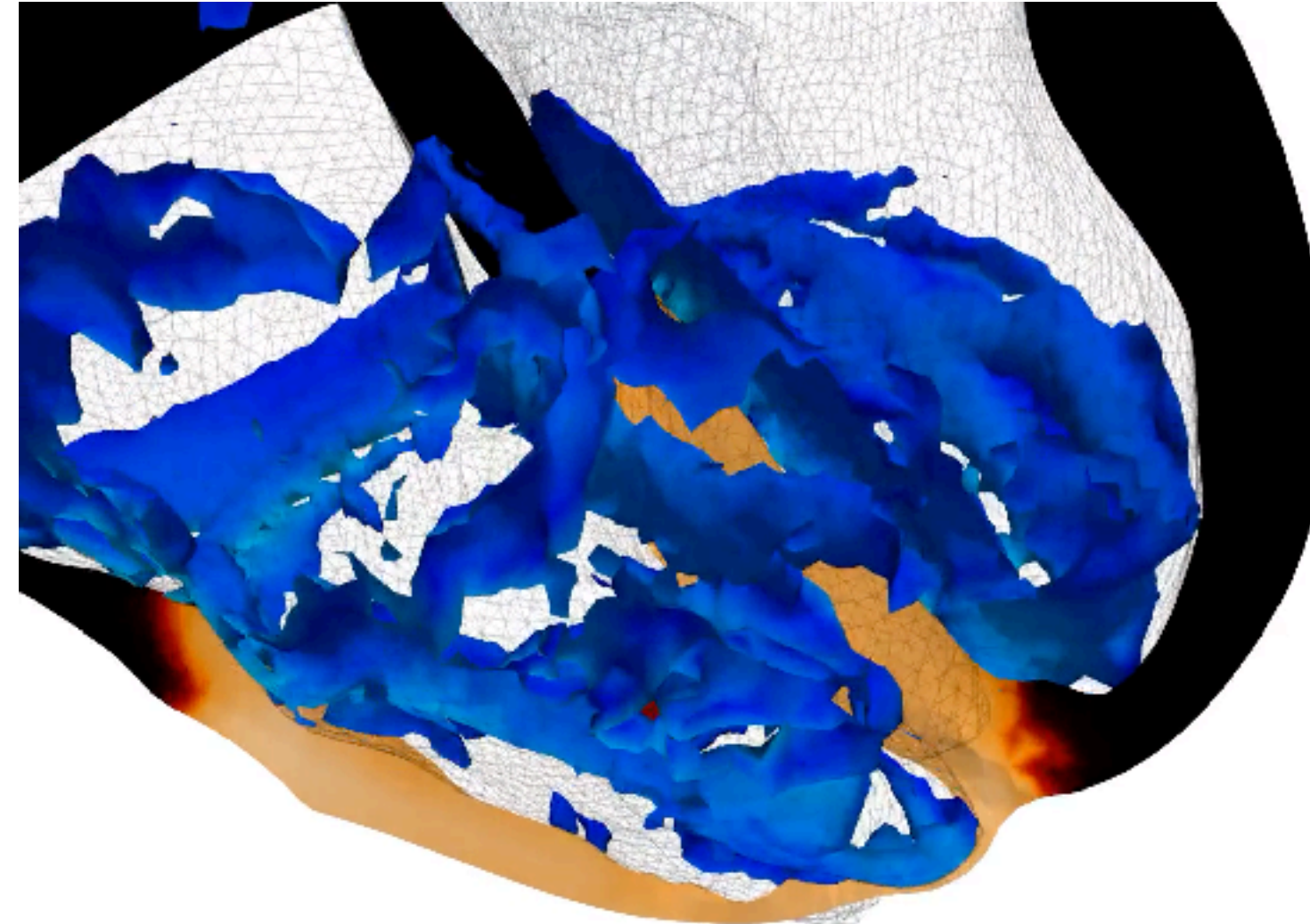
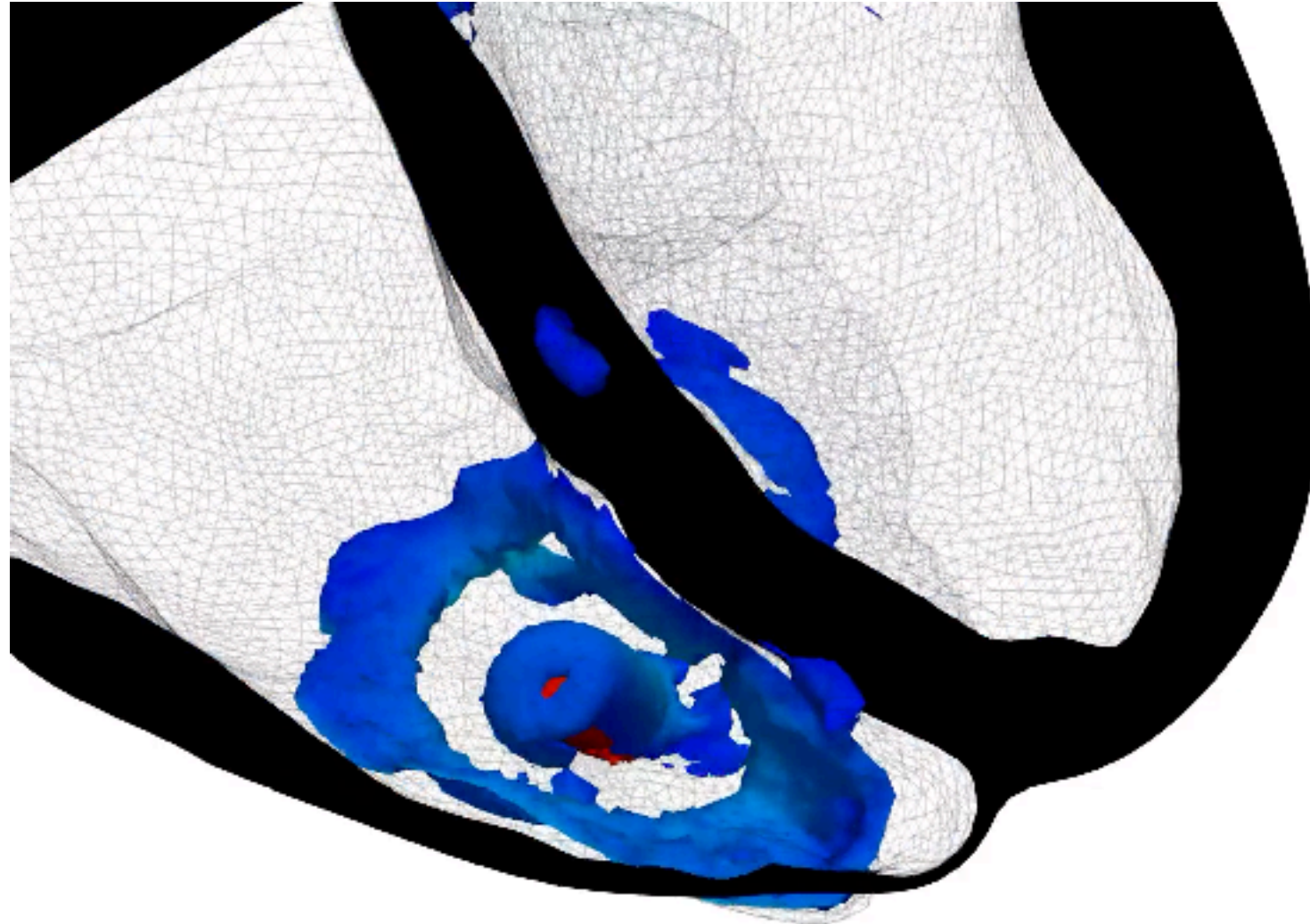
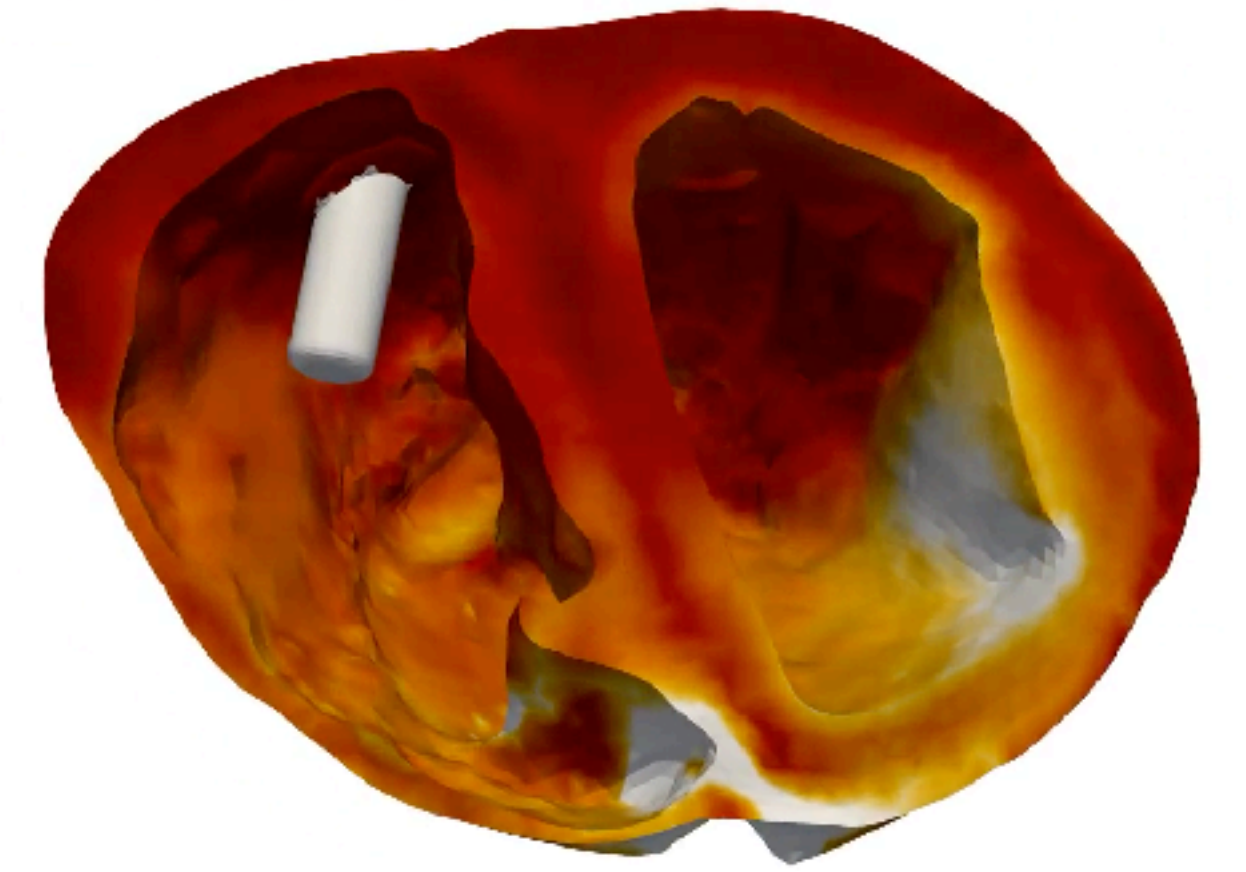
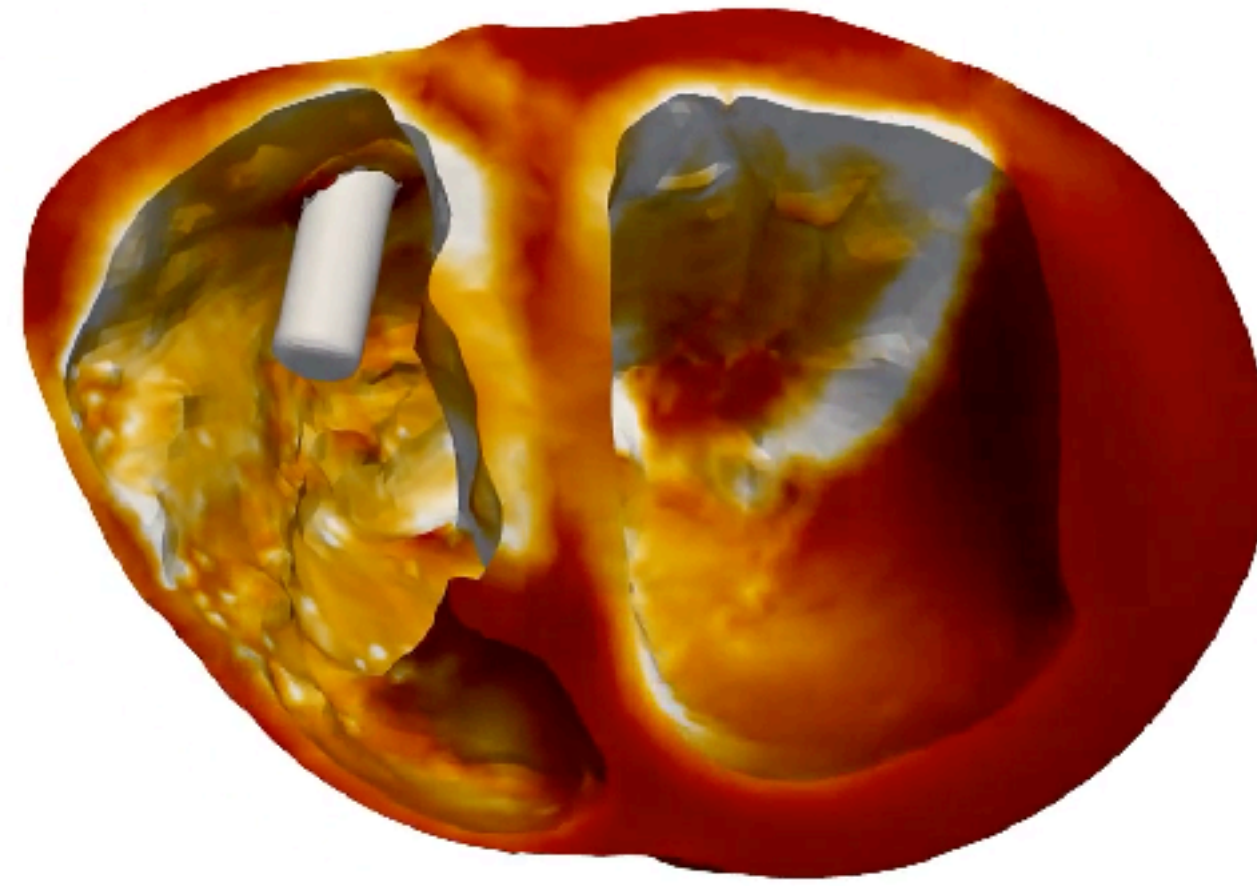
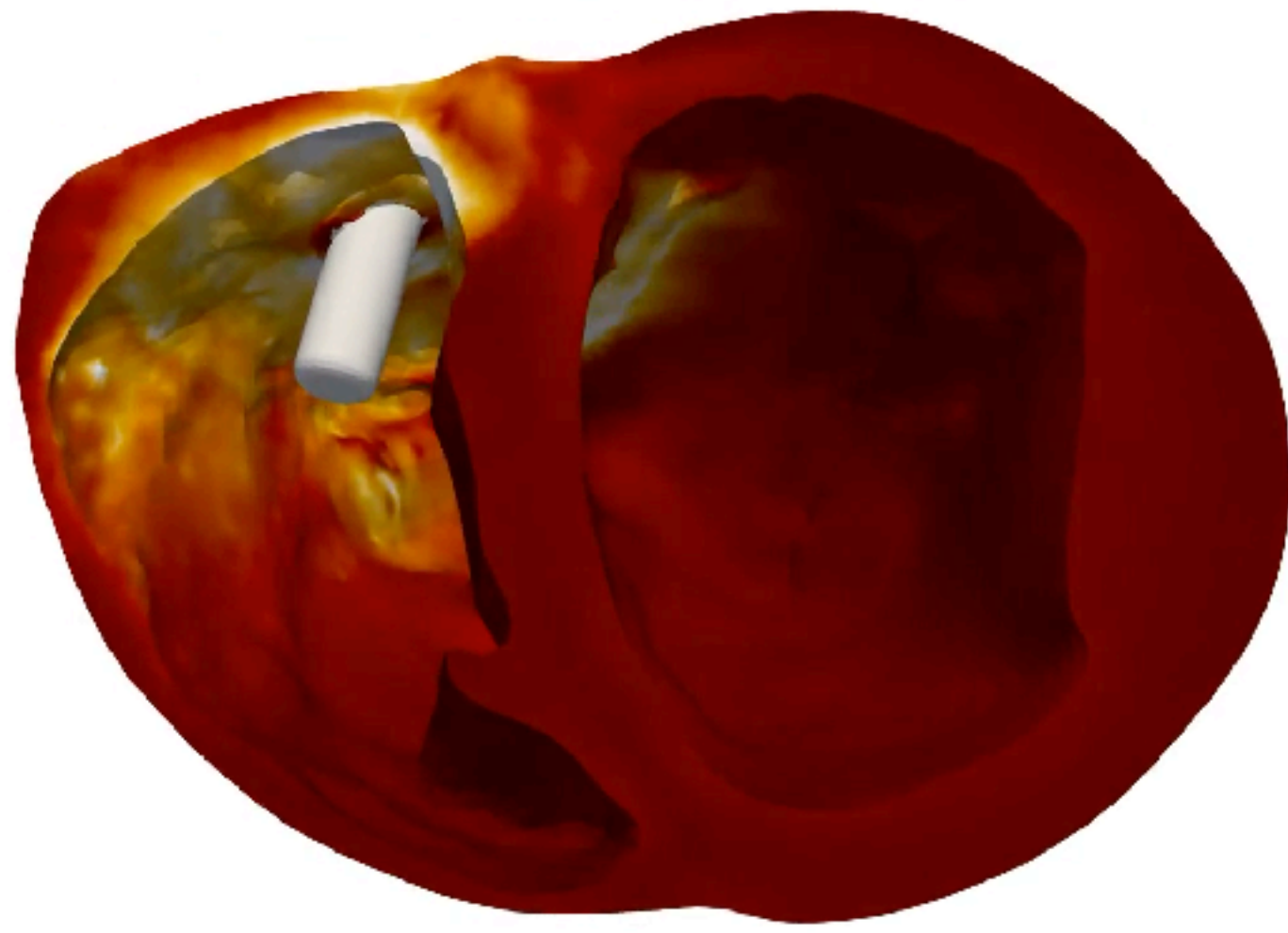
FDA (US)

ATRIOVENTRICULAR BLOCK

CARDIAC RESYNCHRONISATION THERAPIES



SANTIAGO, A., AGUADO-SIERRA, J., ZAVALA-AKÉ, M., DOSTE-BELTRAN, R., GÓMEZ, S., ARÍS, R., CAJAS, J.C., CASONI, E. AND VÁZQUEZ, M., 2018. FULLY COUPLED FLUID-ELECTRO-MECHANICAL MODEL OF THE HUMAN HEART FOR SUPERCOMPUTERS. INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN BIOMEDICAL ENGINEERING, 34(12), P.E3140.

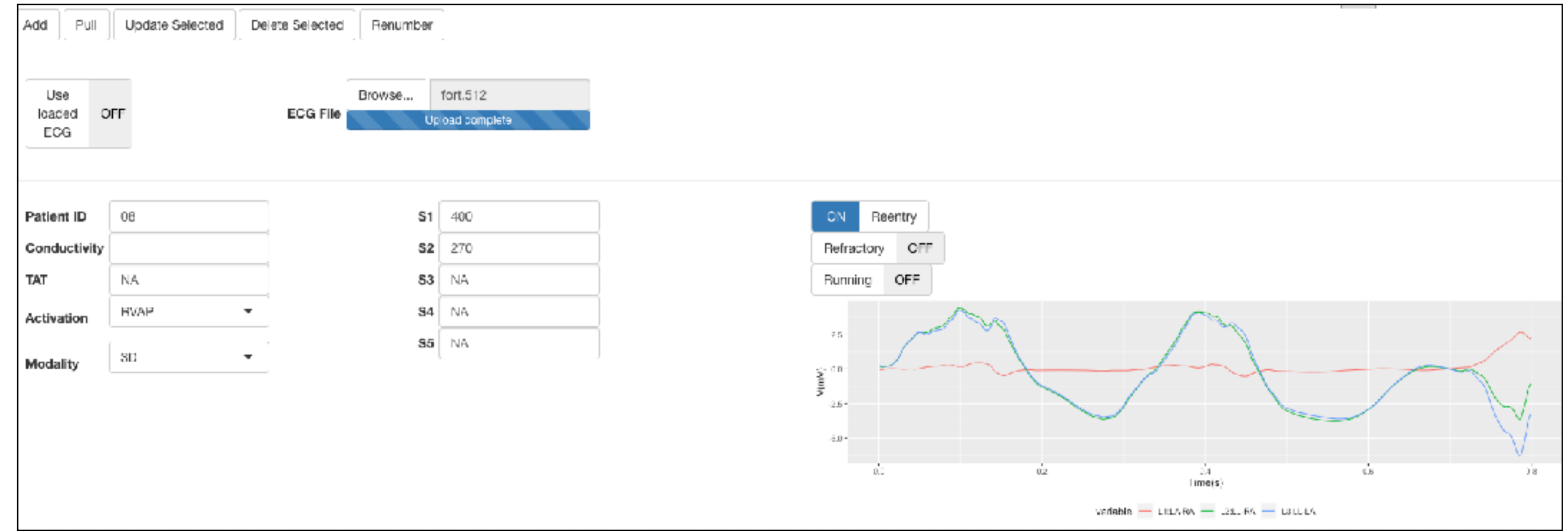


HPC-CLOUD DEPLOYED

VIRTUAL MODELLING
TOOL FOR INSILICO
CLINICAL TRIALS

FEMALE, MALE, CHILDREN
HEALTH, DISEASE AND
TREATMENT

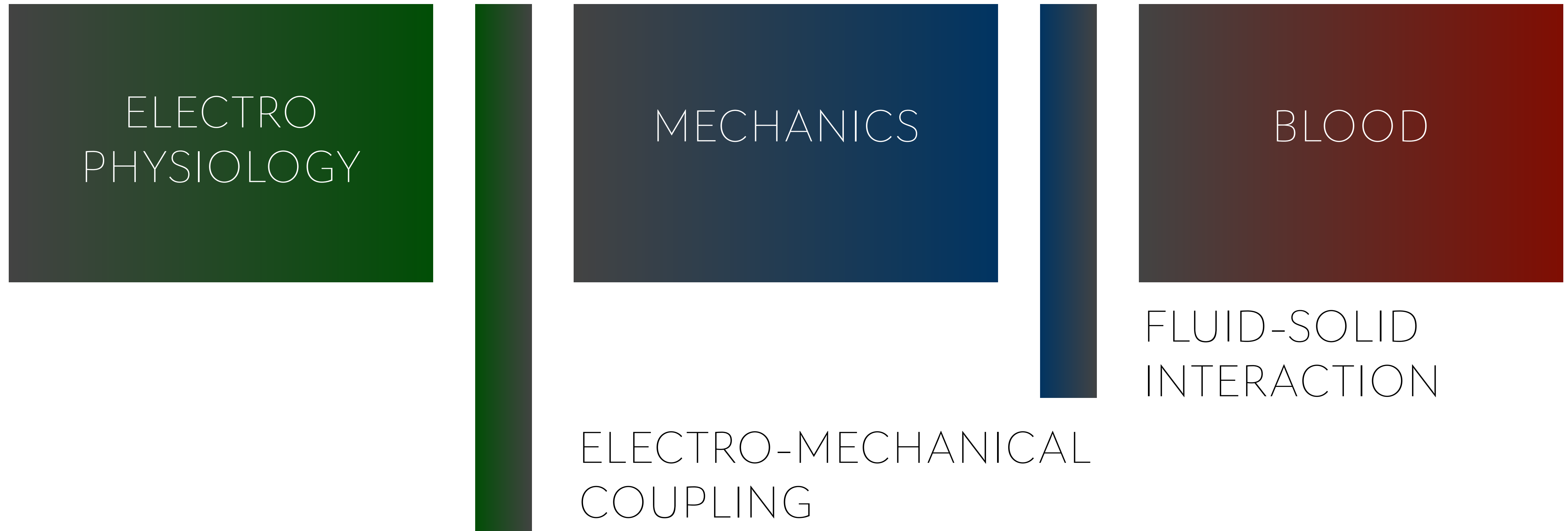
WITH REGULATORY
IMPACT



The screenshot shows the bottom part of the software interface. At the top, there are buttons for 'Edit' (set to 'OFF'), 'Save', and 'Reload'. Below these, there are several toggle buttons for 'S1', 'S2', 'S3', 'S4', 'S5', 'Refractory', 'Running', 'Conductivity', 'TAT', 'Activation', 'L1', 'L2', and 'L3'. A 'Show' dropdown is set to '10 entries'. Below the toggles is a table with columns for PatientId, Modality, S1, S2, S3, Reentry, L1, L2, and L3. The table contains 10 rows of data. A search bar is located on the right side of the table. At the bottom, there is a 'Showing 1 to 10 of 50 entries' message and a pagination control with 'Previous', '1', '2', '3', '4', '5', and 'Next' buttons.

	PatientId	Modality	S1	S2	S3	Reentry	L1	L2	L3
1	02	2D	400	250	250	true			
2	02	2D	400	230	NA	false			
3	07	3D	400	270	NA	false			
4	01	2D	400	280	NA	false			
5	01	3D	400	280	NA	false			
6	05	2D	400	280	NA	false			
7	05	3D	400	280	NA	false			
8	07	2D	400	270	NA	false			
9	07	3D	400	280	NA	false			
10	08	2D	400	280	NA	true			

THE VIRTUAL HEART ENGINEERING VIEWPOINT



SANTIAGO, A., AGUADO-SIERRA, J., ZAVALA-AKÉ, M., DOSTE-BELTRAN, R., GÓMEZ, S., ARÍS, R., CAJAS, J.C., CASONI, E. AND VÁZQUEZ, M.,
2018. FULLY COUPLED FLUID-ELECTRO-MECHANICAL MODEL OF THE HUMAN HEART FOR SUPERCOMPUTERS. INTERNATIONAL
JOURNAL FOR NUMERICAL METHODS IN BIOMEDICAL ENGINEERING, 34(12), P.E3140.

THE VIRTUAL HEART

ENGINEERING VIEWPOINT

ANATOMY & PHYSIOLOGY

ELECTRO
PHYSIOLOGY

MECHANICS

BLOOD

RESULTS ANALYSIS

VALIDATION & VERIFICATION

V-HEART WITH ALYA RED

COMPUTATIONAL ASPECTS

FULL CONTROL AND PORTABILITY: NO DEPENDENCY WITH THIRD-PARTY LIBRARIES (ONLY MPI), WITH CONTINUUM PERFORMANCE ANALISYS,

HYBRID OPENMP / MPI PARALLELIZATION

DYNAMIC LOAD BALANCE (BSC'S DLB) AND CO-EXECUTION

OFF-LOAD OF OUR GPU PARALLEL SOLVER

MULTI-CODE COUPLING: COUPLED PARALLEL INSTANCES OF ALYA (IN THIS CASE, THREE)

MPI POINT-TO-POINT COMMUNICATION

MULTI-LEVEL DATA TRANSFER: CONSERVATIVE OPERATORS BETWEEN MESHES

ANISTROPIC MESH REFINEMENT

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Centro Nacional de Supercomputación

