HPC-based multi-physics simulations for the energy realm

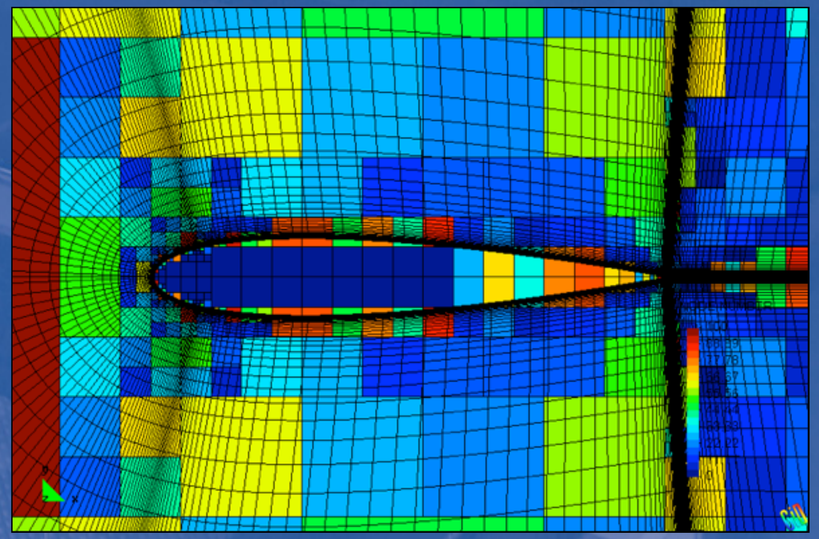
M. Vázquez, G. Houzeaux, J.M. Cela

M. Hanzich, J. de la Puente

A. Folch, D. Mira

Barcelona Supercomputing Center

Spain



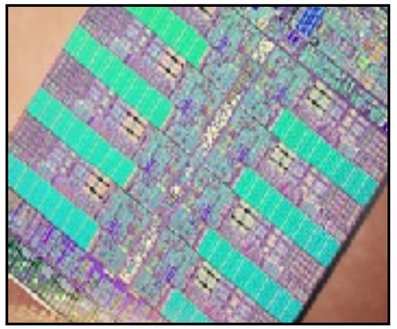
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

CASE: The BSC’s applications department

BSC Research Departments

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

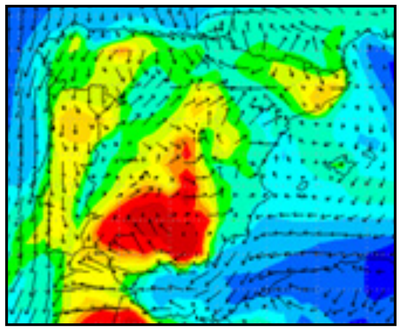


Computer Science

Tools, storage, cloud...

Computer architectures

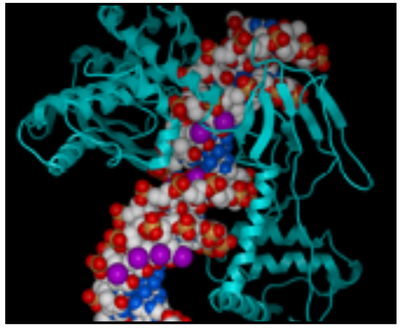
Programming models



Earth Science

Climate

Air quality



Life Science

Bioinformatics for Genomics

Computational Biochemistry

Computer Applications in Science and Engineering

CASE

AMC TV Show *Halt and Catch Fire*

“Computers are not *the thing*, computers are the thing that gets us to *the thing*.”

AMC TV Show *Halt and Catch Fire*

Computer Applications in Science and Engineering (CASE)

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

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

More than 65 researchers:

Post-docs, students, programmers

Computer Science, Physicists, Mathematicians, Engineers

CASE Research lines

Physical and Numerical Modeling

Numerical Solution Algorithms: from stabilisation to solvers
Multi-physics and multi-scale coupling

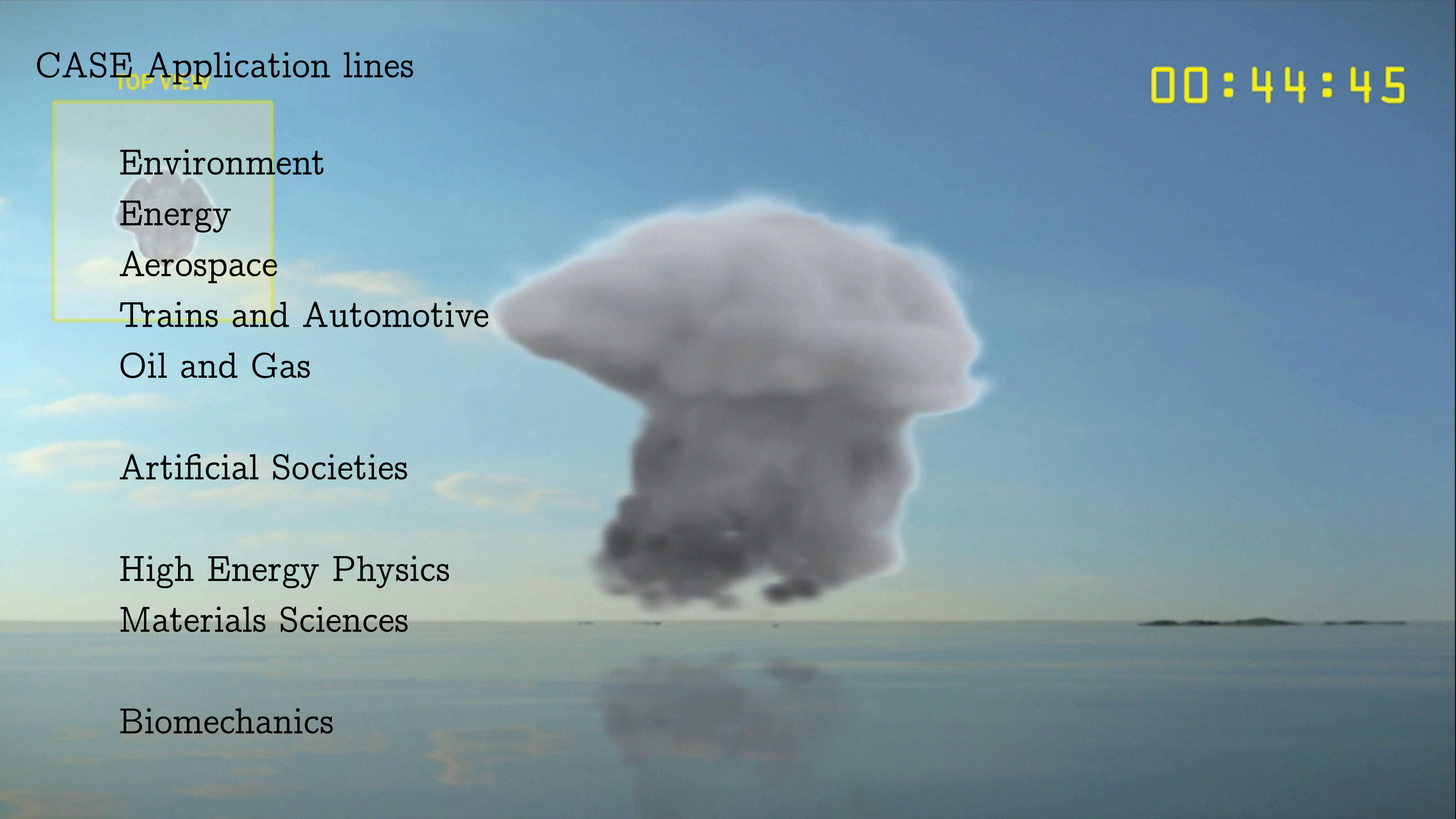
High Performance Computing in CM (HPCM)
Parallelisation in Distributed and Shared memory machines

Mesh Generation

Scientific Visualisation & Big Data

Optimisation

CASE Application lines



Environment
Energy
Aerospace
Trains and Automotive
Oil and Gas

Artificial Societies

High Energy Physics
Materials Sciences

Biomechanics

Application projects' keywords:

Complex geometries

Complex, unconventional physical / mathematical models

Complex pre-process (meshing) and post-process (visualization and analysis)

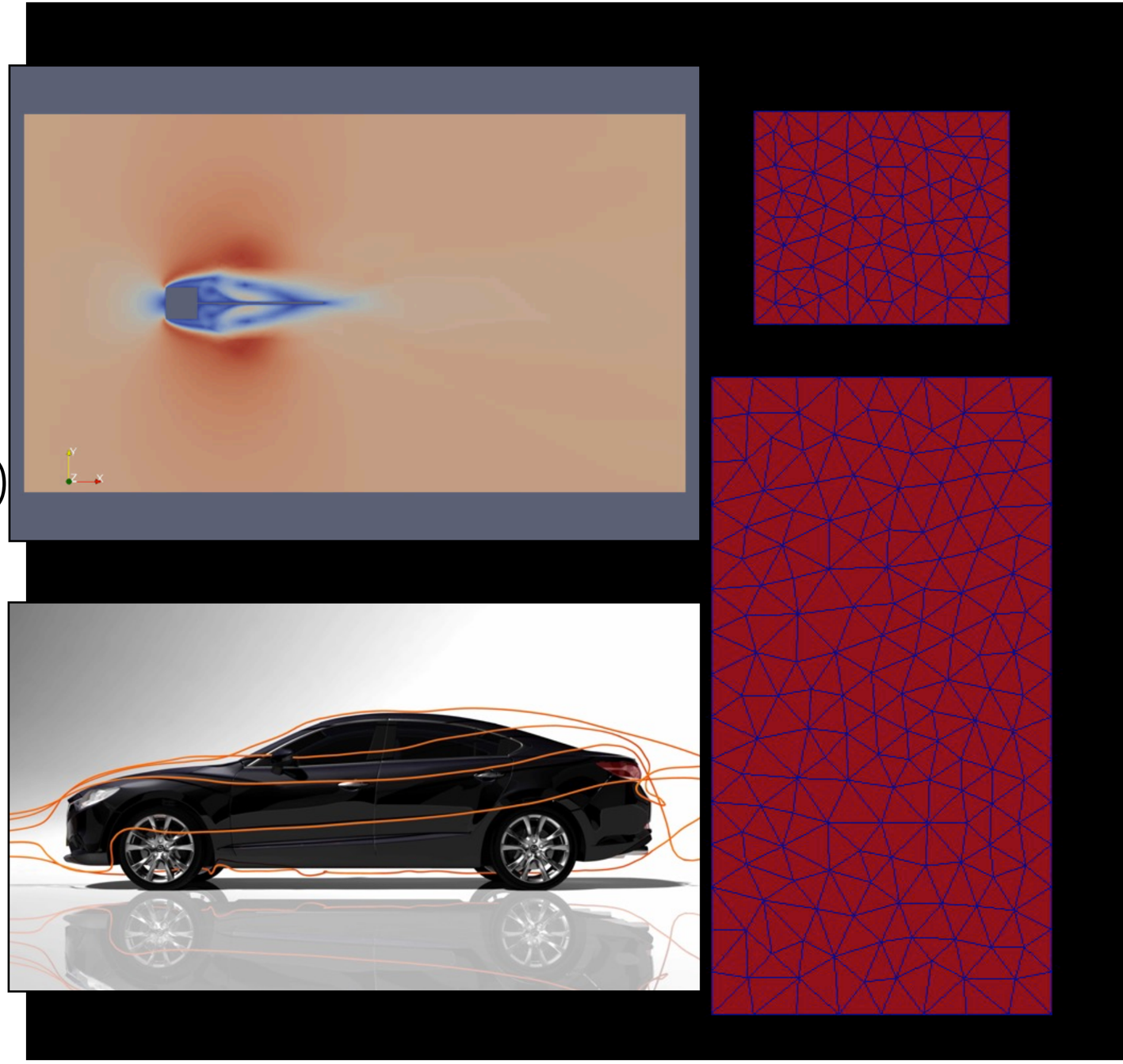
Large-scale simulations

Multi-physics problems

Automatic optimization

Big data management and visualization

Efficient and accurate software for supercomputers



The BSC’s simulation software

CASE simulation parallel software stack

Partial differential equations on cartesian meshes

Partial differential equations on non-structured meshes

Agent-based methods

CASE simulation parallel software stack

Partial differential equations on cartesian meshes

Exploit the well-ordered data for both access and operations

Simple numerics, allowing equal work distribution among threads, stencils

High order schemes preferred: DG, FEM or FD (although low order possible)

Simple geometries

Small code kernel

Well suited for GPUs

CASE simulation parallel software stack

Partial differential equations on non-structured meshes

Flexible platforms for complex problems, specially coupled multi-physics

Complex (always evolving) numerics, unequal work on threads, conditionals...

Low order preferred (>= 2): FEM, FV (although high order possible)

Complex geometries

Large code kernel

Well suited for CPUs

CASE simulation parallel software stack

Alya: non-structured meshes, coupled multi-physics

Waris: cartesian (staggered) meshes, well-defined numerics, one code - one problem - one physics

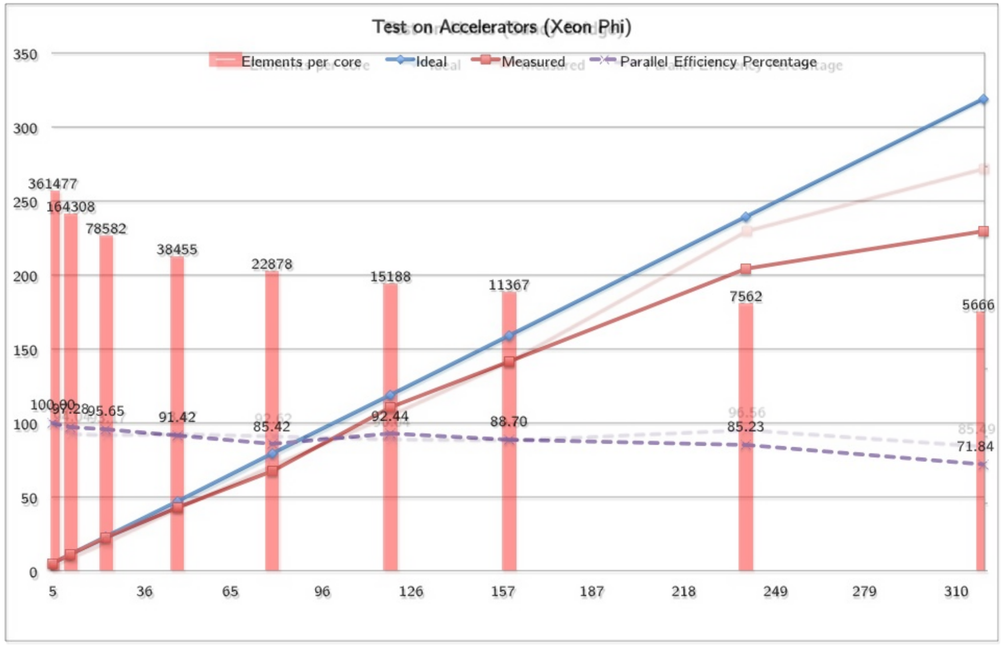
Saiph: DSL for cartesian meshes (with Computer Science Dpt.)

Pandora: agent-based simulations

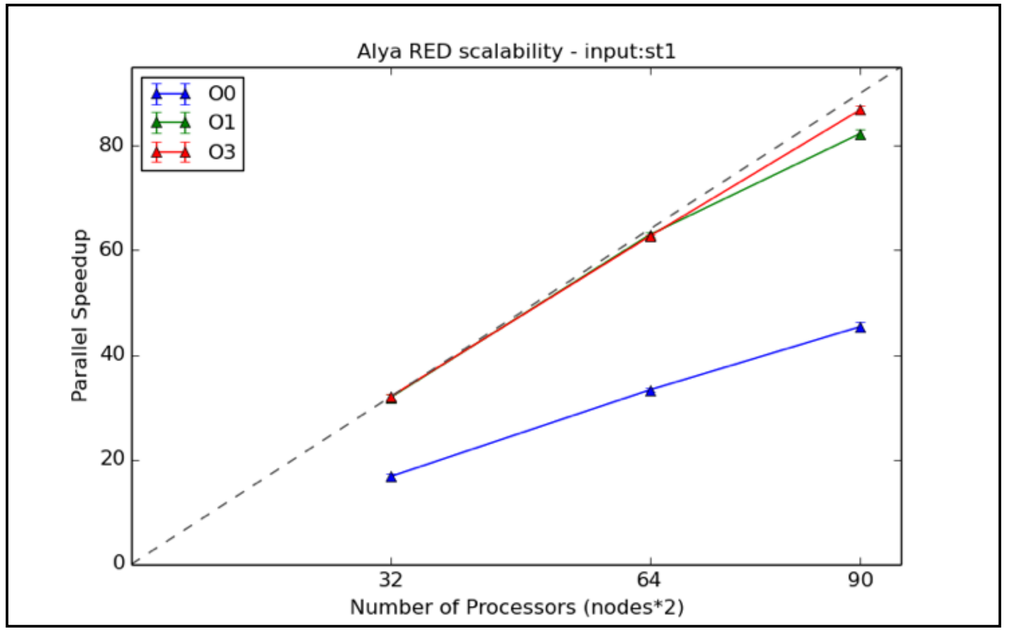
Alya

Porting to new architectures

Intel Xeon Phi



Arm CPUs



Defining parallel multi-physics coupling

How do you define a physical system?

Just the governing equations?

Then what is multiphysics coupling?

How do you define a physical system?

Equations + space/time domain + boundary/initial conditions

How do you define a physical system?

Equations + space/time domain + boundary/initial conditions

After applying a numerical method,

Equations + space/time domain + boundary/initial conditions + discretization

How do you define a physical system?

Equations + space/time domain + boundary/initial conditions

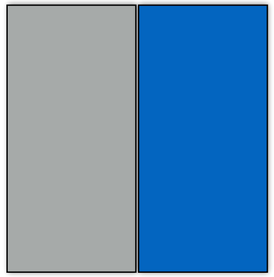
After applying a numerical method,

Equations + space/time domain + boundary/initial conditions + discretization

This widens up the concept of “multi-physics coupling”:

Two or more coupled problems, where at least one of the terms above varies.

Very generally speaking and to fix ideas..



Contact domains:

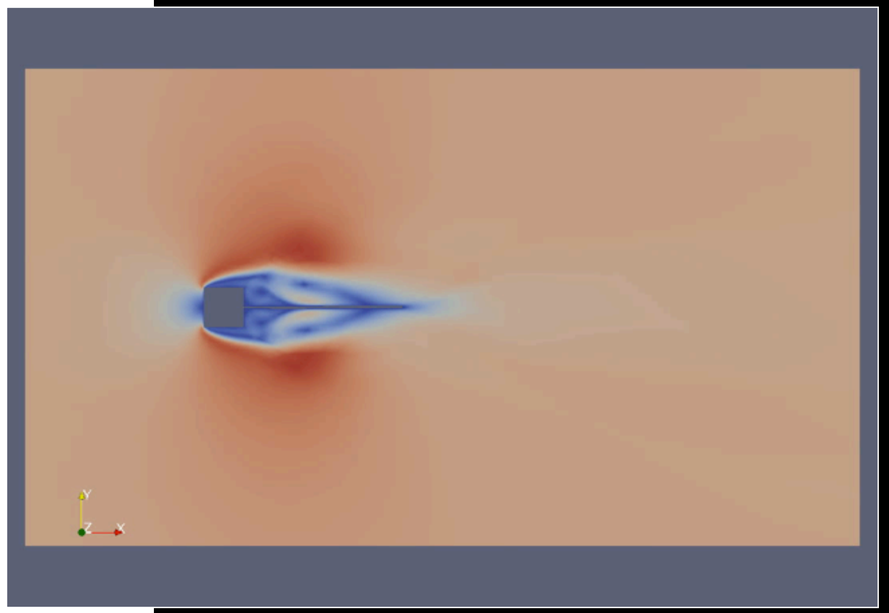
Fluid-structure interaction

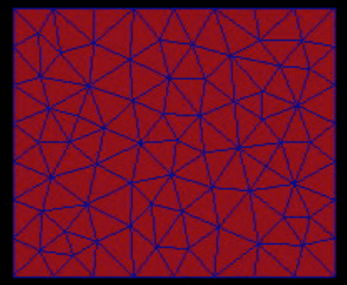
Contact and impact problems

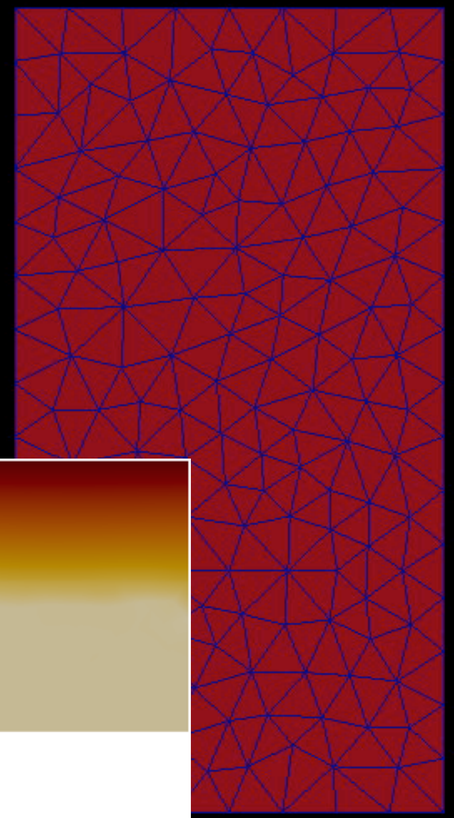
N-bodies collisions

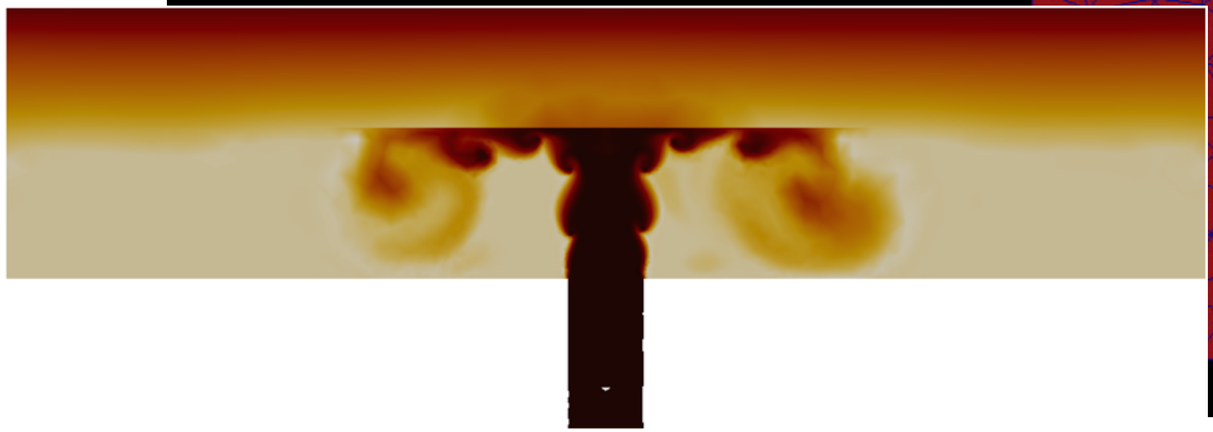
Heat transfer

Meshes can/cannot coincide

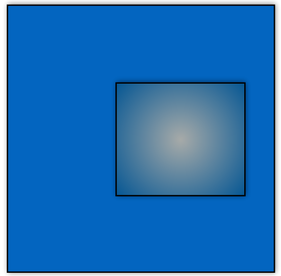








Very generally speaking and to fix ideas...



Overlapping domains:

Overset meshes and Chimera

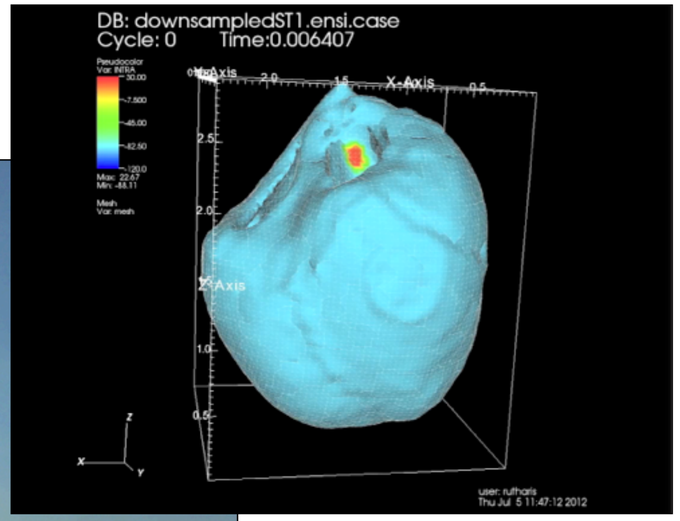
Electromechanical cardiac model

RANS modelled turbulence

Multi-scale problems

Particles and immersed bodies

Meshes can/cannot coincide



Issues

Coupling connectivity among MPI tasks

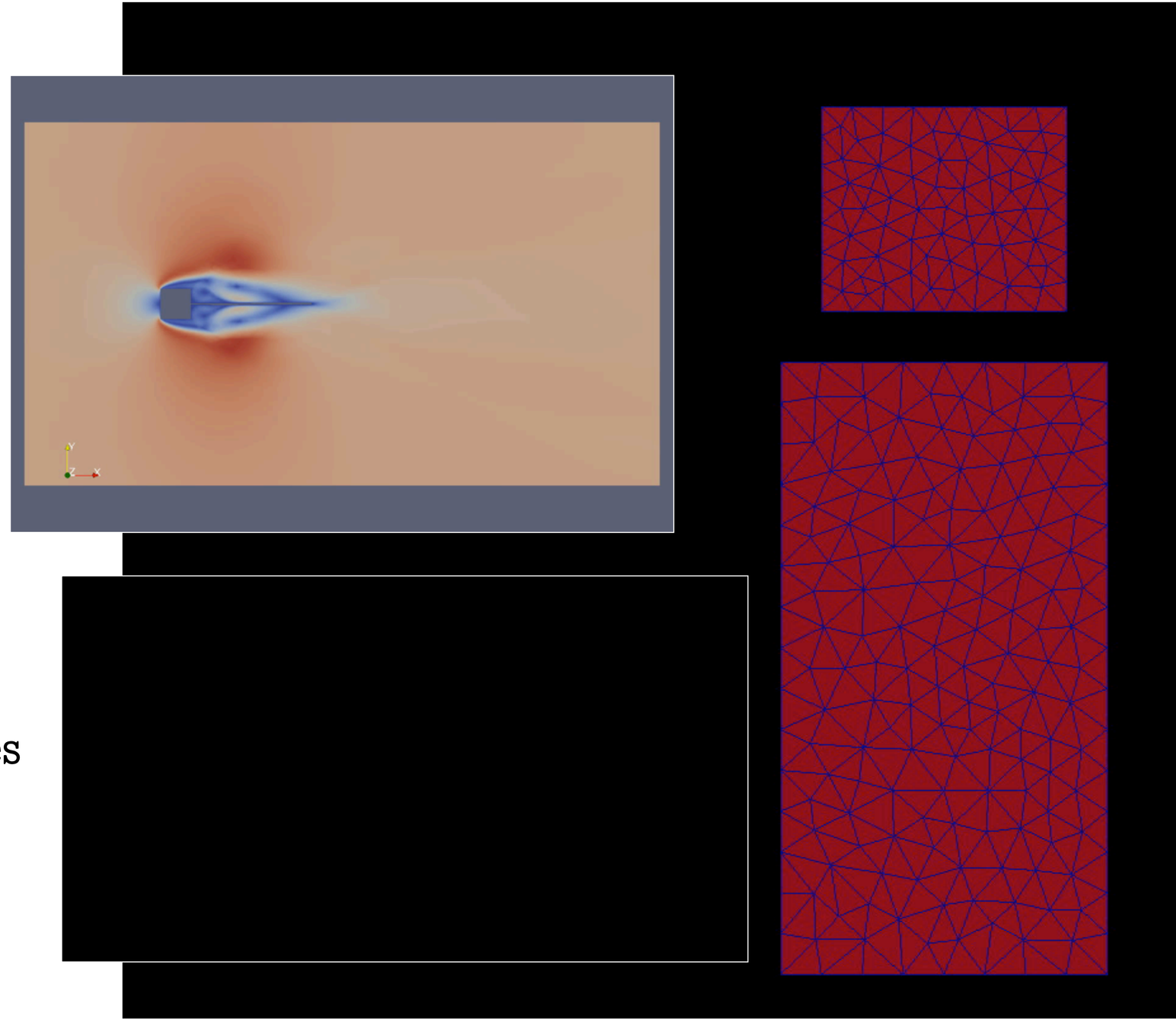
Numerically stable coupling algorithms

Preconditioners for the coupled scheme

Time-scale disparity

Synchronous/Asynchronous schemes

Coupling different codes (multi-codes)

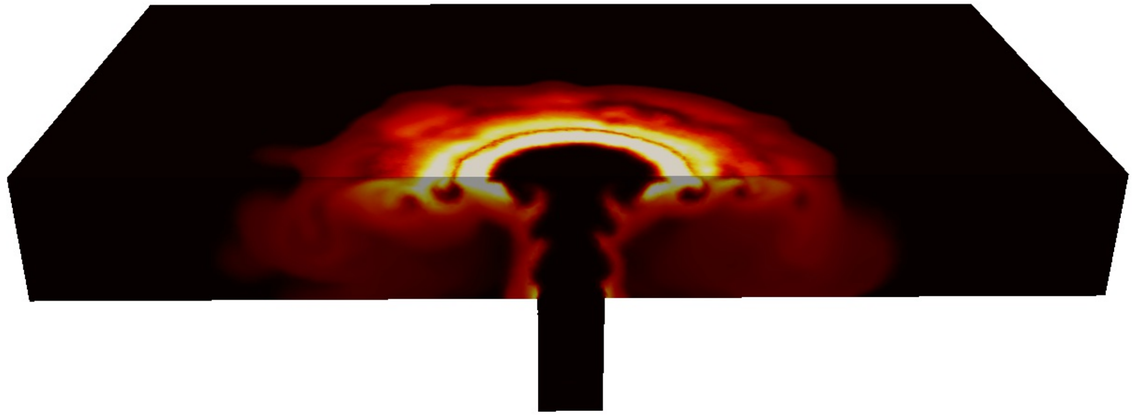


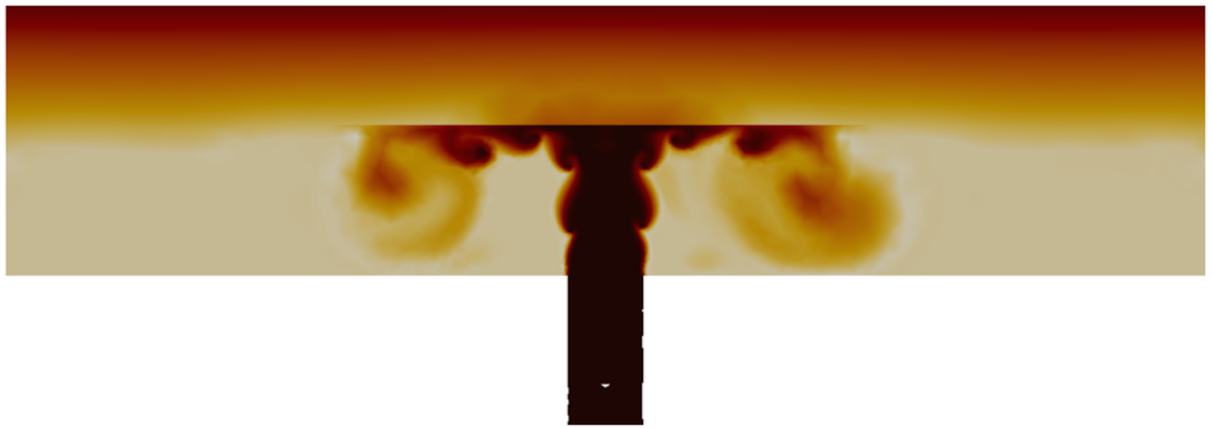
Alya

Parallel multi-physics code developed at BSC

Parallel coupling strategies:

- Code coupling
  - Several instances of Alya
  - Alya with other codes
- Couplers
  - In-house, integrated in Alya
  - PLE (with EDF, France)
  - PreCICE (with TUM, Germany)
  - Adan (with LNCC, Brazil)





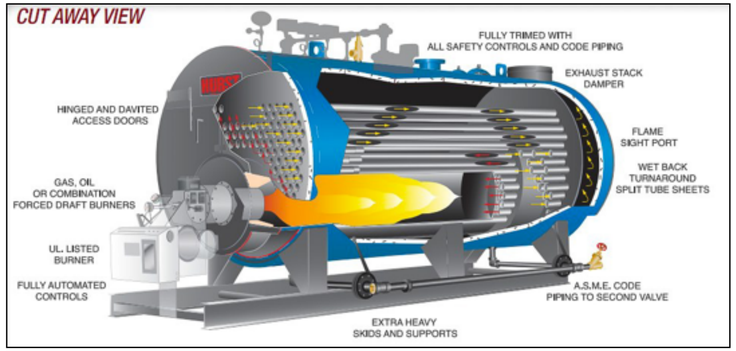
Simulations for Industry:

The energy realm

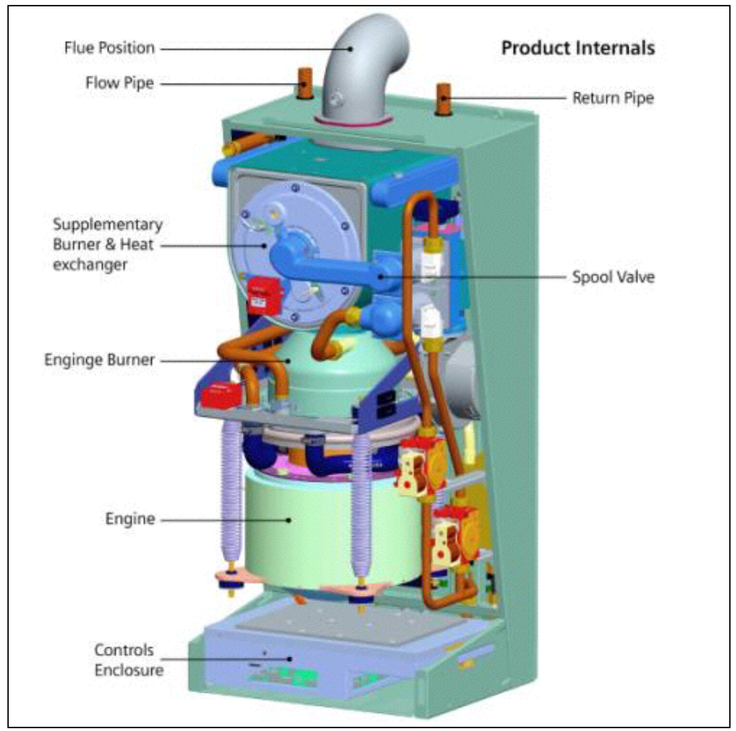
Multi-physics:

Chemical reactions and Combustion

Boilers



Combined Heat and Power (cogeneration)



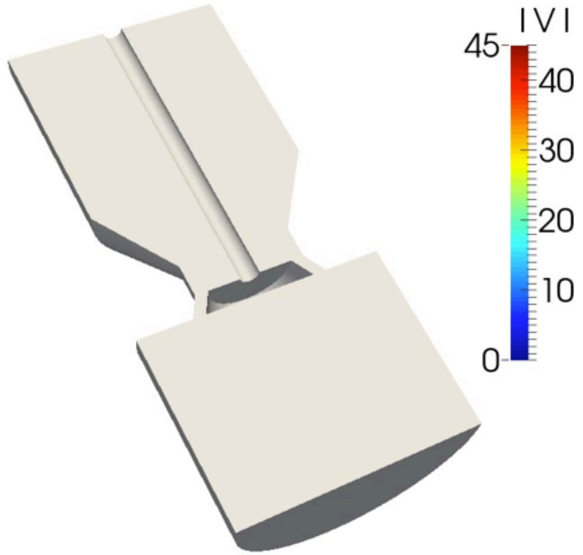
High-fidelity numerical simulations of practical combustors

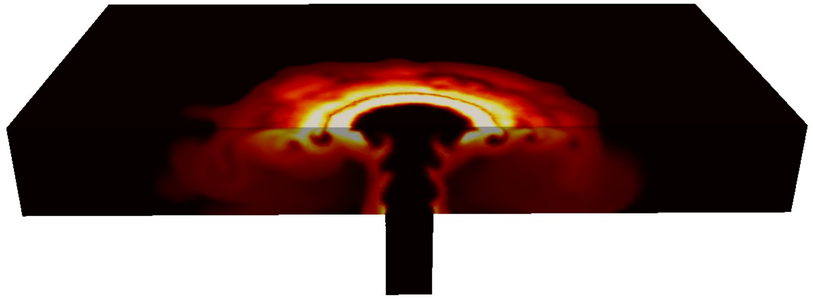
Prediction of performance and pollutants emission

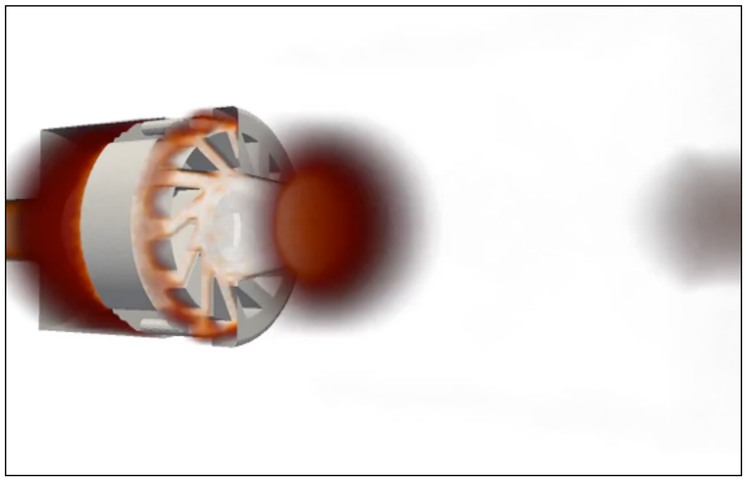
Prediction of noise and instabilities

Optimisation designs for heat and power generation with:

- Low emissions
- Highly efficient
- Energy saving







Compressible / Incompressible flows

Chemical reactions and species

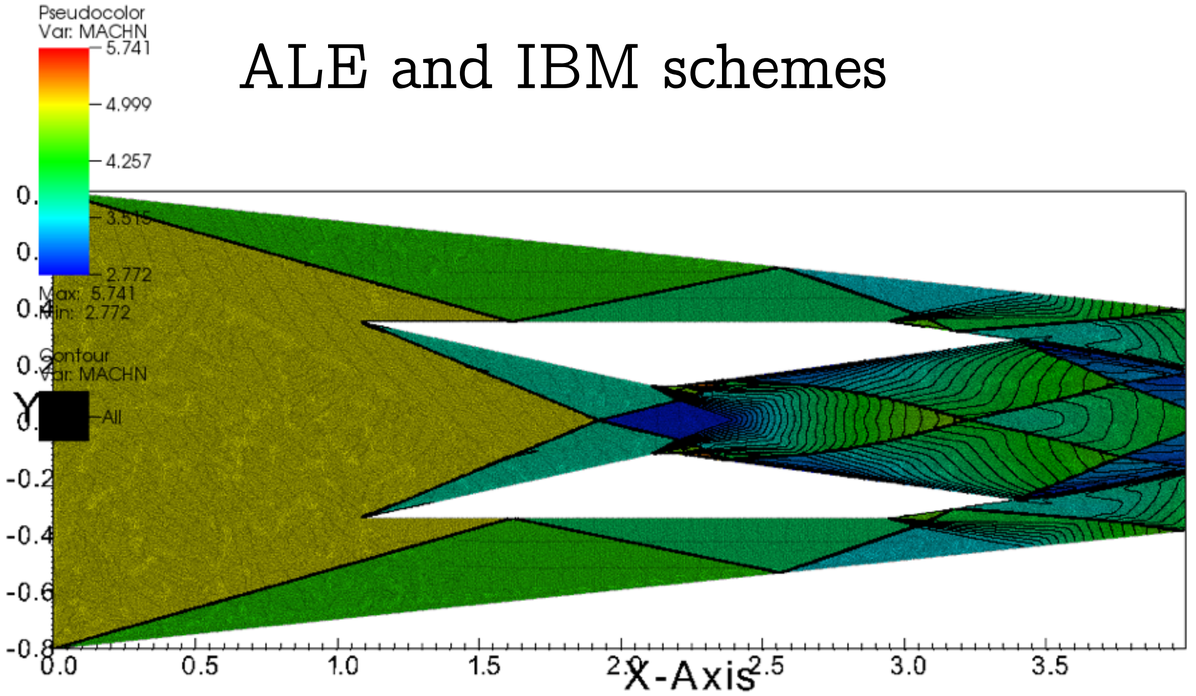
Combustion

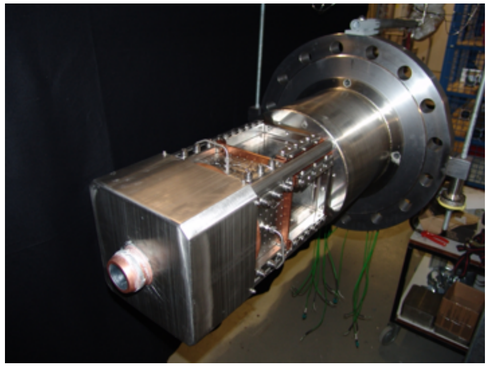
Heat transfer

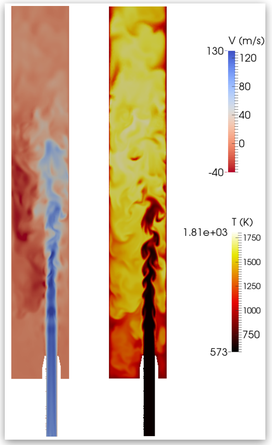
Multi-codes coupling

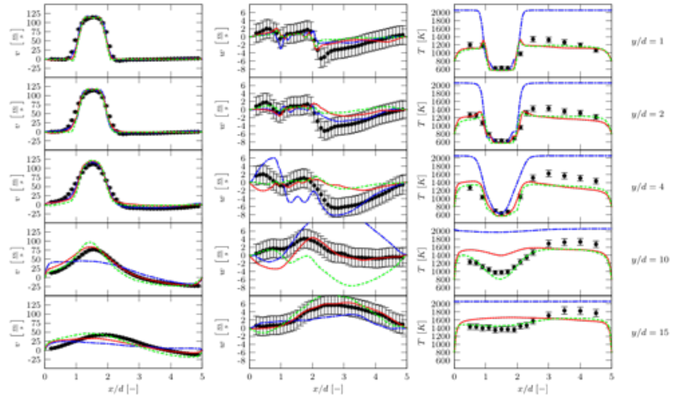
Local preconditioners for low Mach numbers

ALE and IBM schemes

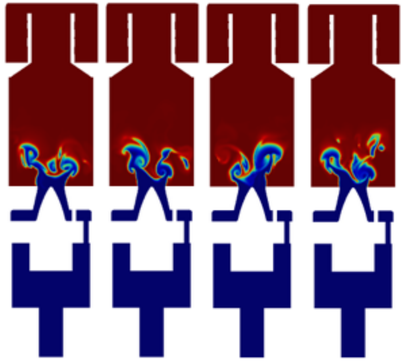


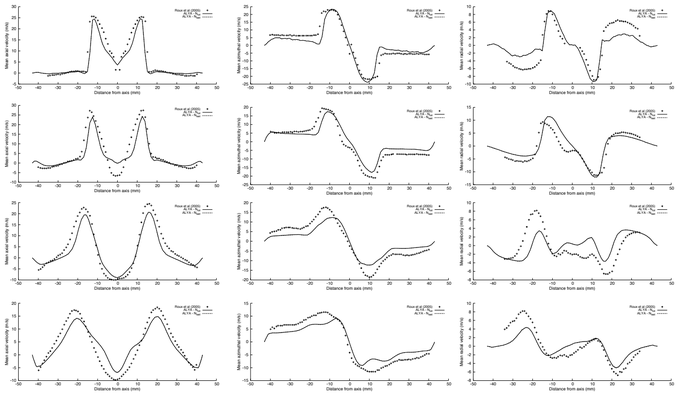




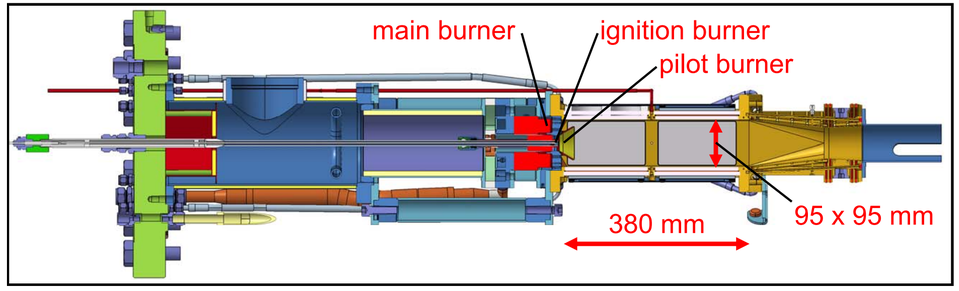


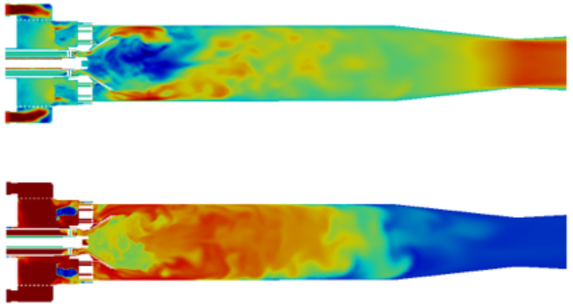
FLOX®
combustor DLR





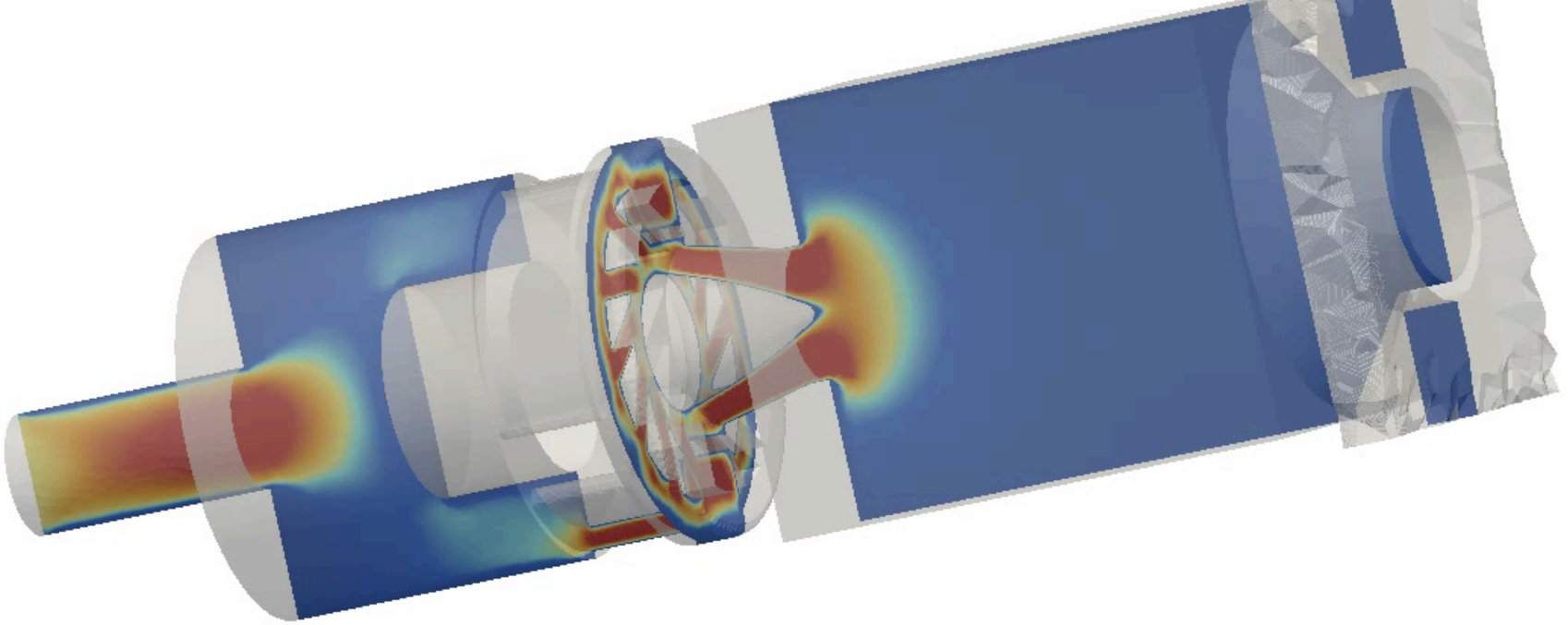
PRECCINSTA
DLR

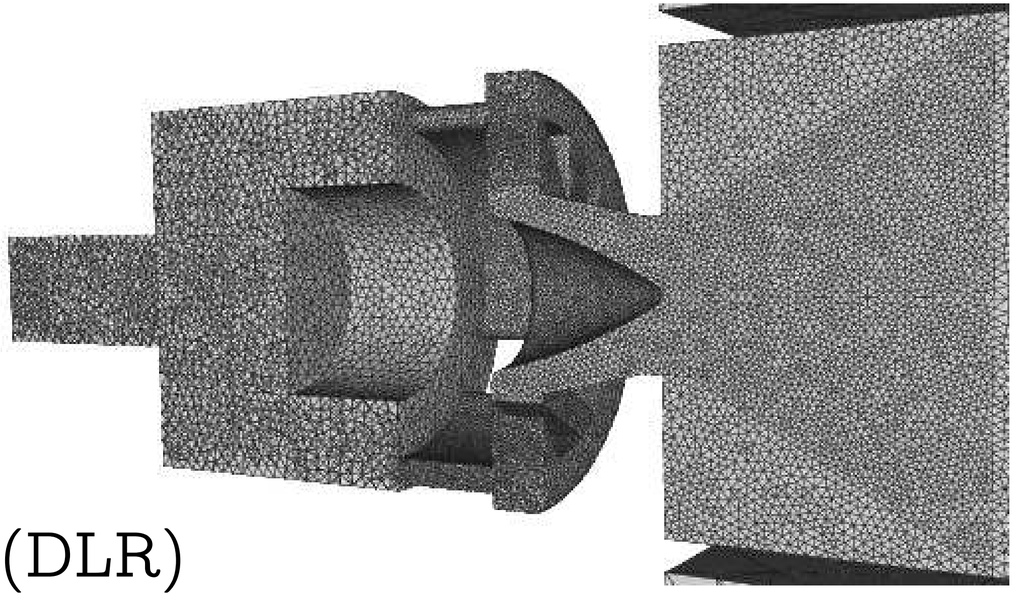




PCS
SIEMENS

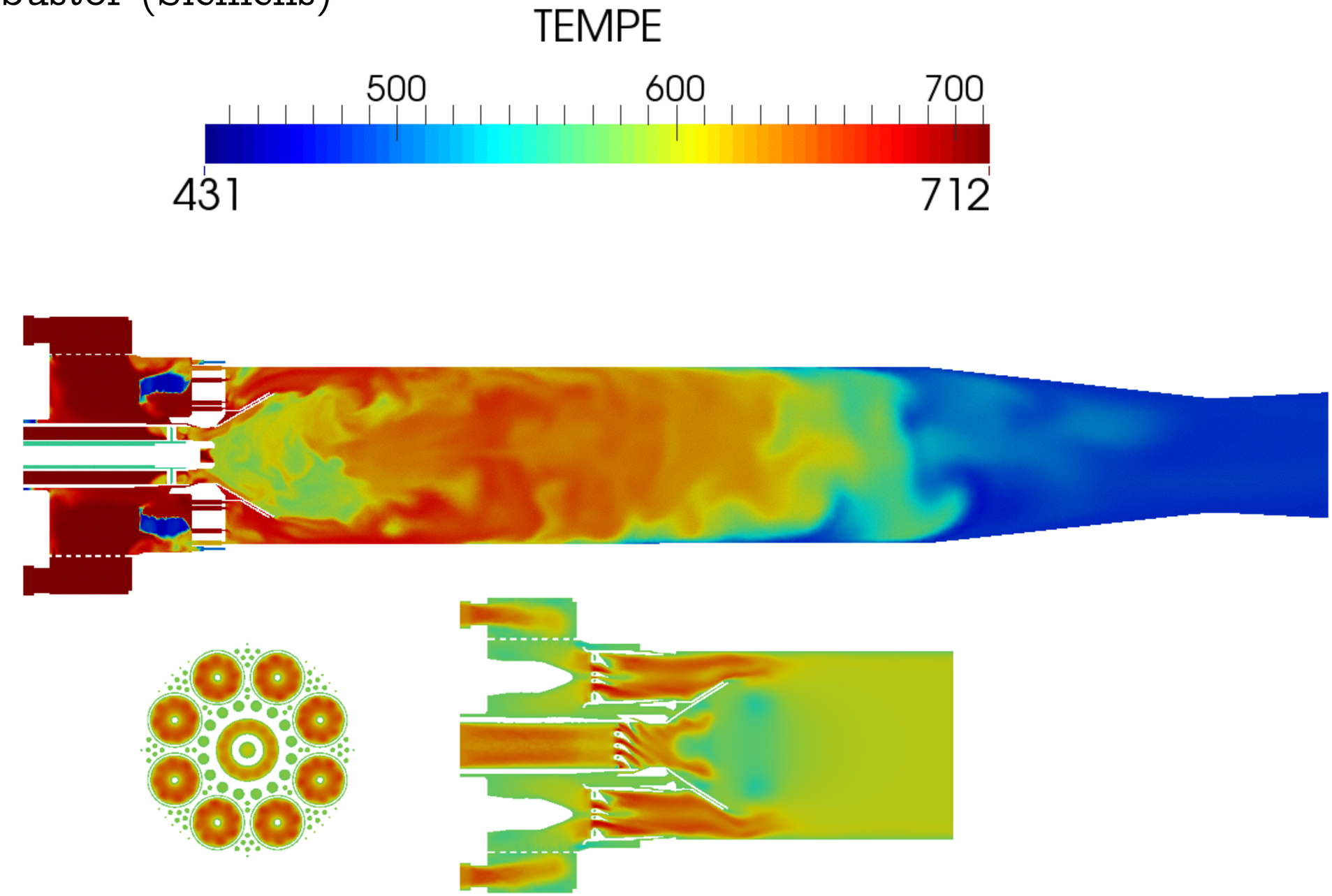
PRECCINSTA Burner





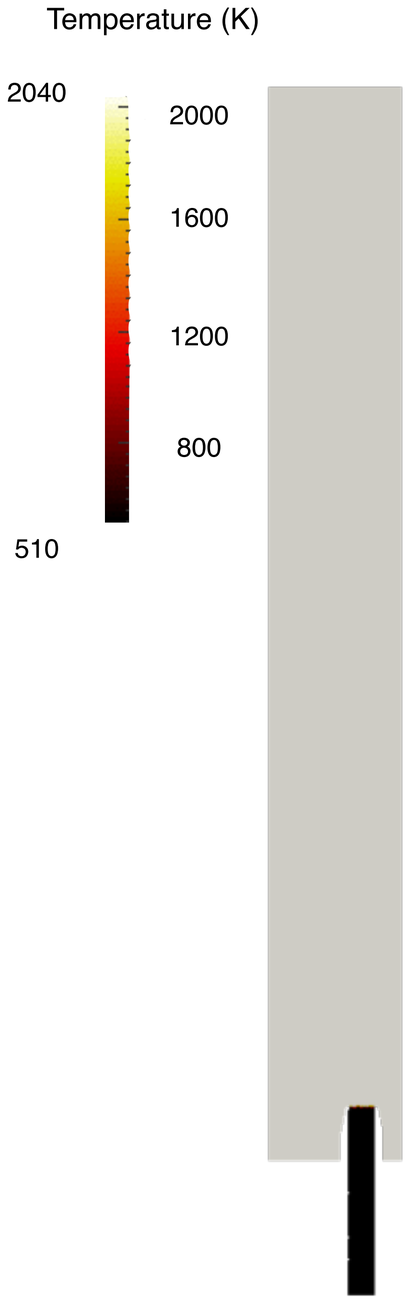
Experimental facility (DLR)

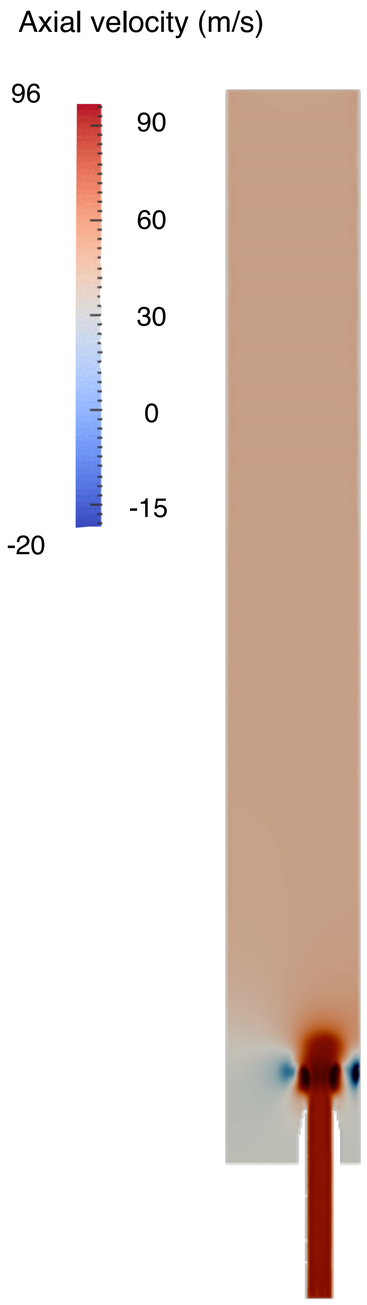
PCS combustor (Siemens)

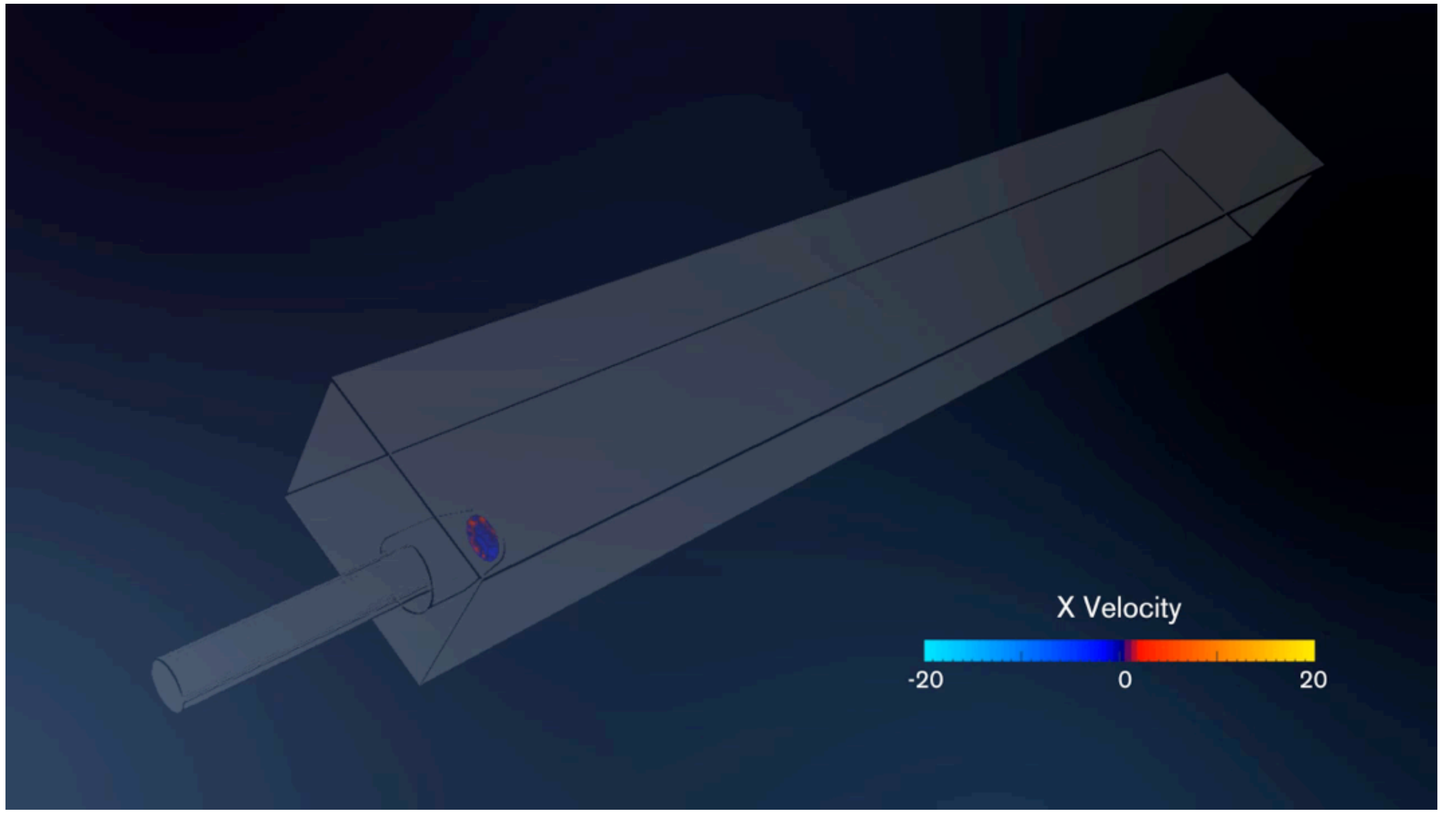


Dynamic thickened flame models (TFLES)

DLR Siemens combustor







The REPSOL -BSC research center

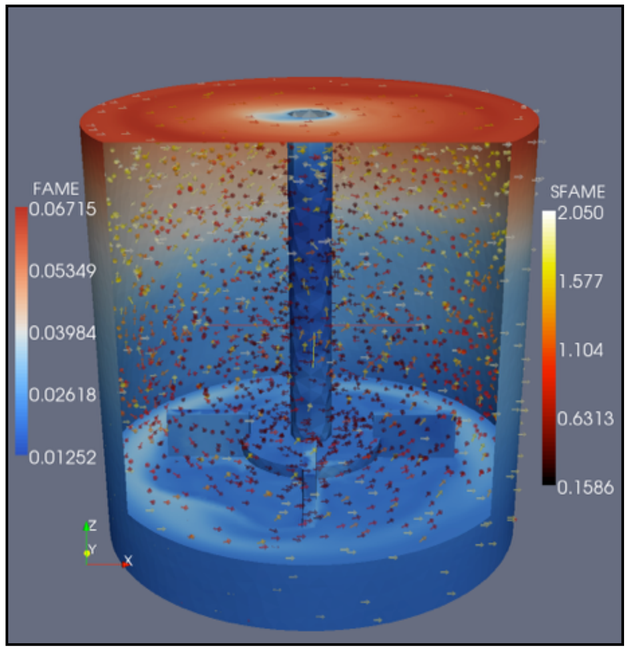
As a start, one particular problem selected... then, the project grows

Oil business is very large: plenty of problems and opportunities for HPC-based simulations

In some of its sectors, simulation is in their core business: geophysics and reservoir modeling

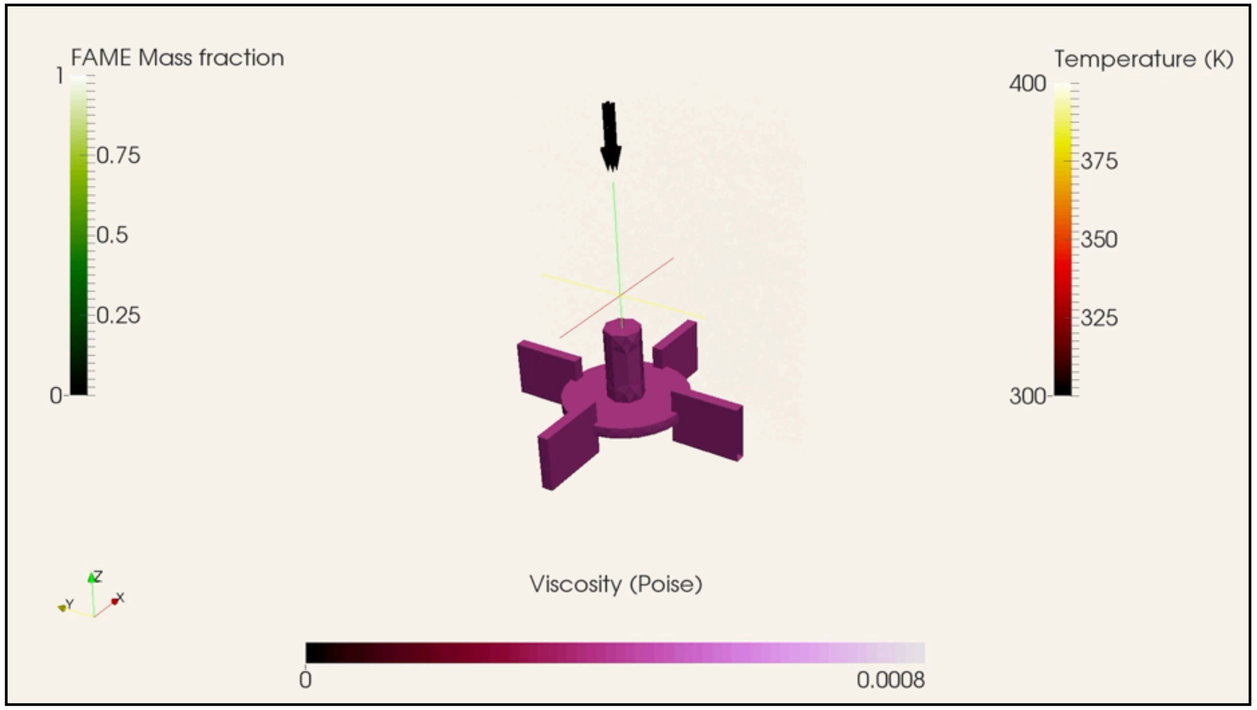
Other sectors are prone to copy the model.

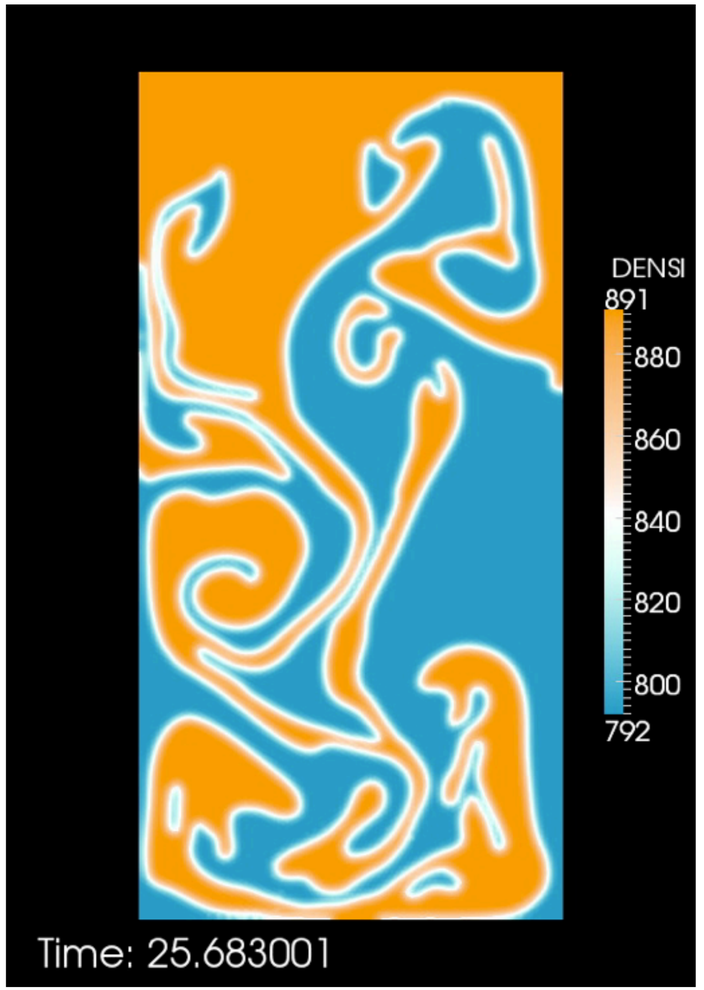
Keywords:
Geophysics, Batteries, Chemical Reactors, Reservoir Modelling



Trans-esterification

Incompressible flow + Chemical reactions + Heat





Decantation of vegetal oil in methanol

Incompressible flow + level sets

Reverse Time Migration (BSIT)

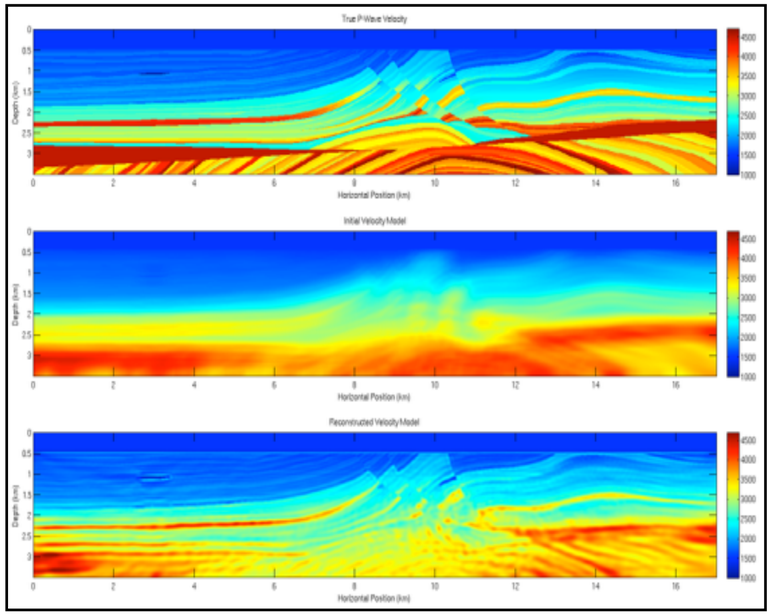
Full Waveform Inversion (Waris)

Elastic Wave Propagation (Waris)

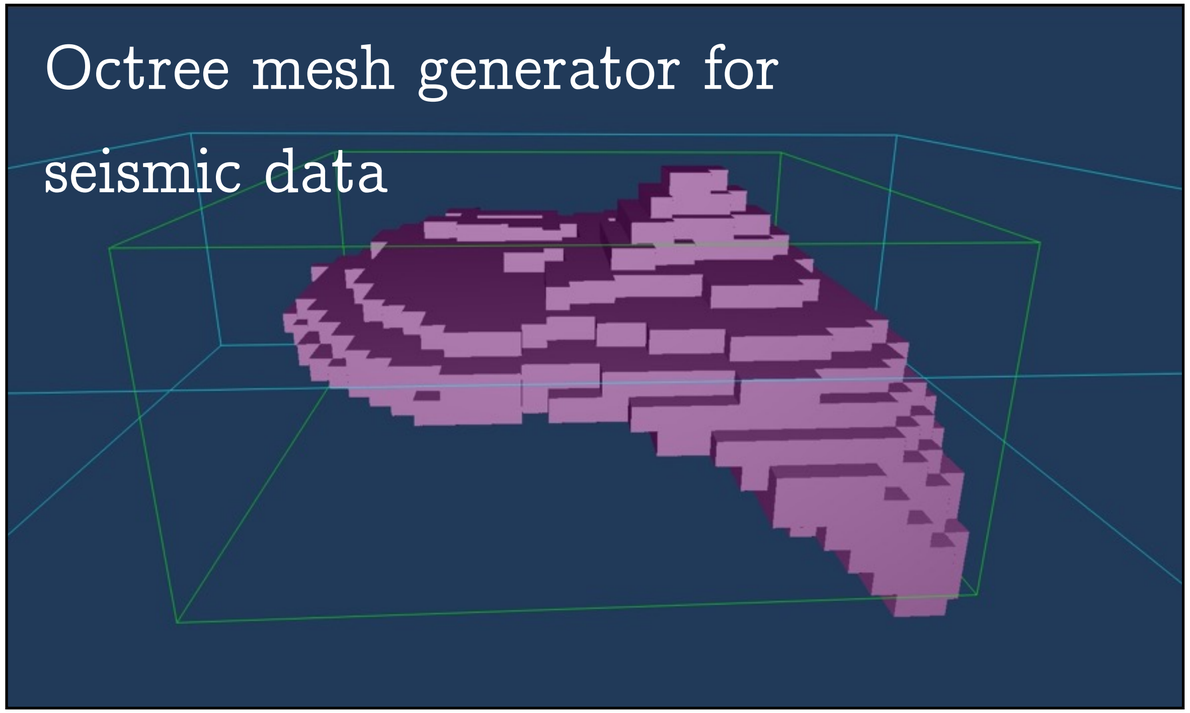
Control-source Electromagnetic Model (Alya)

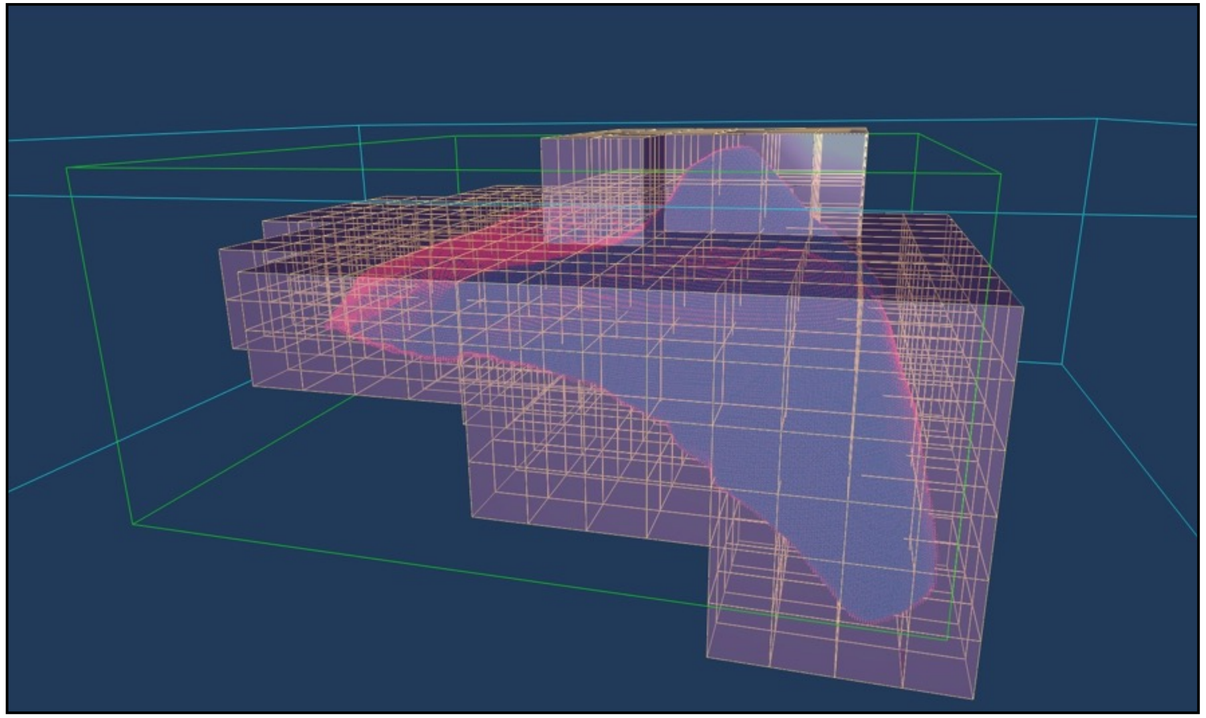
Adjoint-based optimization methods (Alya-Waris)

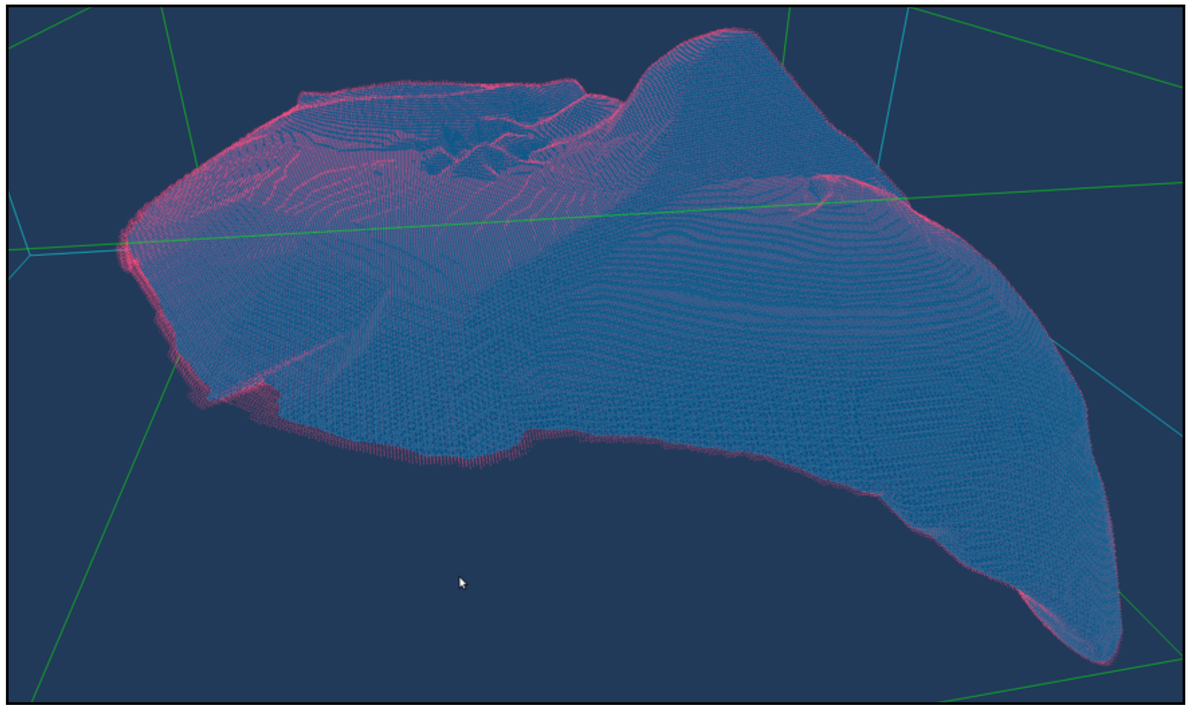
Software development for GPUs and multicores (Waris)

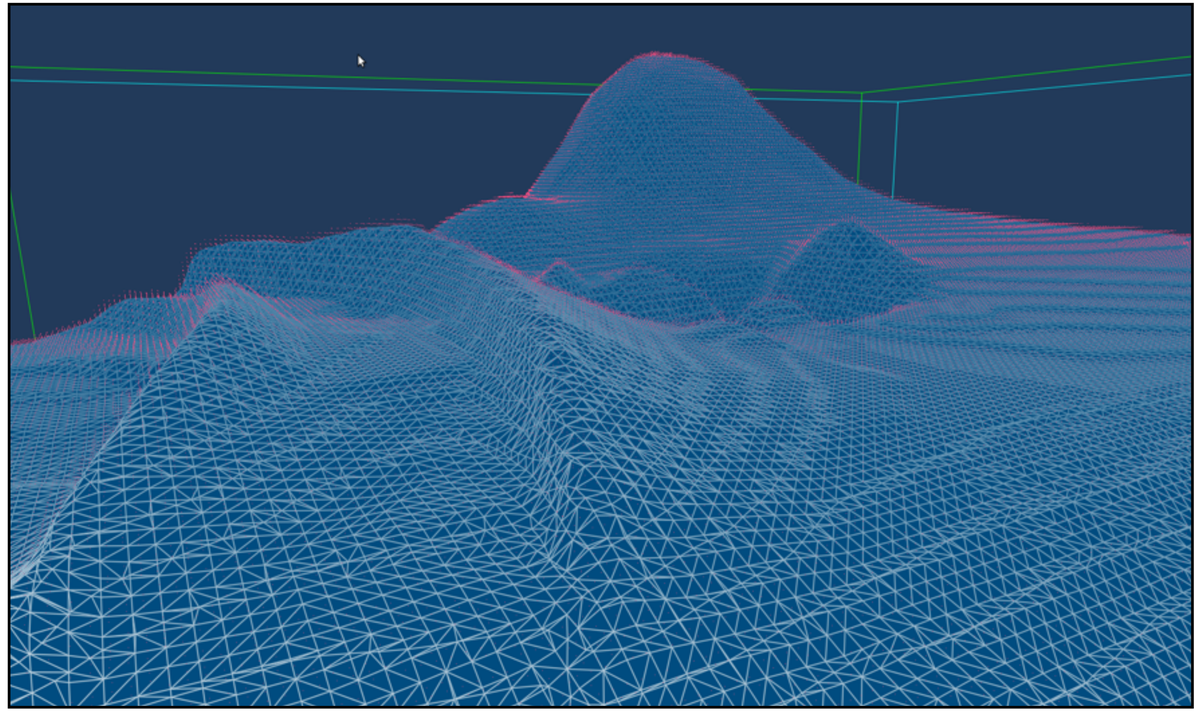


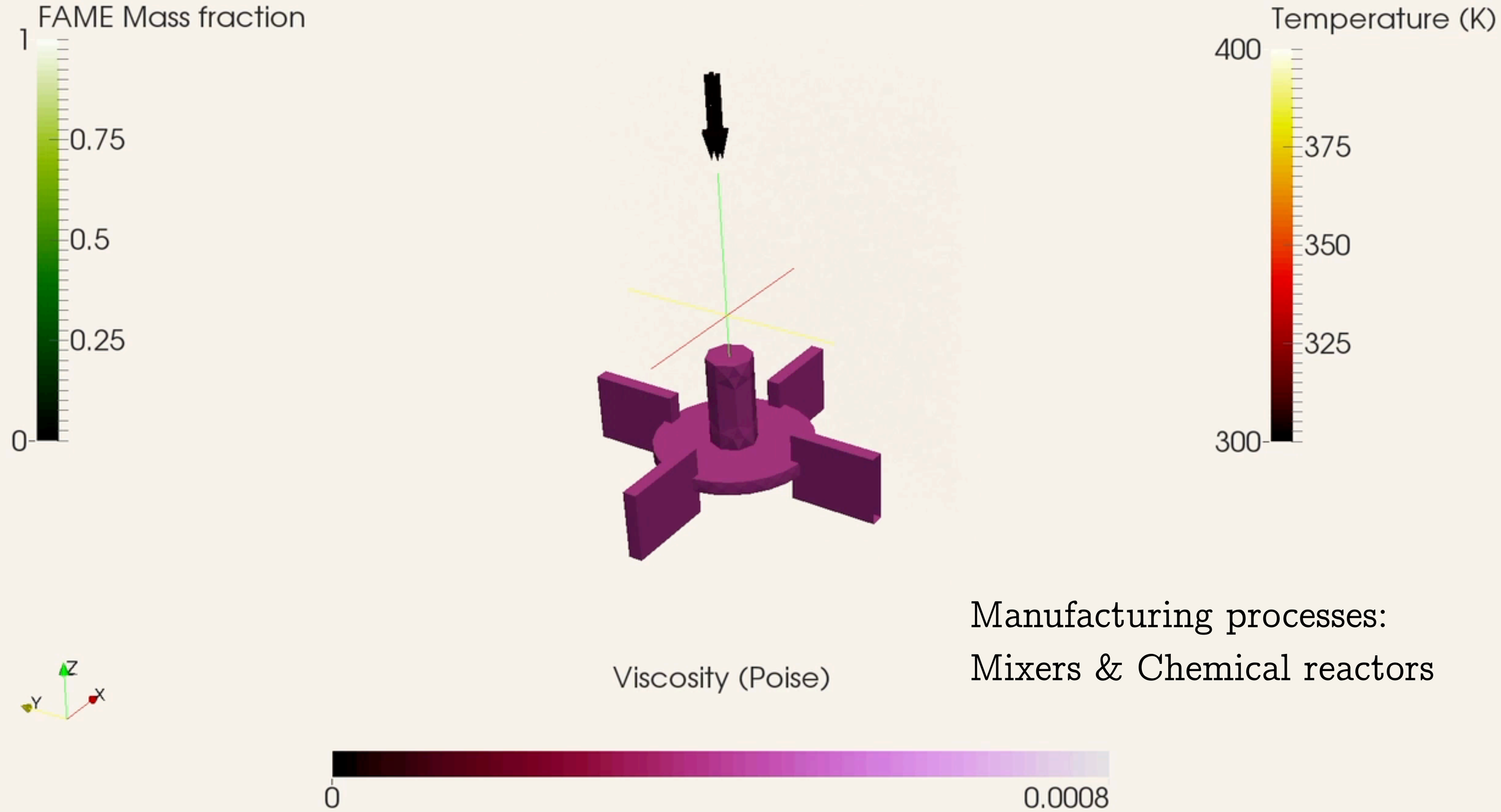
Octree mesh generator for seismic data









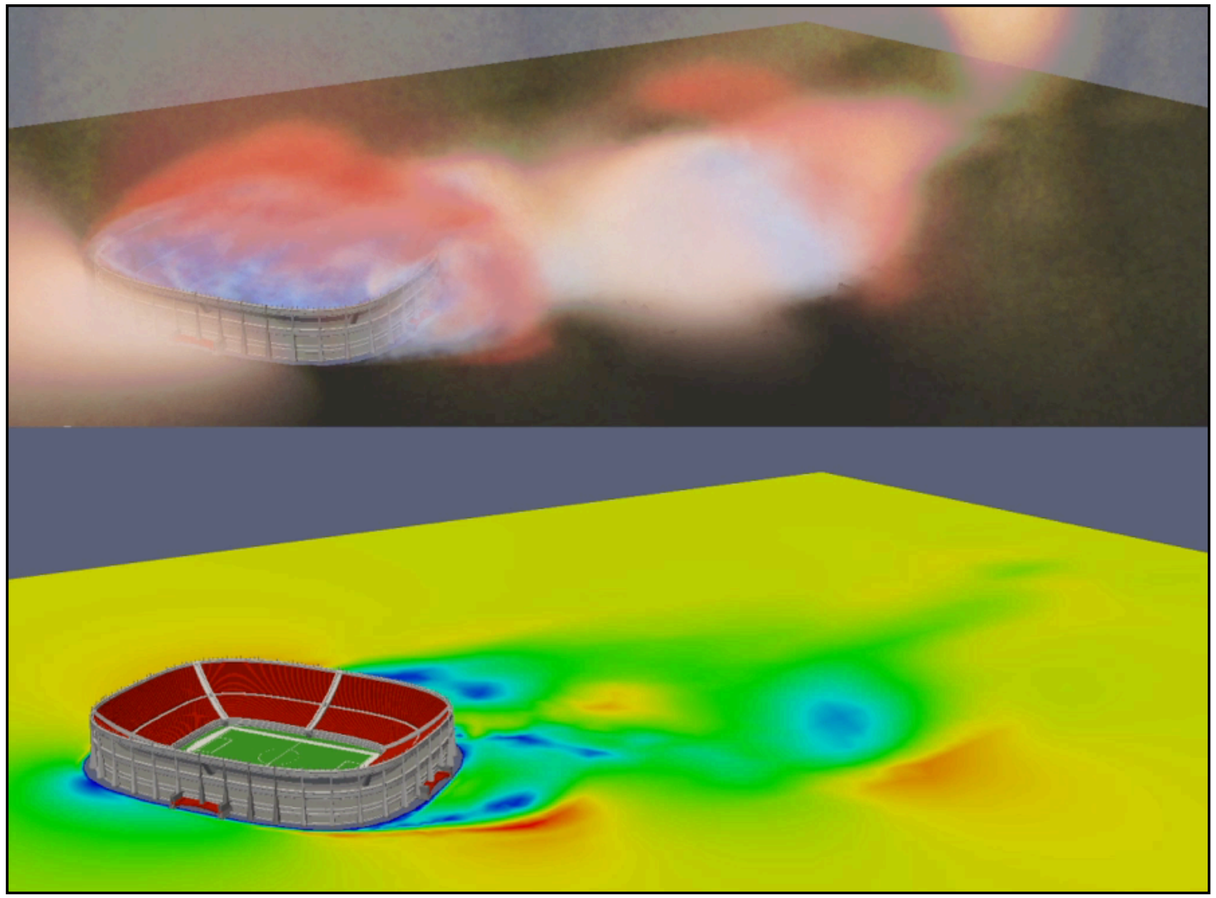


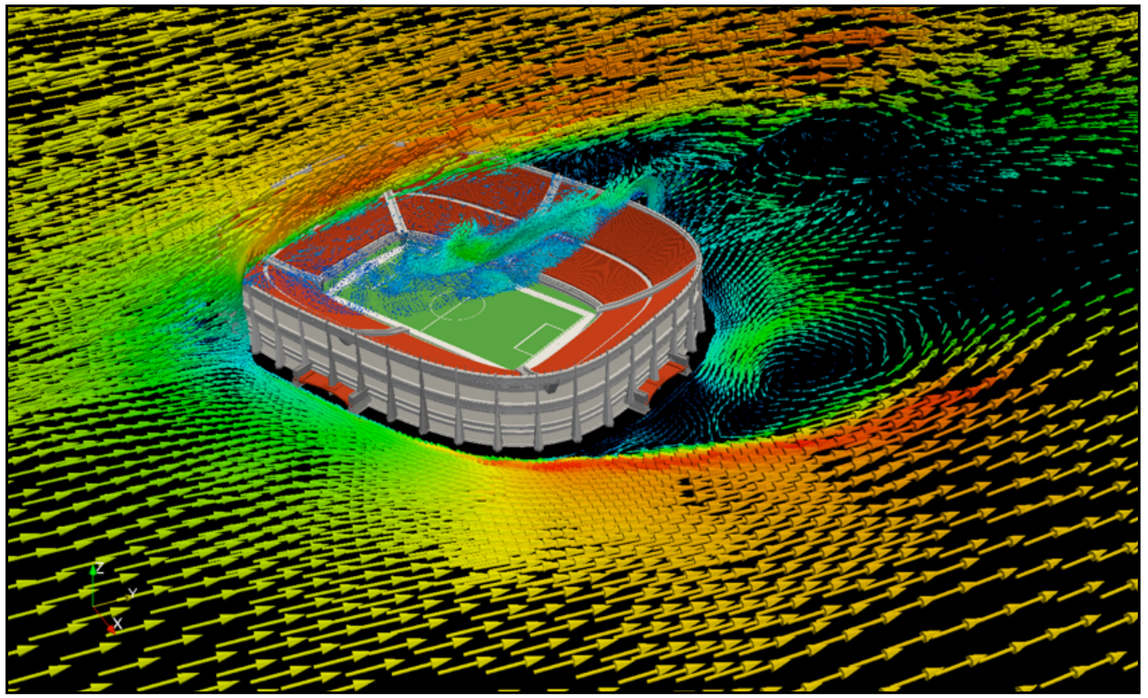
Manufacturing processes:
Mixers & Chemical reactors

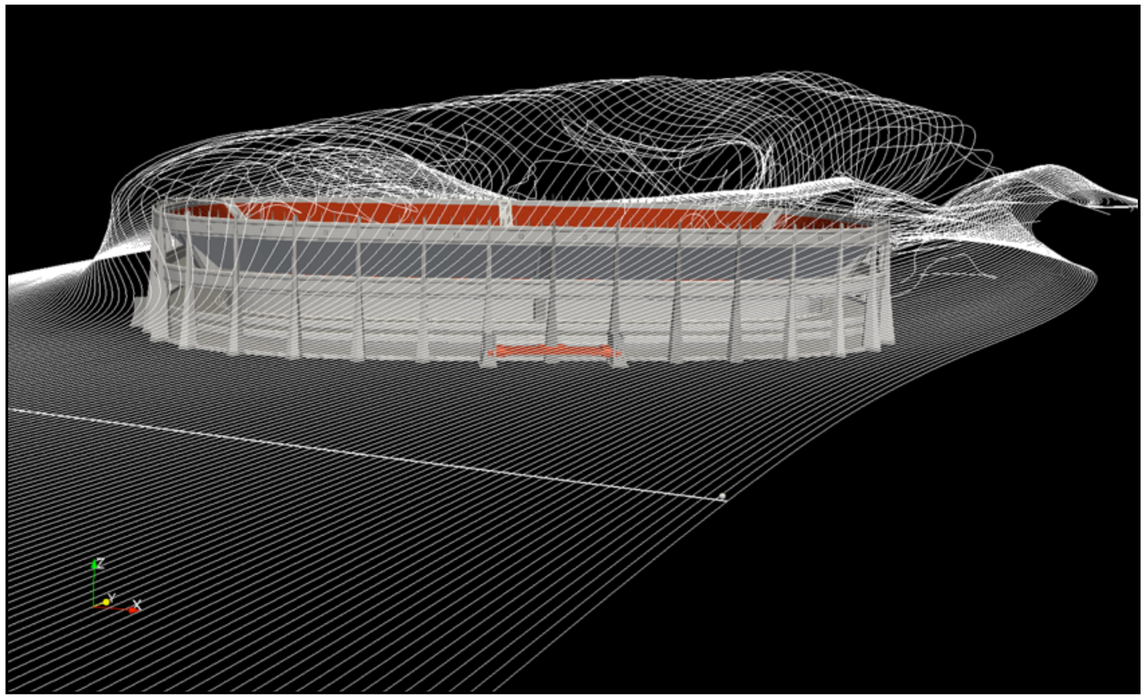
The wind and the environment

ATMOST Spanish project

Wind in urban environments

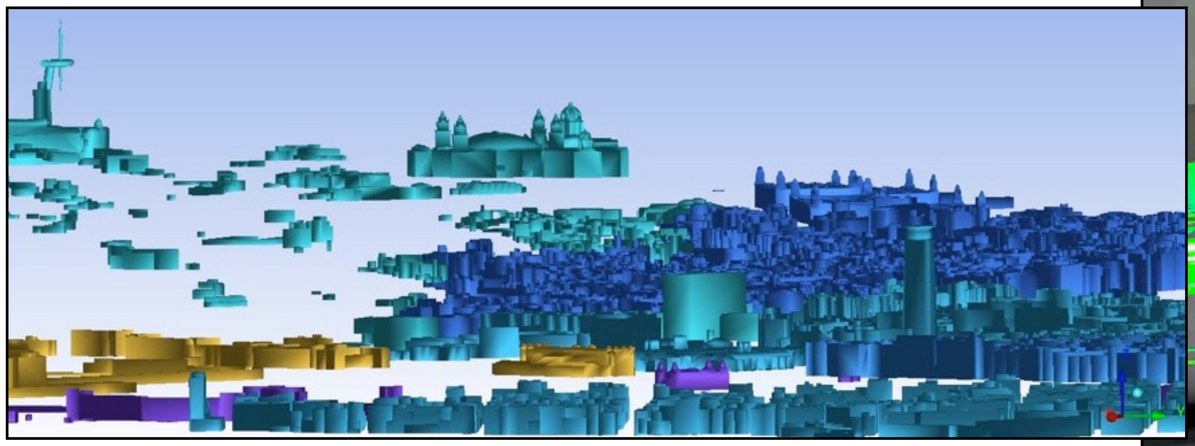


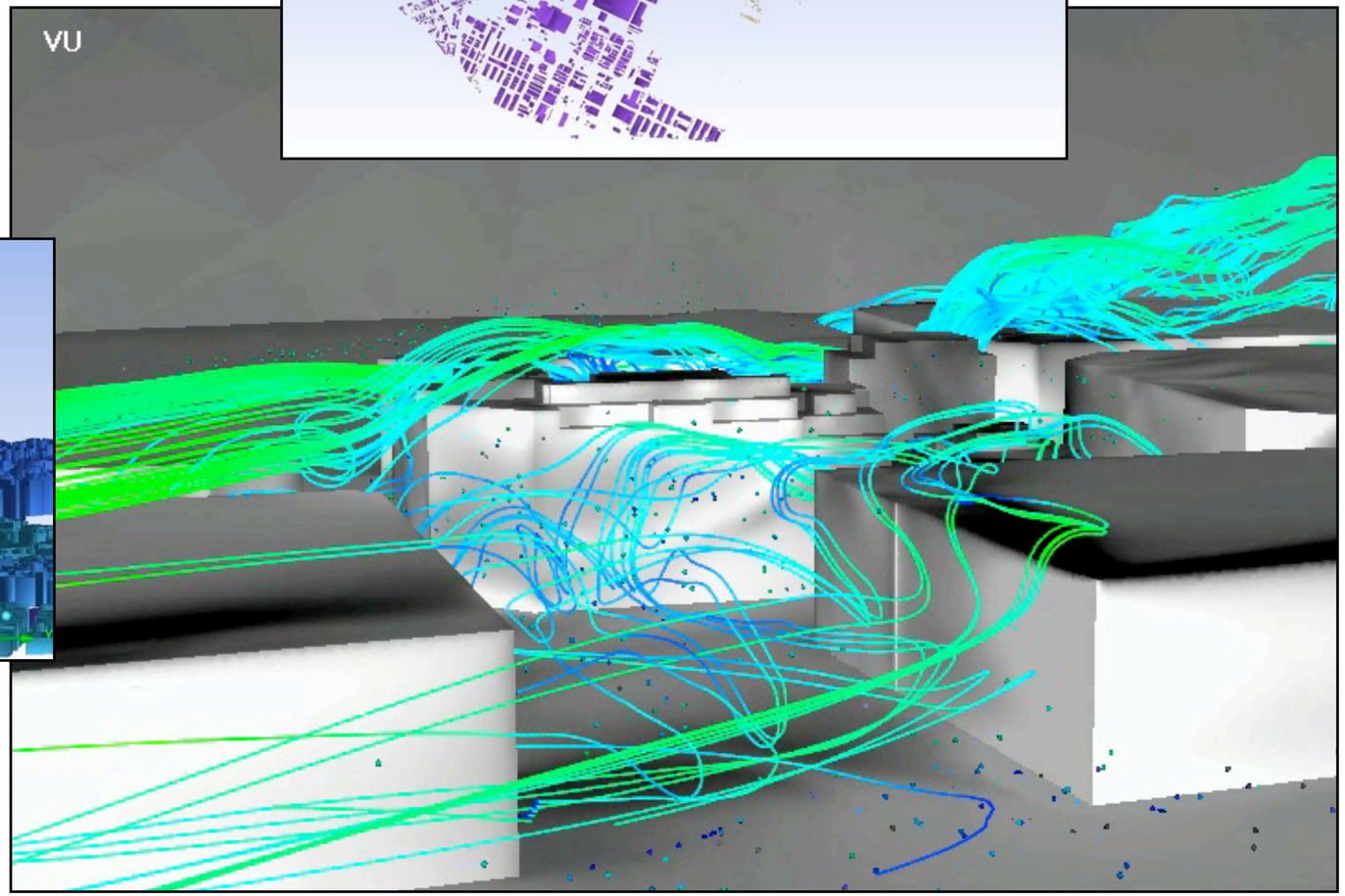




ATMOST Spanish project

Wind in urban environments





IBERDROLA + BSC + CENER

Convenio Iberdrola (SEDAR) and S4E (proyecto Plan Nacional)

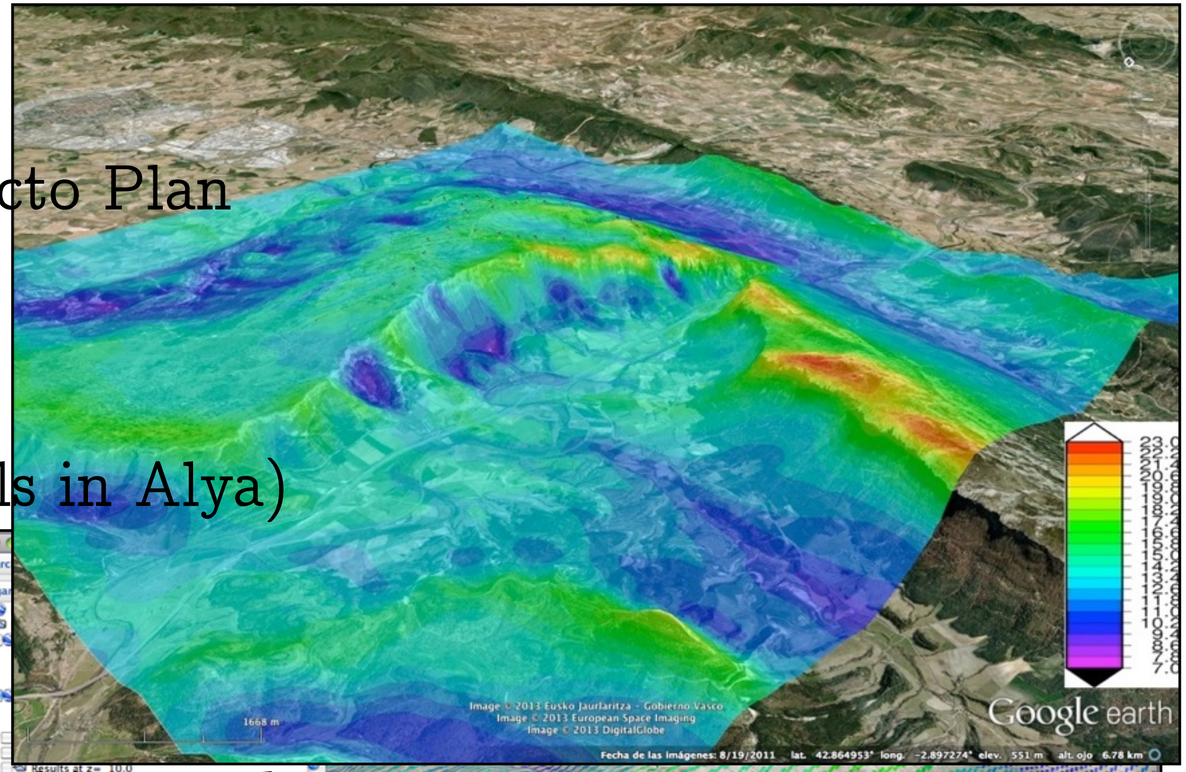
Wind farm modelling

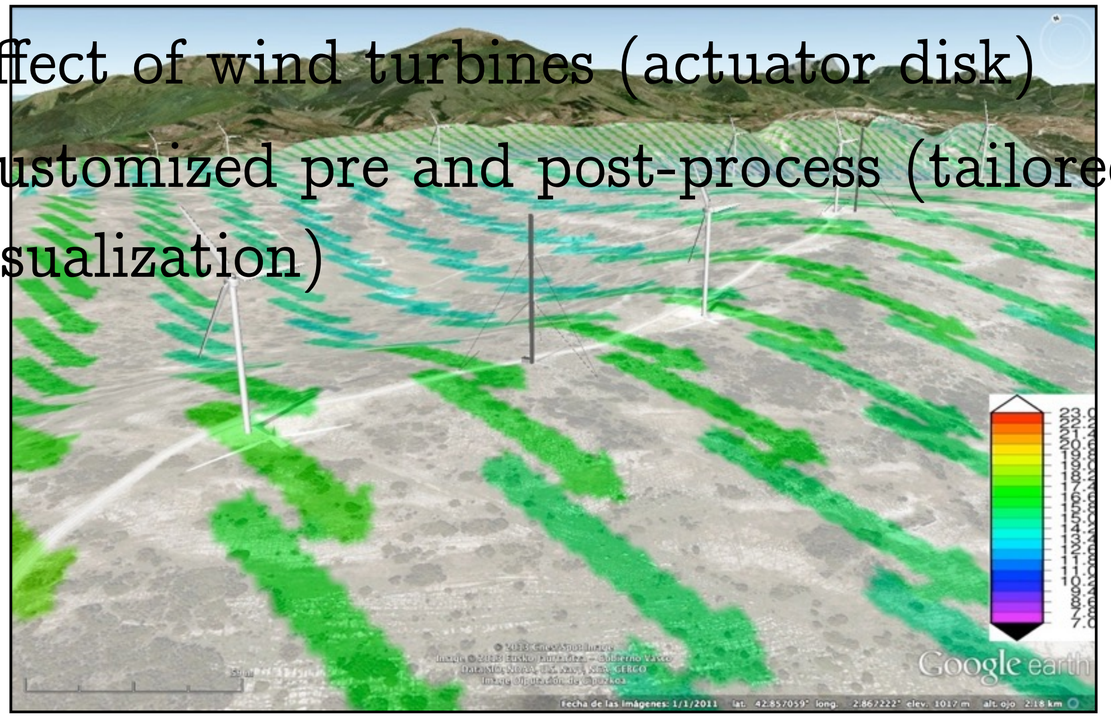
High-resolution wind modelling (RANS models in Alya)

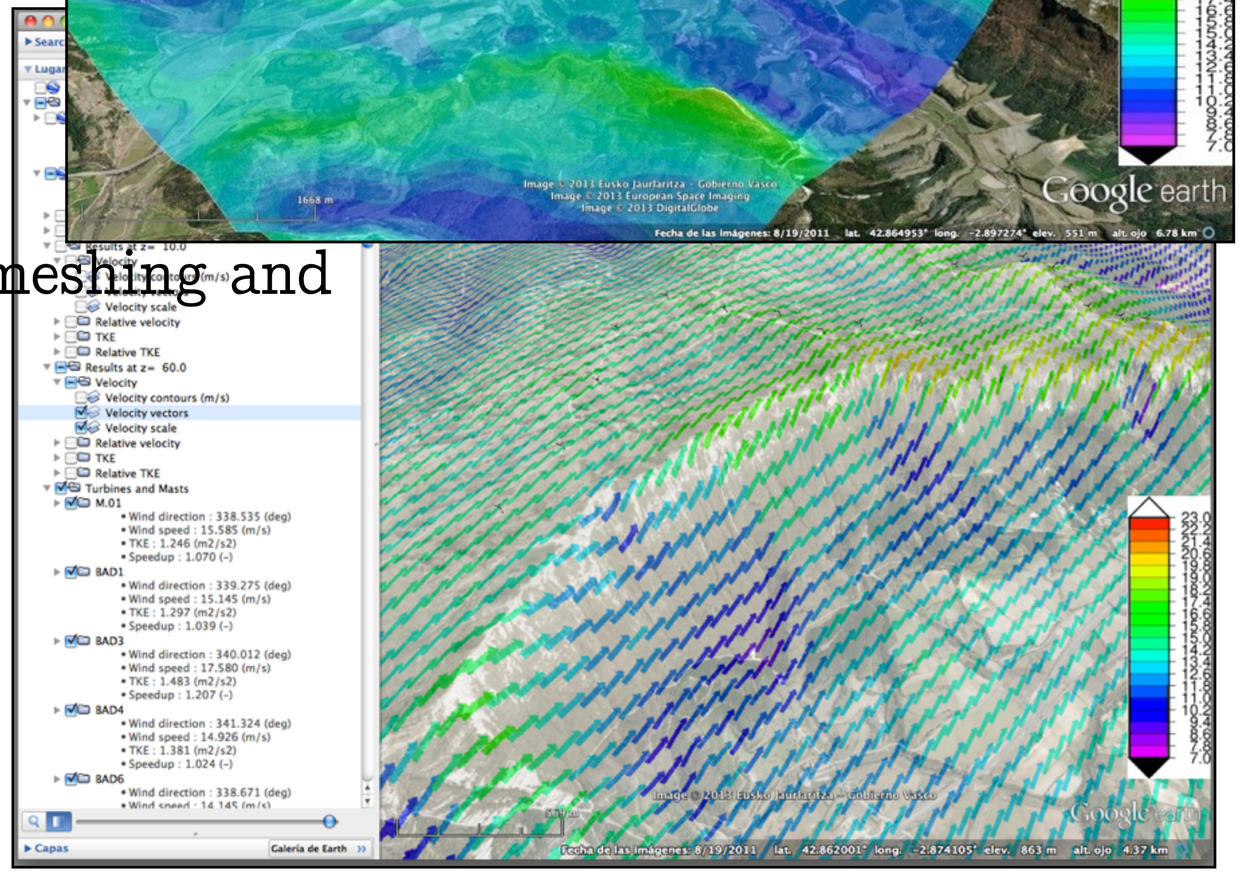
Thermal coupling

Effect of wind turbines (actuator disk)

Customized pre and post-process (tailored meshing and visualization)

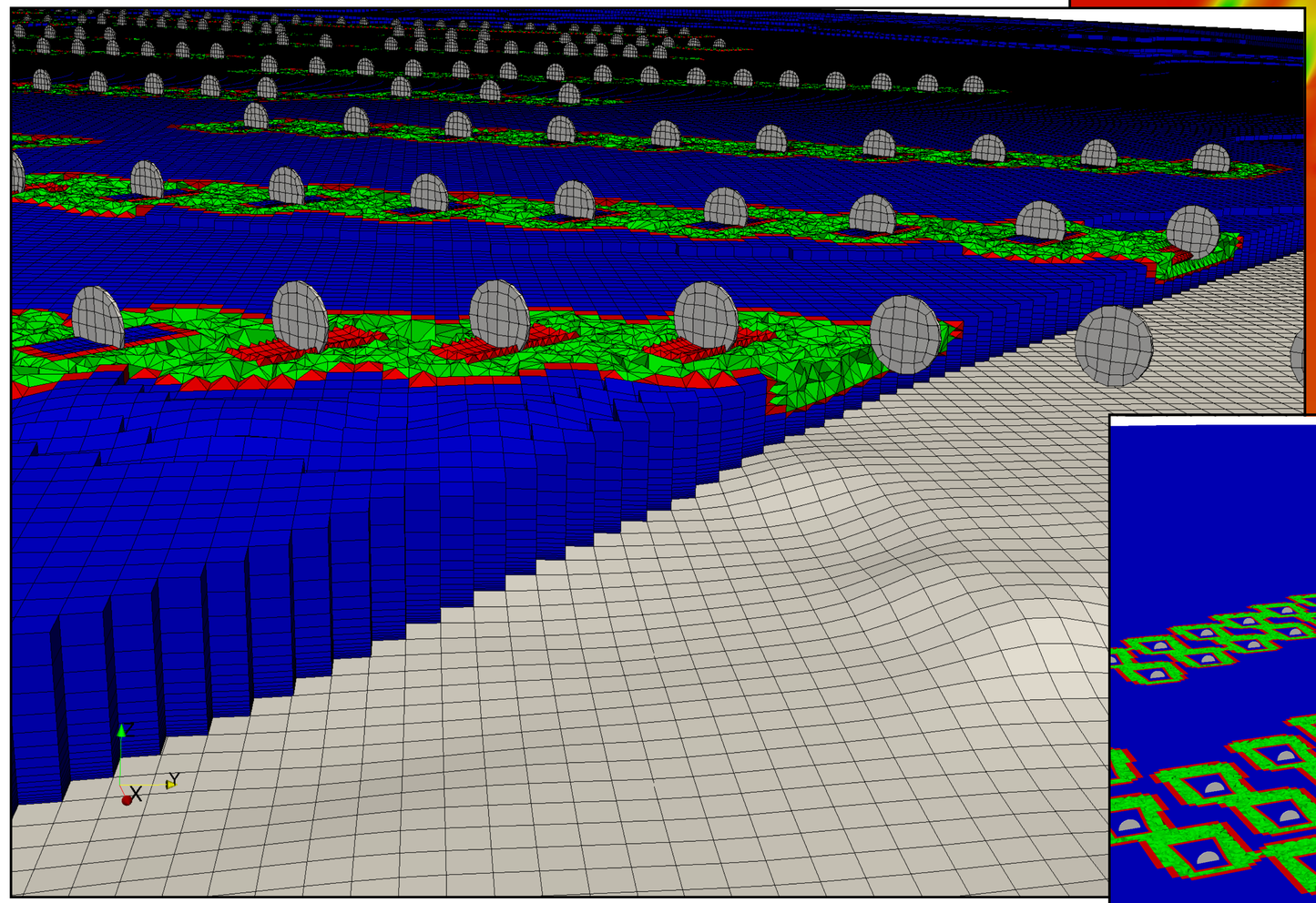


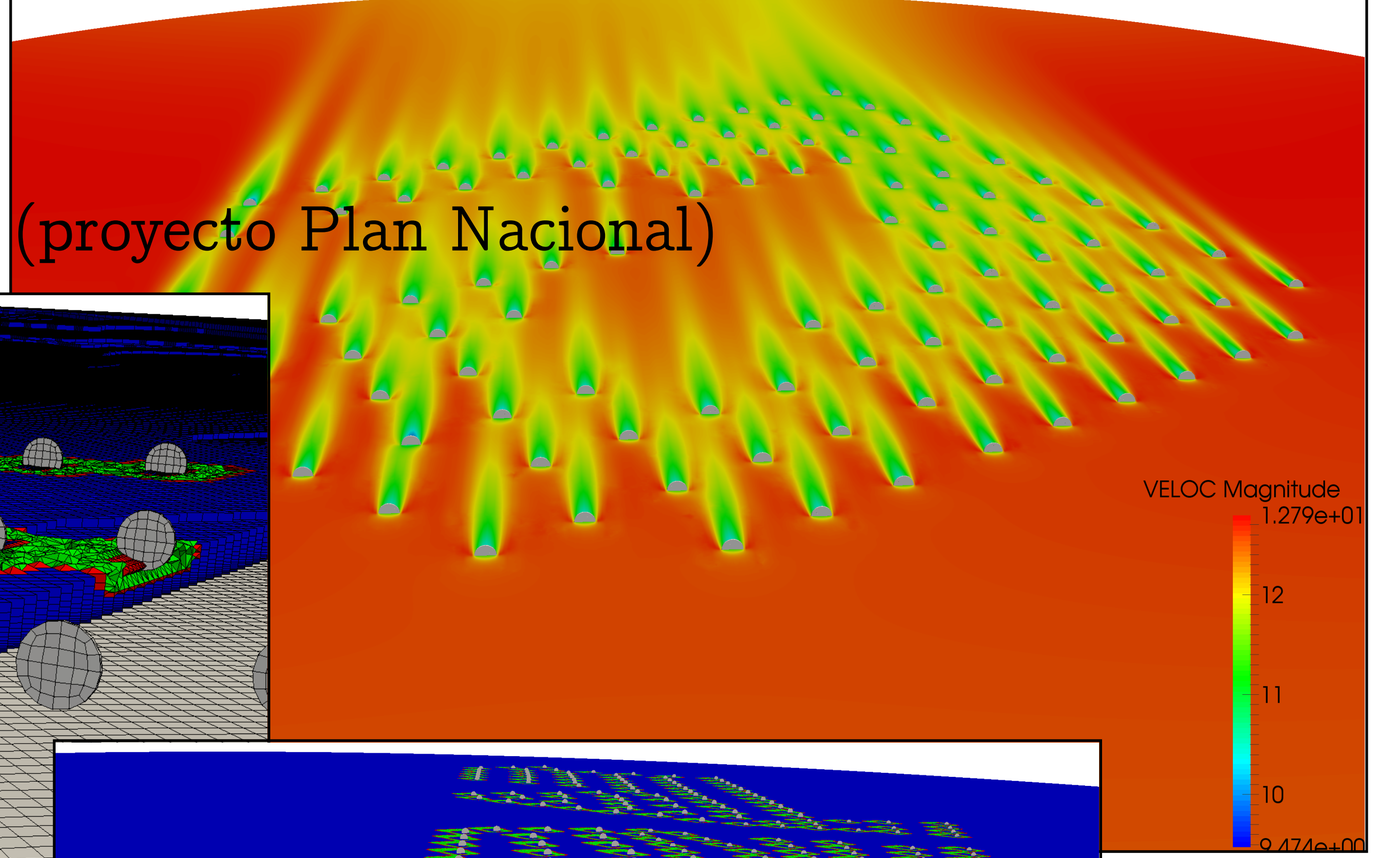


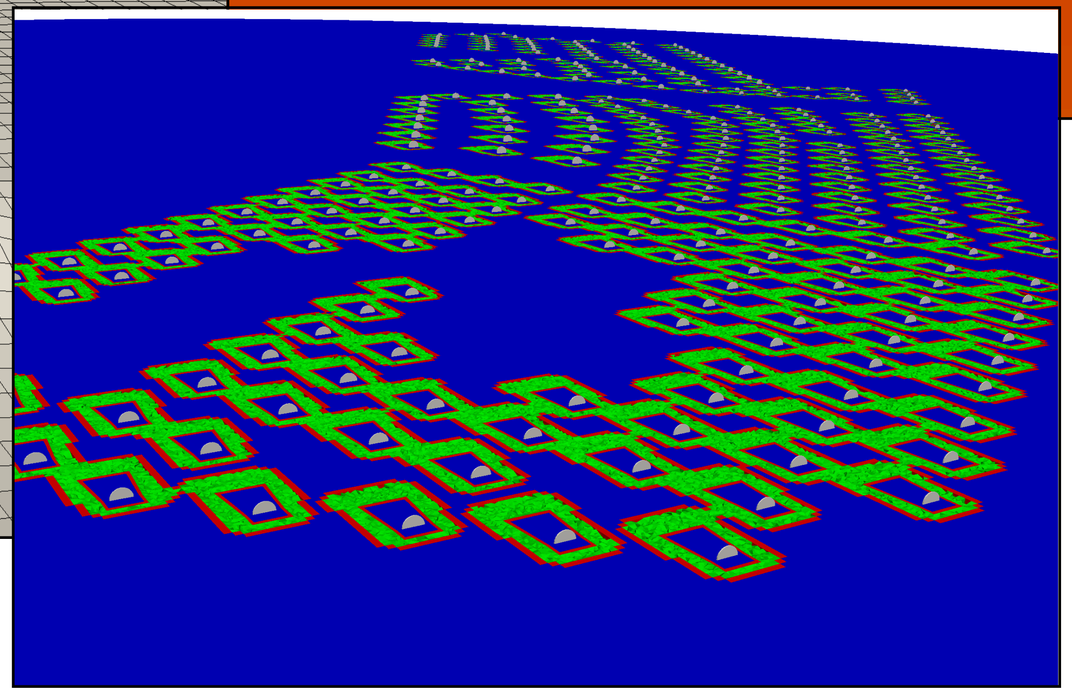


IBERDROLA + BSC + CENER

Convenio Iberdrola (SEDAR) and S4E (proyecto Plan Nacional)



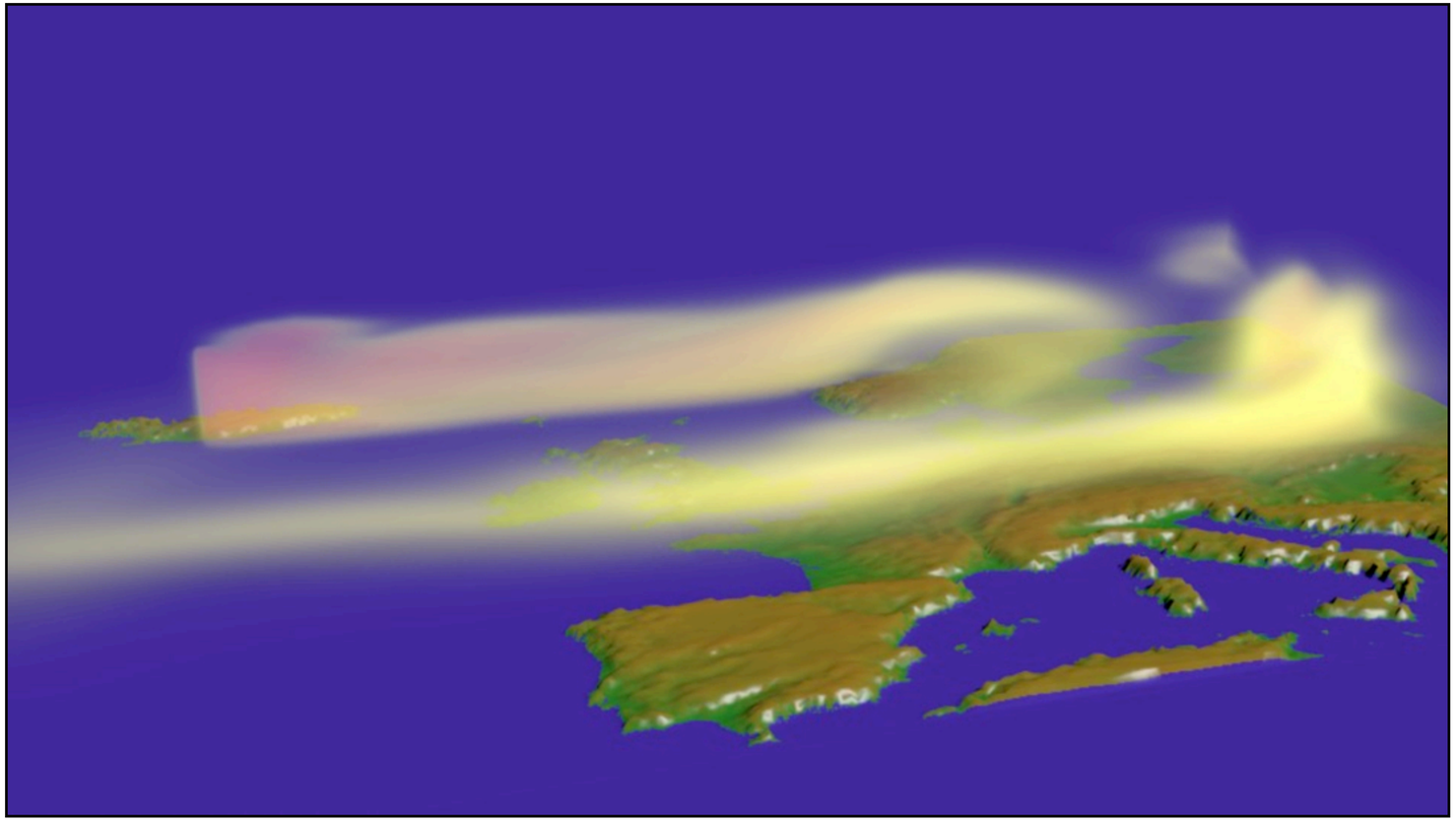


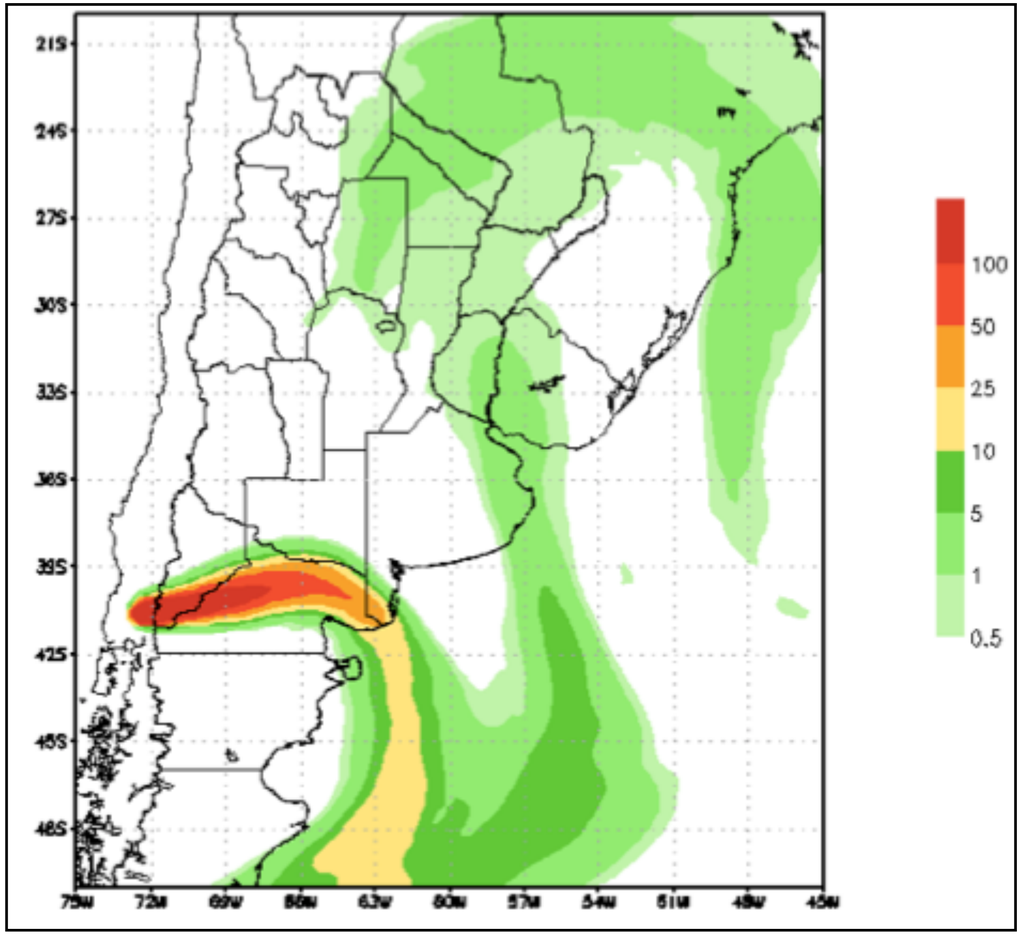


NEMOH FP7 European Project

Modelling of volcanic process and hazard

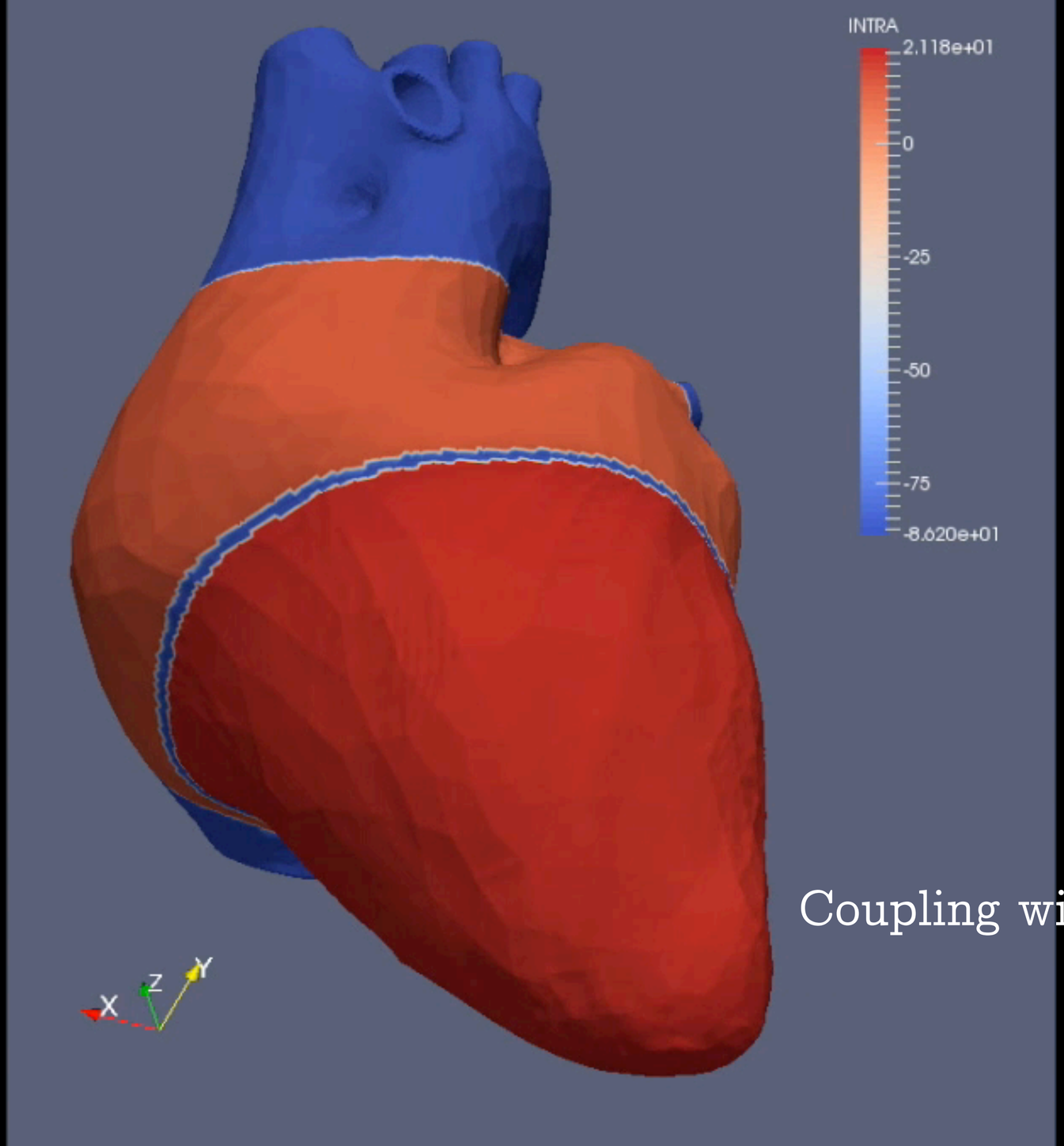
Volcanic ash transport and deposition

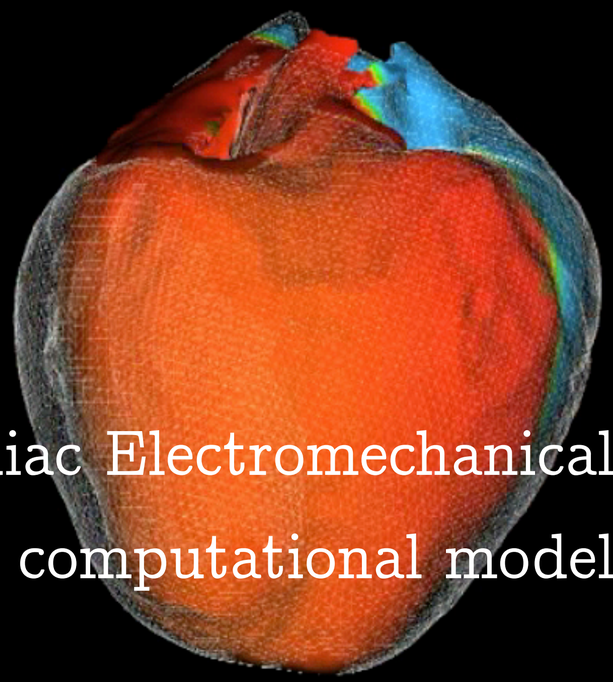




Previous BSC - Brazil initiatives:

EU-Brazil Cloud Connect

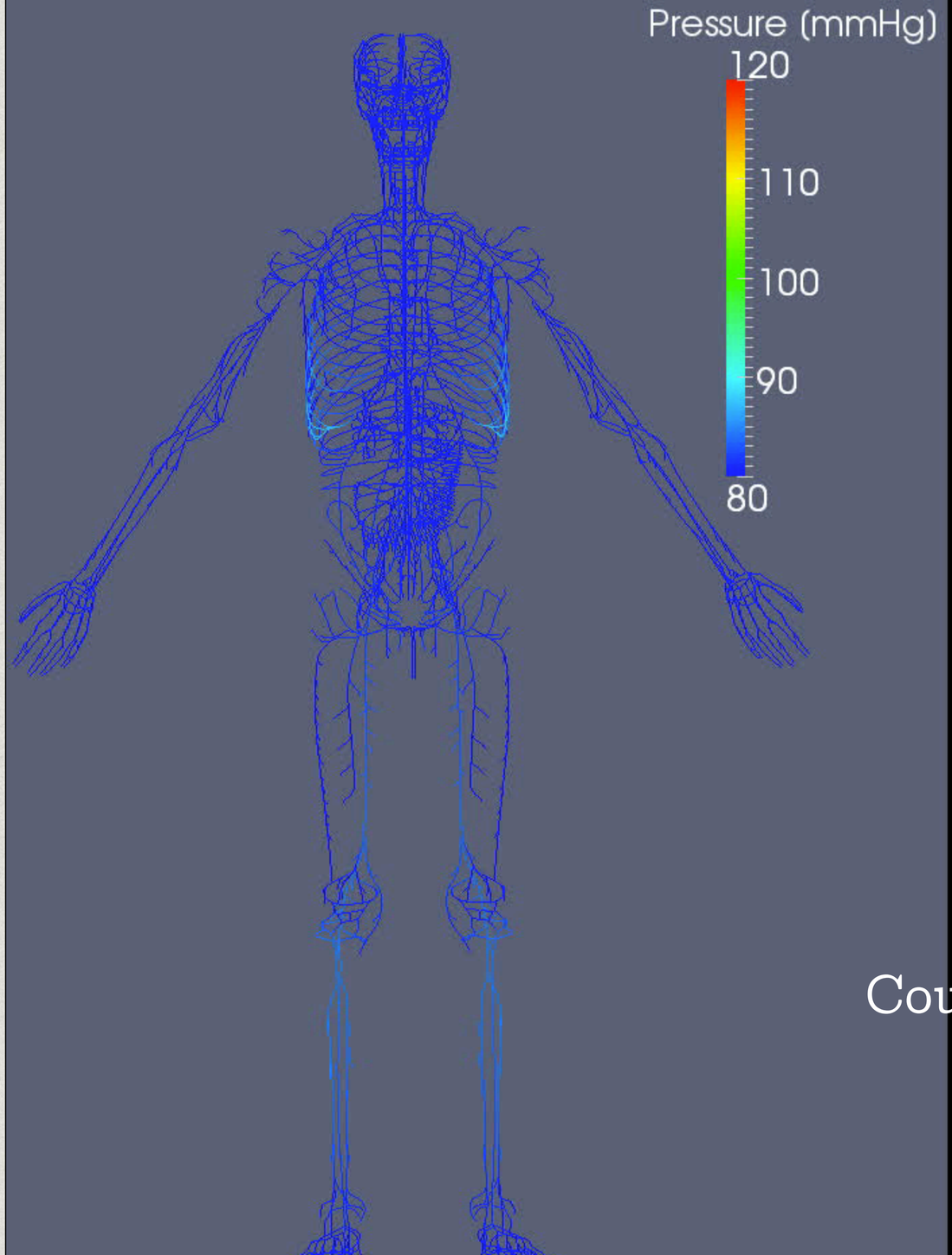


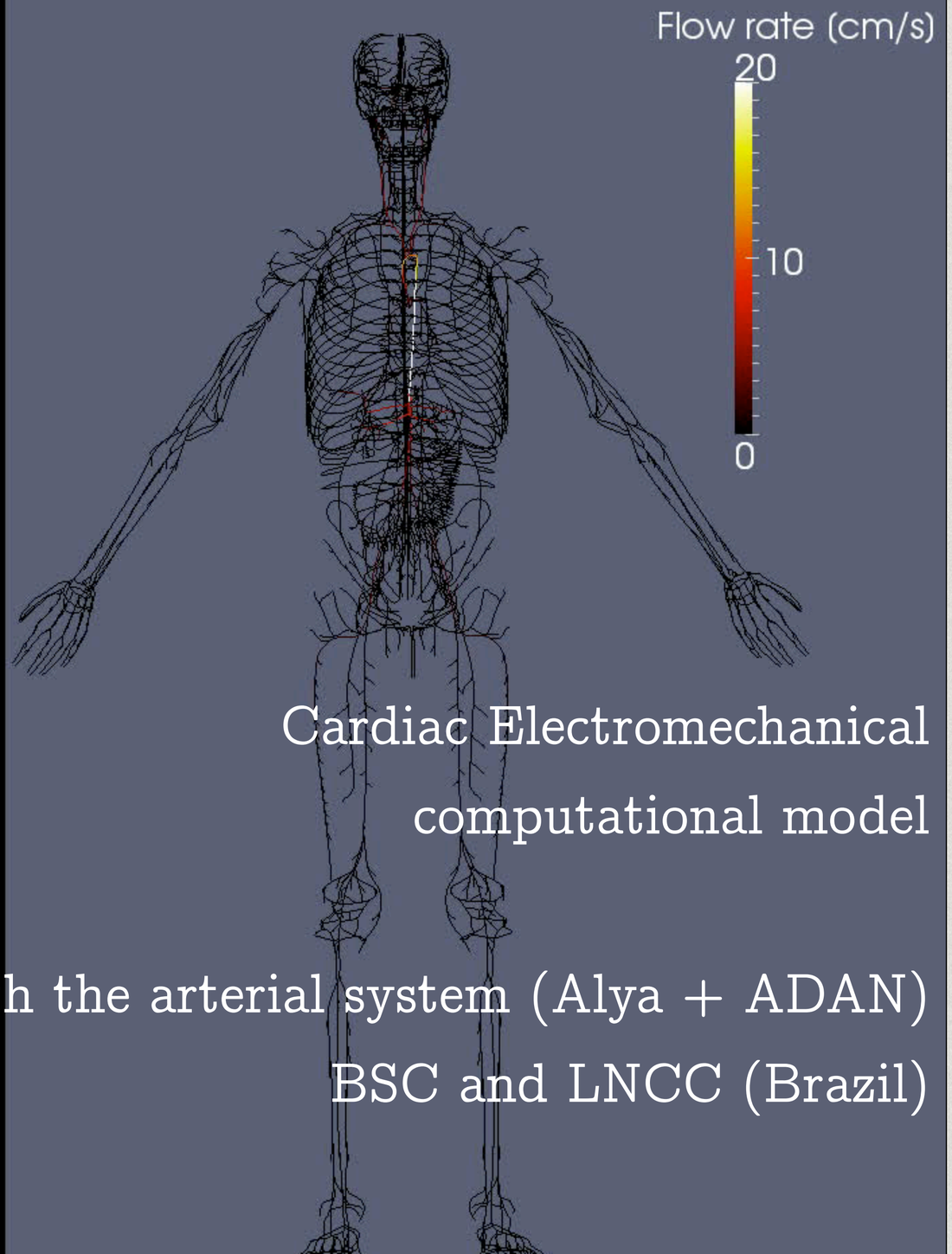


Cardiac Electromechanical computational model

Coupling with the arterial system (Alya + ADAN)

BSC and LNCC (Brazil)





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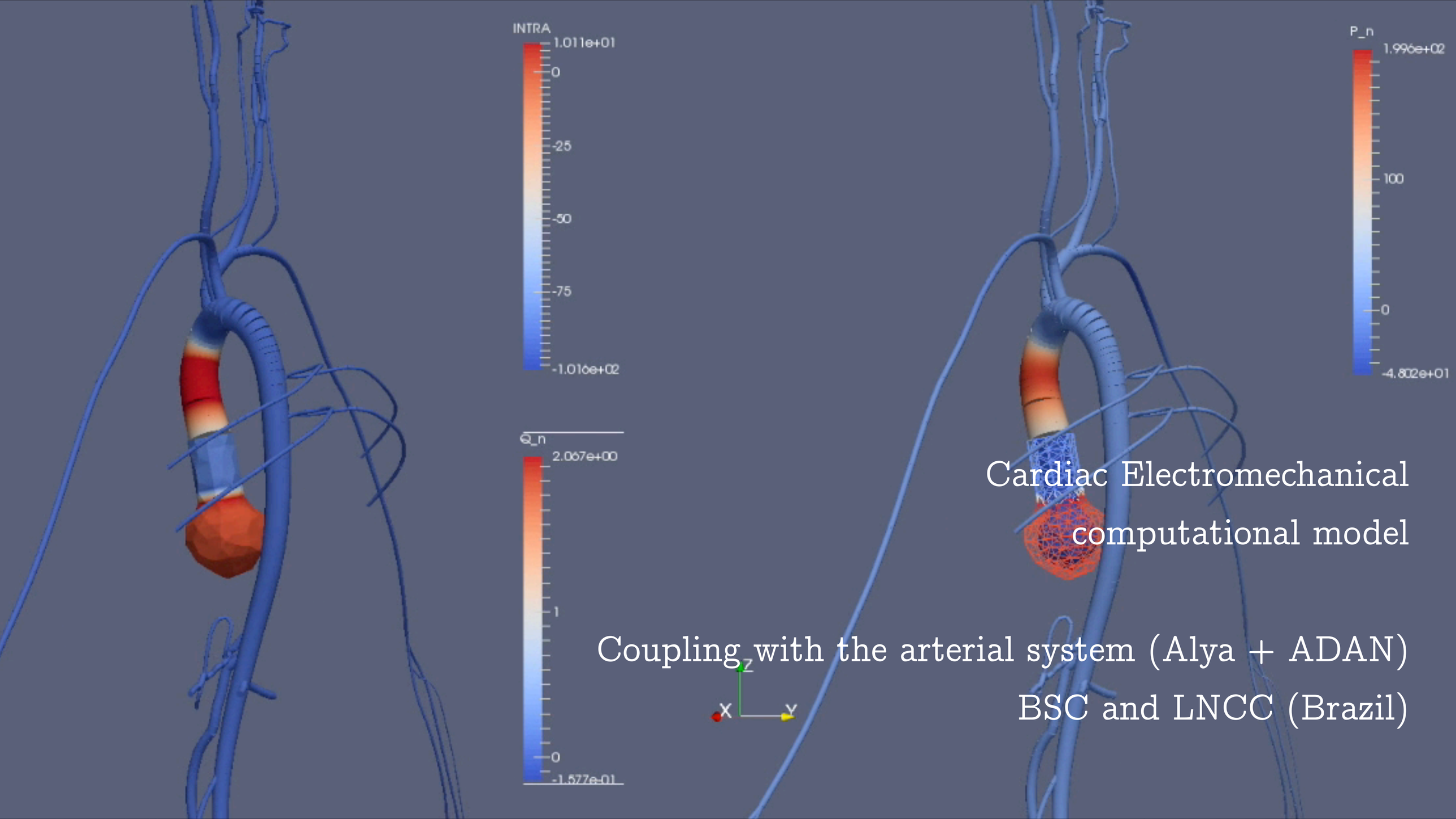


Cardiac Electromechanical computational model

Coupling with the arterial system (Alya + ADAN)

BSC and LNCC (Brazil)

Current BSC - Brazil initiatives:

HPC4E

HPC4E (HPC for Energy)

EU - Brazil collaboration project

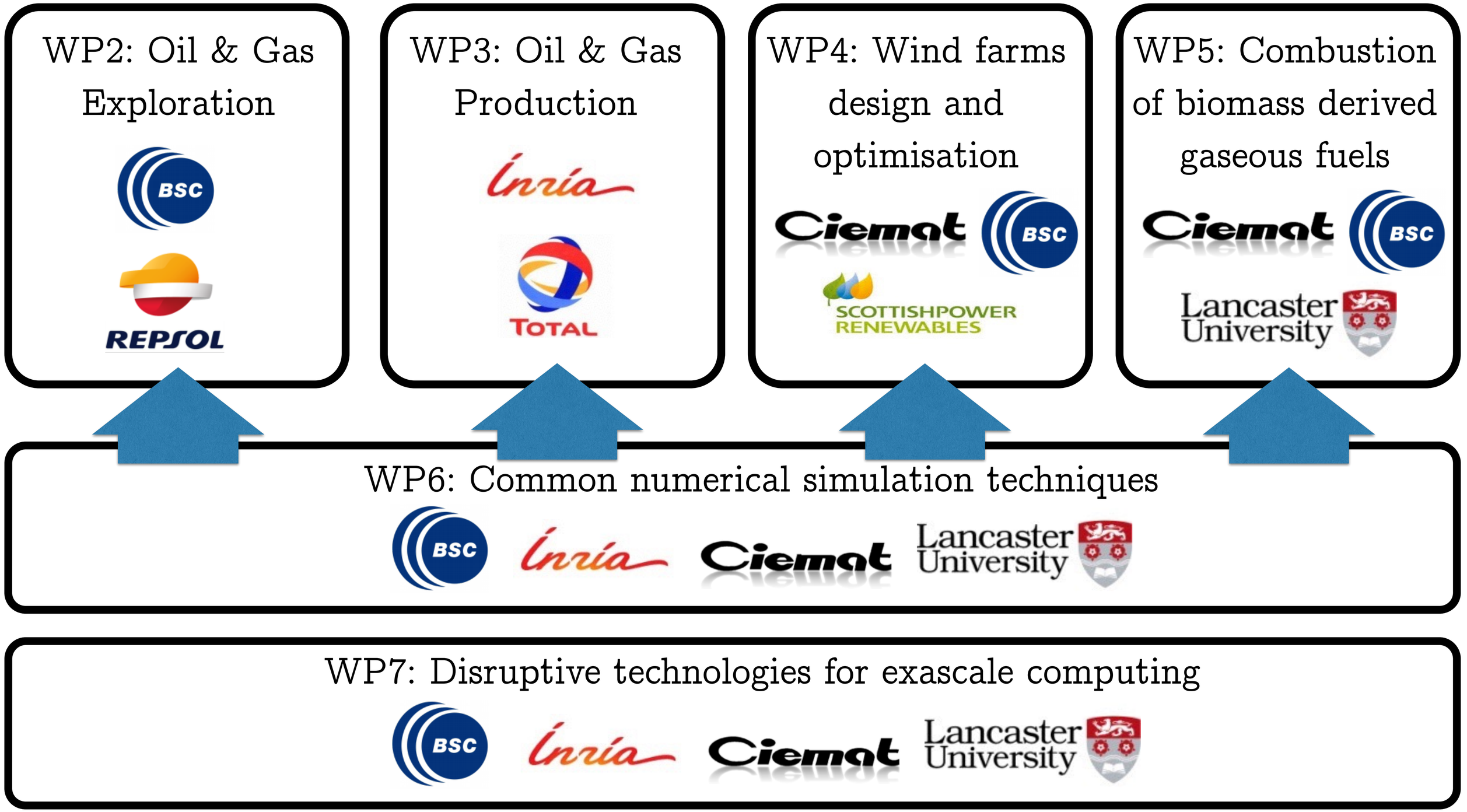
H2020-EUB-2-2015:

High Performance Computing

2 Million Euro for European partners alone

“Apply Exascale HPC technology to energy industry simulations”

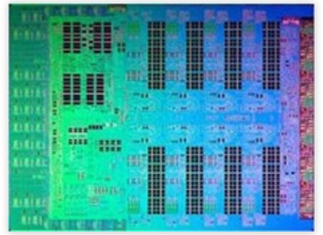
Wind + Oil and Gas + Biomass


WP2: Oil & Gas Exploration
BSC
REPSOL
WP3: Oil & Gas Production
Inria
TOTAL
WP4: Wind farms design and optimisation
Ciemat
BSC
SCOTTISHPOWER RENEWABLES
WP5: Combustion of biomass derived gaseous fuels
Ciemat
BSC
Lancaster University
WP6: Common numerical simulation techniques
BSC
Inria
Ciemat
Lancaster University
WP7: Disruptive technologies for exascale computing
BSC
Inria
Ciemat
Lancaster University

Hydrocarbon Energy

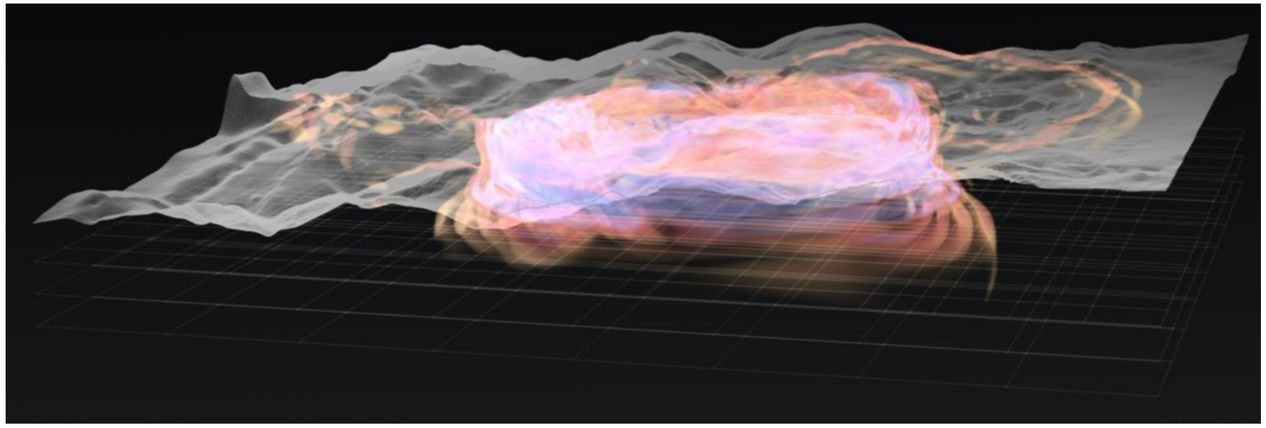
Exascale-level computational kernels (x5 performance and energy efficiency)

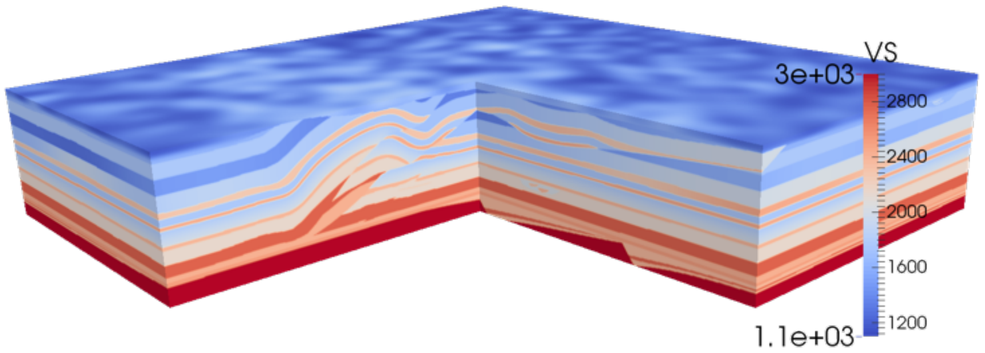
- Multiscale Hybrid-Mixed methods + DG/CG (frequency domain)
- Mimetic deformed grid FD (time domain)



Exploration risk reduction through uncertainty quantification

Industry-driven benchmarks for geophysical imaging





Wind farm design and optimisation

Goal: To overcome some of the existing limitations by developing models for atmospheric boundary layer winds in complex terrains and its HPC implementation to evaluate the technical and economic feasibility of wind farms

- Implementation in the in-house ALYA code of atmospheric boundary layer models for neutral and non-neutral (thermal coupling) atmospheric stability
- Transient coupling with mesoscale meteorological models
- Wake modelling. Characterizing numerically the downwind effects of rotors by solving complex turbulent rotating flows

Biomass energy

- Generation and assessment of chemical kinetics mechanisms describing the chemical pathways for the combustion of biomass-derived gaseous blends.

- Extending the use of HPC to investigate biomass-derived-fuels with focused on combustion dynamics, stability and pollutant formation in stationary gas turbines.

- Generation of an optimised industrial guideline for the use of biomass-derived gaseous fuel in industrial systems.

Important issues

- European part Grant Agreement to be signed NOVEMBER 14TH 2015
- Starting date proposed to CE officer: DECEMBER 1ST 2015
- Starting date depends on the Brazilian part Grant Agreement signed... (update?)

Important issues

- HPC4E groups must take profit of PRACE calls, asking for resources in MN (and other PRACE supercomputers...)
  - Project access: code scaling and optimisation

    Cut-off dates every 3 months
  - Preparatory access: large-scale computationally intensive projects

    February and September

Check periodically: http://www.prace-ri.eu/call-announcements/

HPC-based multi-physics simulations for the energy realm

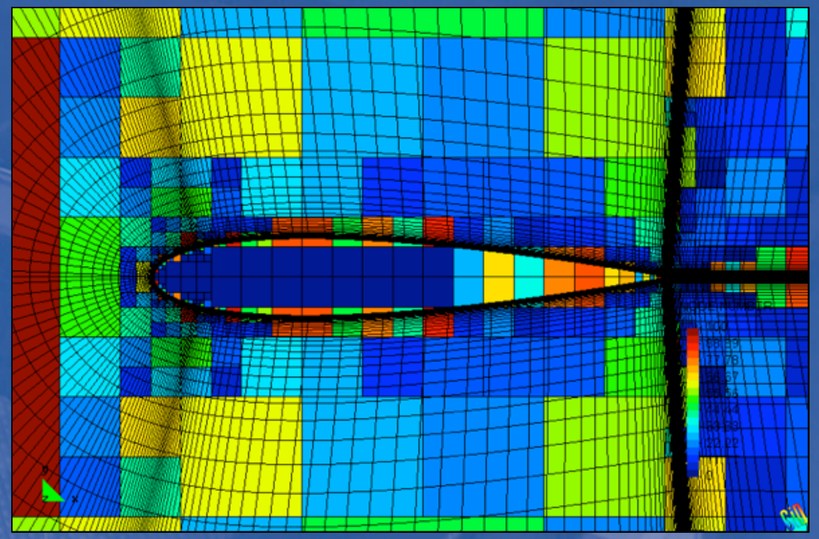
M. Vázquez, G. Houzeaux, J.M. Cela

M. Hanzich, J. de la Puente

A. Folch, D. Mira

Barcelona Supercomputing Center

Spain



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA