The Alya System: HPC simulations for real world problems.

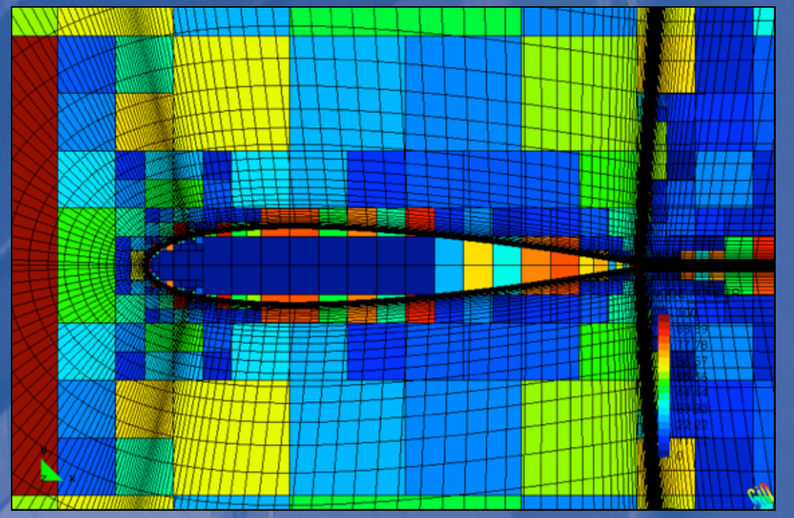
M. Avila, M. Vázquez, G. Houzeaux and CASE Department

Barcelona Supercomputing Center

Spain

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA



HPC methods for Engineering Workshop - Milano, Italy, June 2015

Background

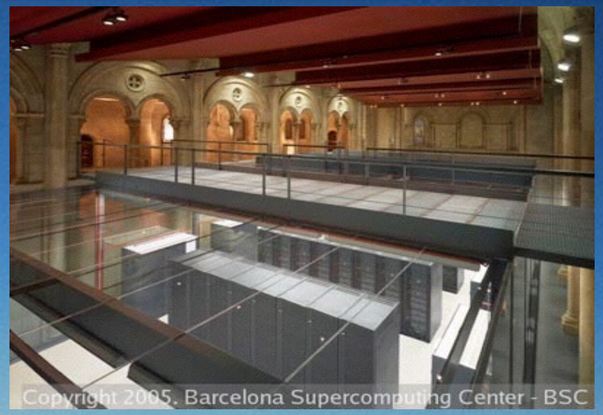
BSC-CNS is the Barcelona Supercomputing Center – Centro Nacional de Supercomputación, the Spanish national supercomputing center

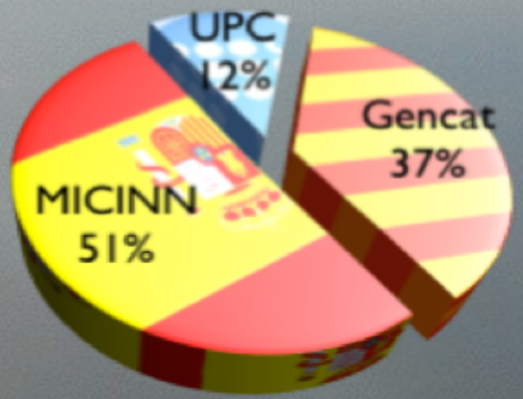
It is a **public center**, co-financed by the Spanish Ministry of Science, the regional government of Catalonia and the UPC (Technical University of Catalonia)

Around 300 researchers from several disciplines

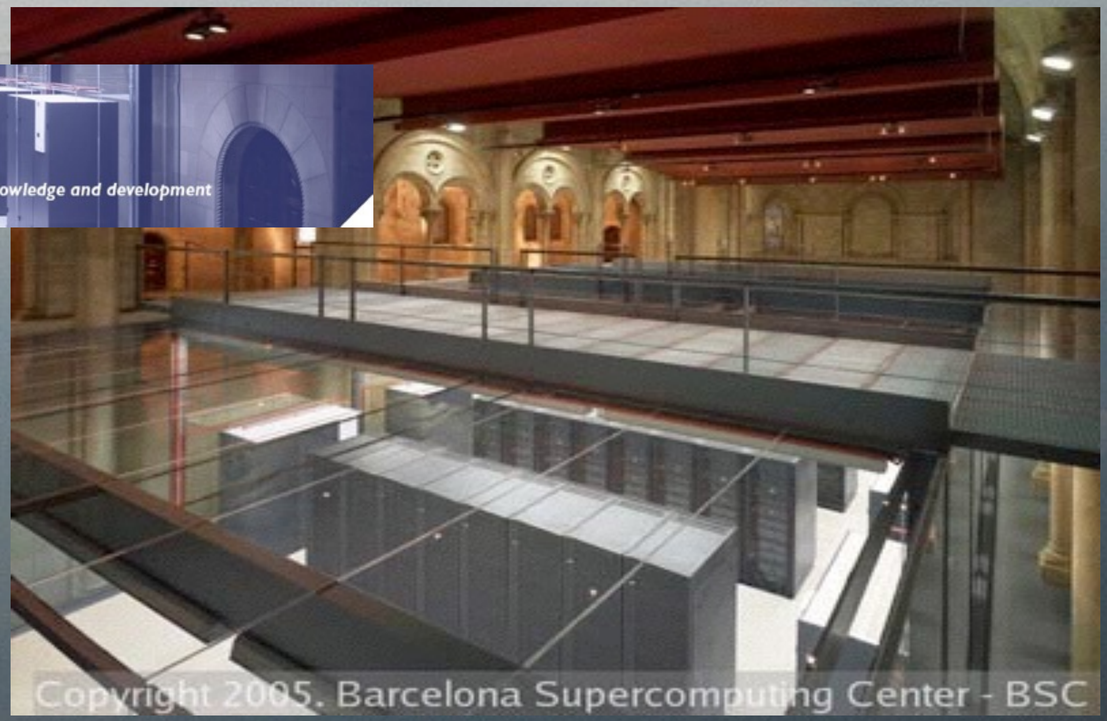
It hosts the **MareNostrum**, 3rd supercomputer in Europe in Nov 2007. 76th in Nov 2008.

Mare nostrum today: 49 000 cpu's, 1PFlop. 19th in Europe and 57th in the World.



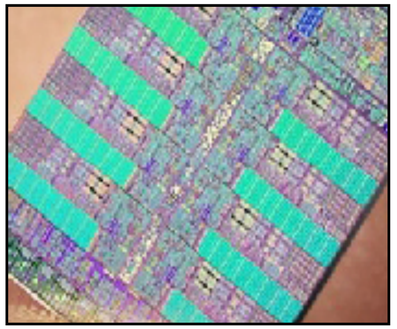


Barcelona Supercomputing Center



BSC Research Departments

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

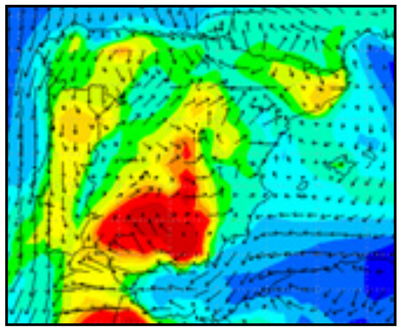


Computer Science

Tools, storage, cloud...

Computer architectures

Programming models

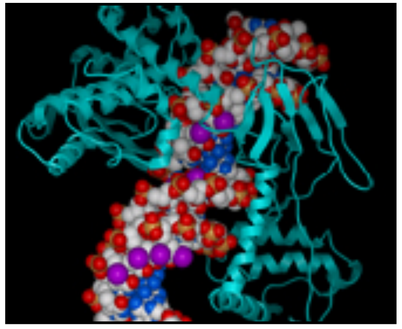


Earth Science

Climate

Air quality

Hardware and software technologies for efficient use supercomputer technologies



Life Science

Bioinformatics for Genomics

Computational Biochemistry

Computer Applications in Science and Engineering

CASE

CASE: The BSC’s applications department

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

From 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 adapted to run onto high-end parallel supercomputers

More than 65 researchers:

Post-docs, students, programmers

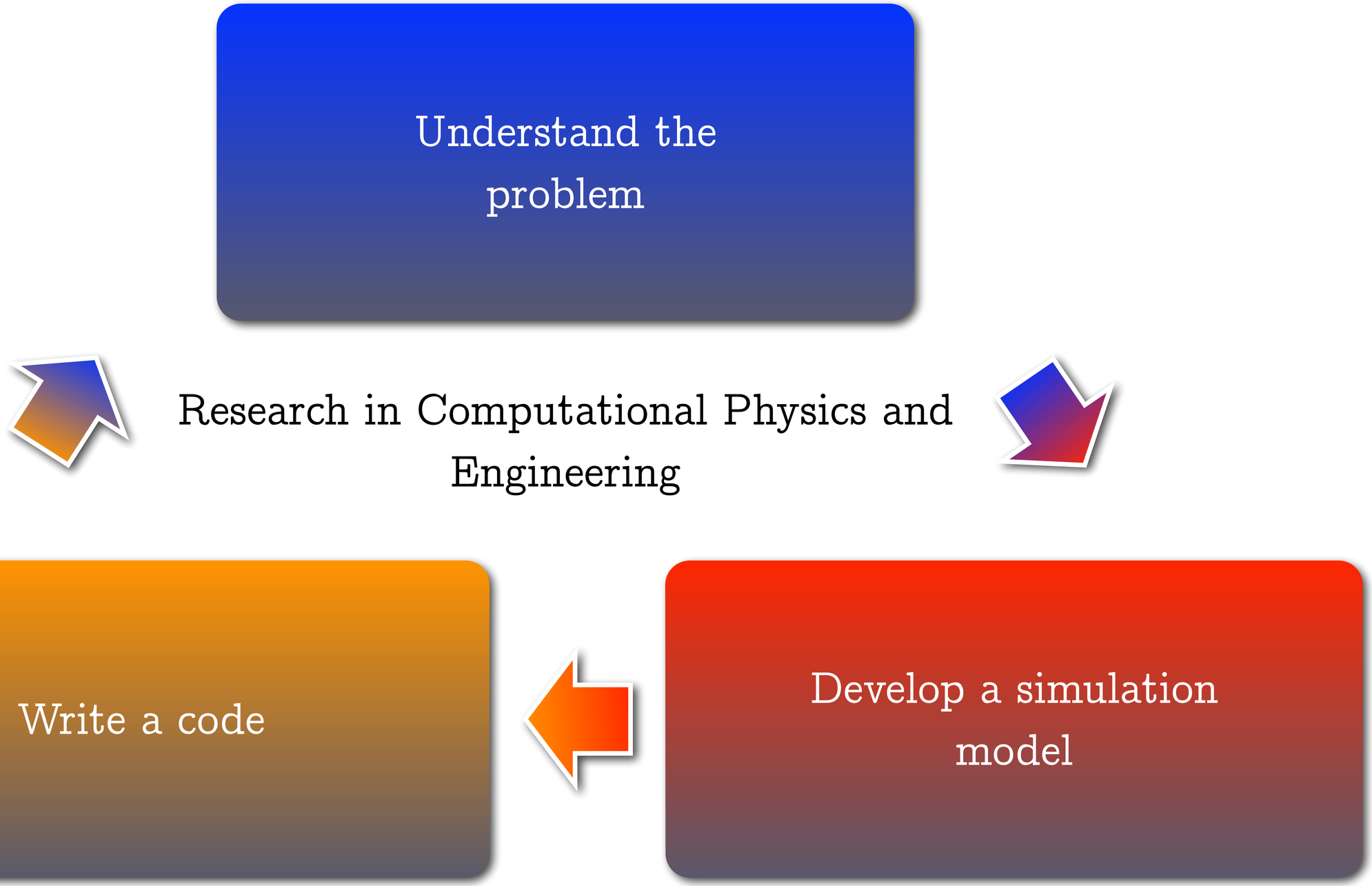
Computer Science, Physicists, Mathematicians, Engineers

Physics

Research in Computational Physics and Engineering

Computer Science

Mathematics


Understand the problem
Research in Computational Physics and Engineering
Develop a simulation model
Write a code

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

Meteorology
Energy
Trains and Automotive
Ship hydrodynamics
Oil and Gas Industry

Artificial Societies (Population dynamics)

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)

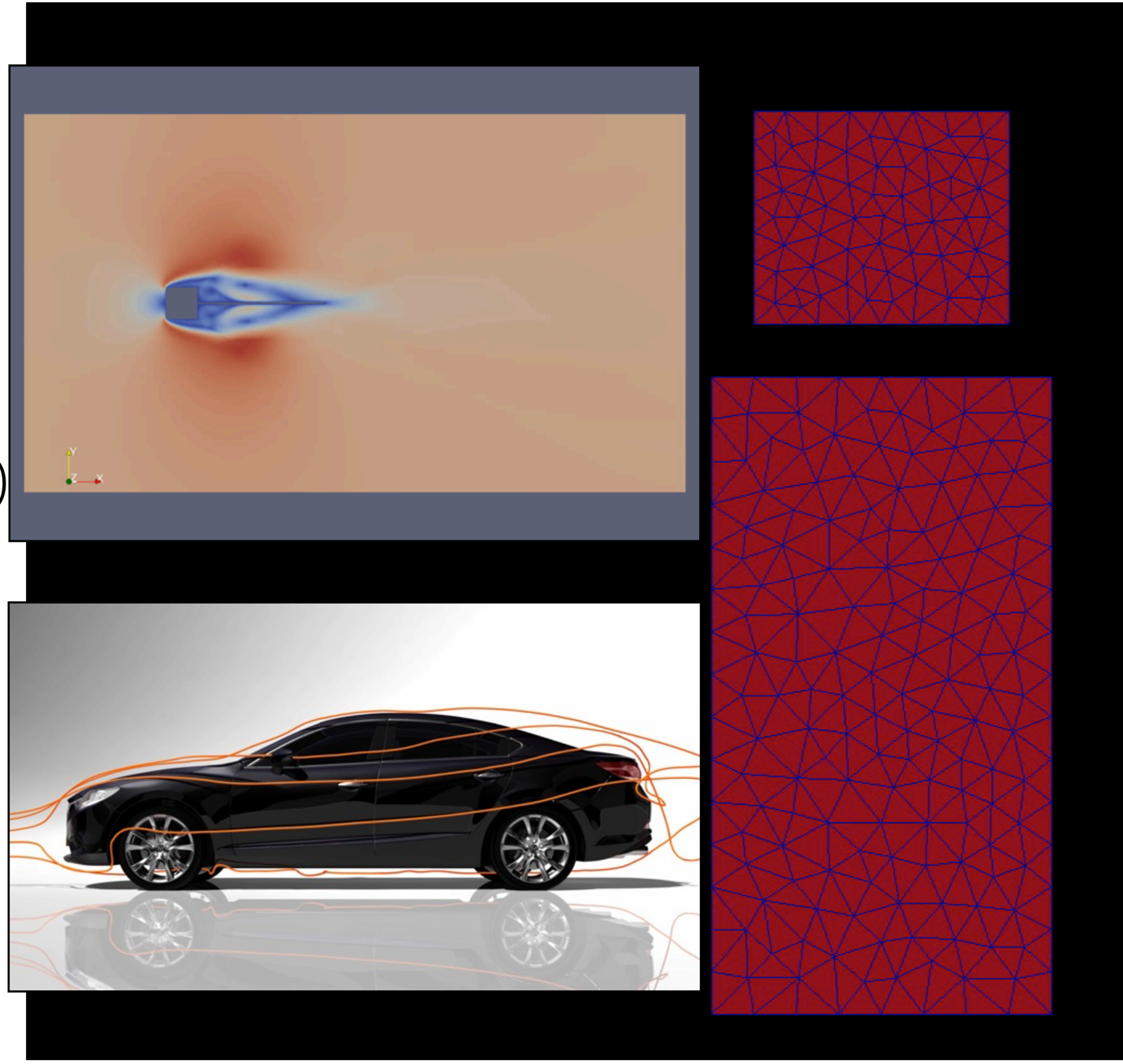
Large-scale simulations

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

Alya: non-structured meshes, coupled multi-physics, complex geometries.

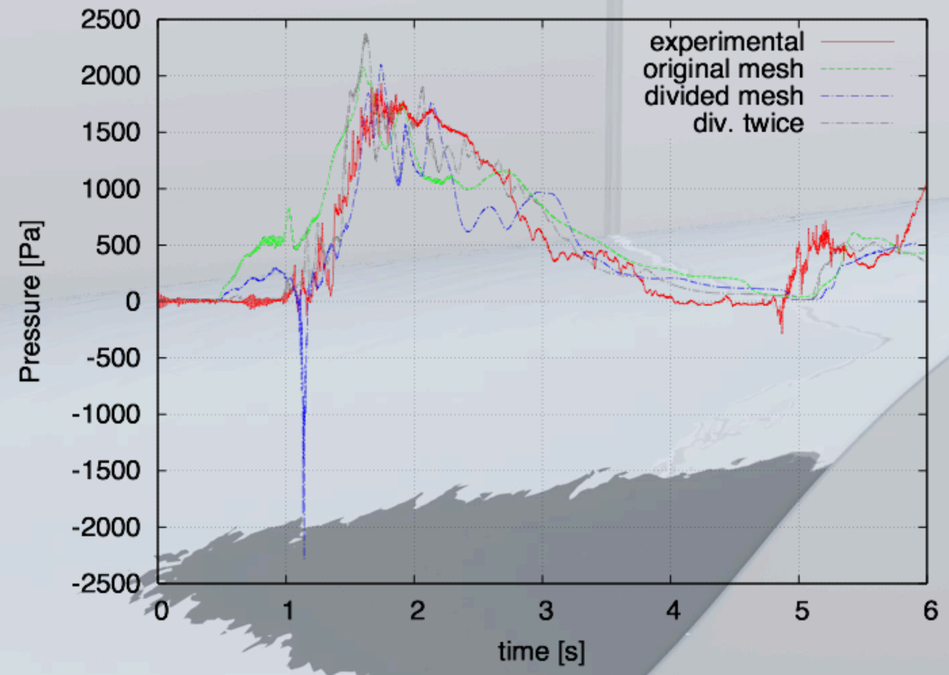
Waris: cartesian (staggered) meshes, well-defined numerics, one code - one problem - one physics.

Pandora: agent-based simulations.

Alya

Parallel multi-physics code developed at BSC

- Coupled PDEs: loosely, strongly, both
- Unstructured meshes
- Explicit and implicit schemes
- Finite Element Variational Multiscale Method
- Modular: kernel, modules, services
- Parallelization based on:
  - MPI tasks and automatic mesh partition using METIS
  - OpenMP threads on loops
  - Both
- Portability is a must
- Porting to new architectures: Cells, GPUs

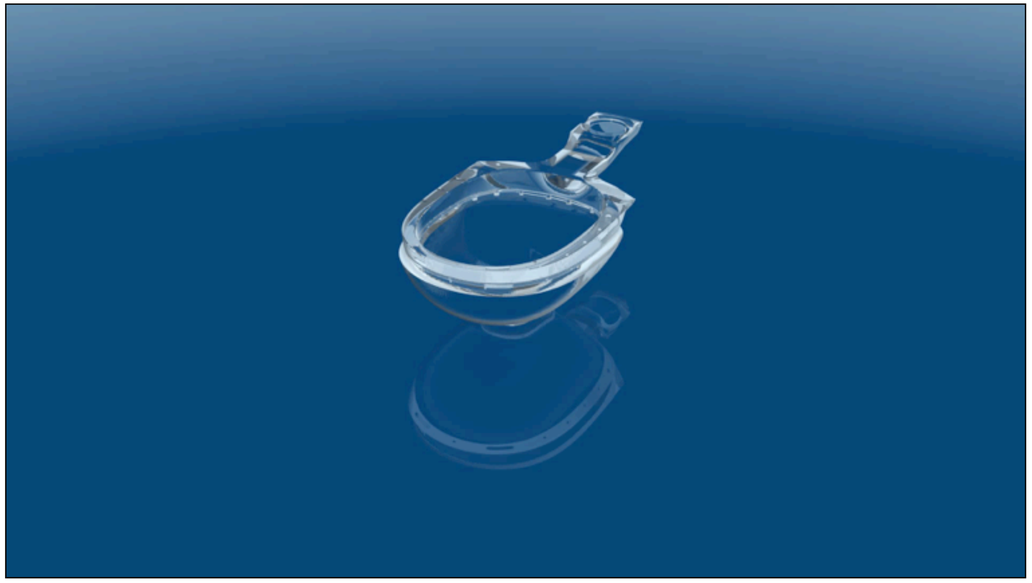


Alya

Parallel multi-physics code developed at BSC

Physics:

- In / Compressible flow, Turbulence, Level Sets
- Chemical reactions, Combustion
- Heat transport
- Non-linear solid mechanics, contact, N-bodies
- Electromagnetism
- Excitable media
- Acoustics
- ALE for FSI
- Adjoint-based optimisation
- Particles (tracers) and Immersed bodies

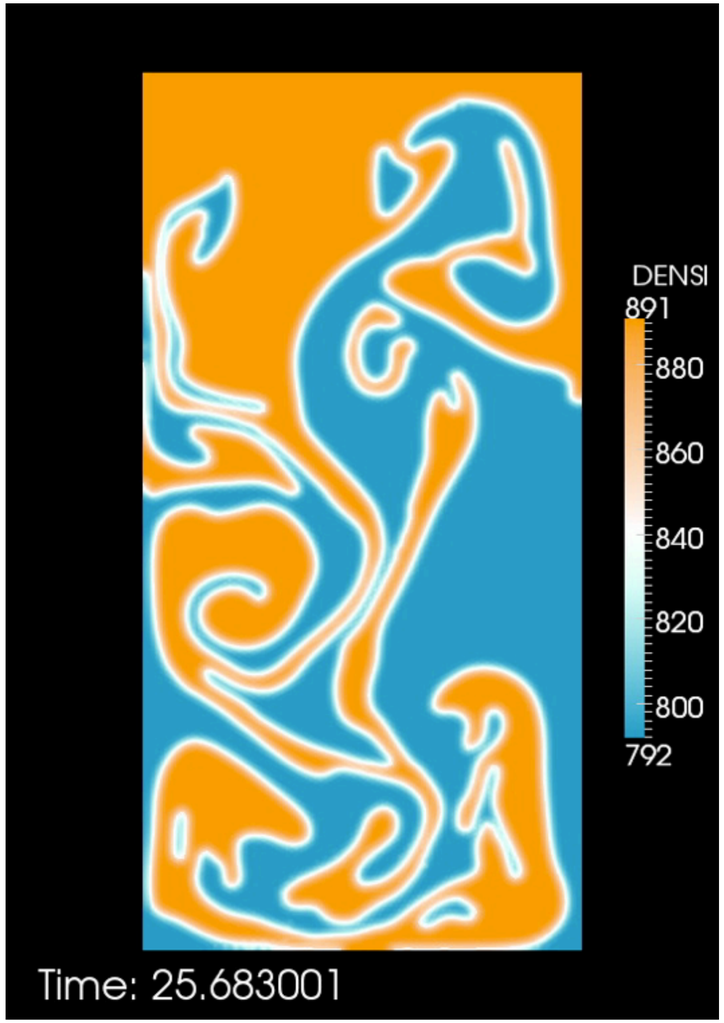


Alya

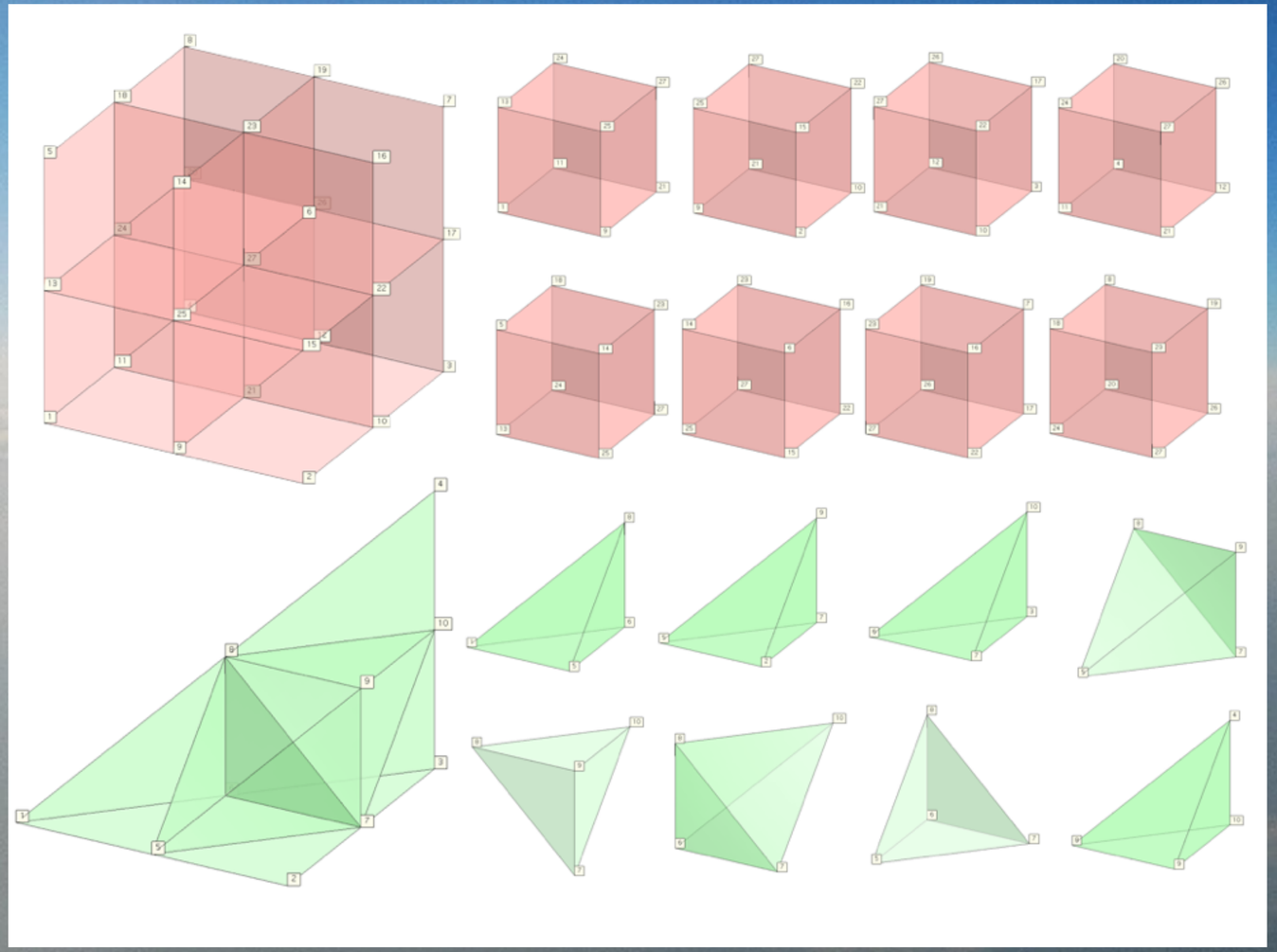
Parallel multi-physics code developed at BSC

Meshing and preprocess:

- Integrated meshing issues
  - Mesh multiplication
  - Implicit Chimera and overset meshes
  - Iris Mesh: octree mesh generator from cloud points
- Hybrid meshes



ALYA - Automatic DIVISOR

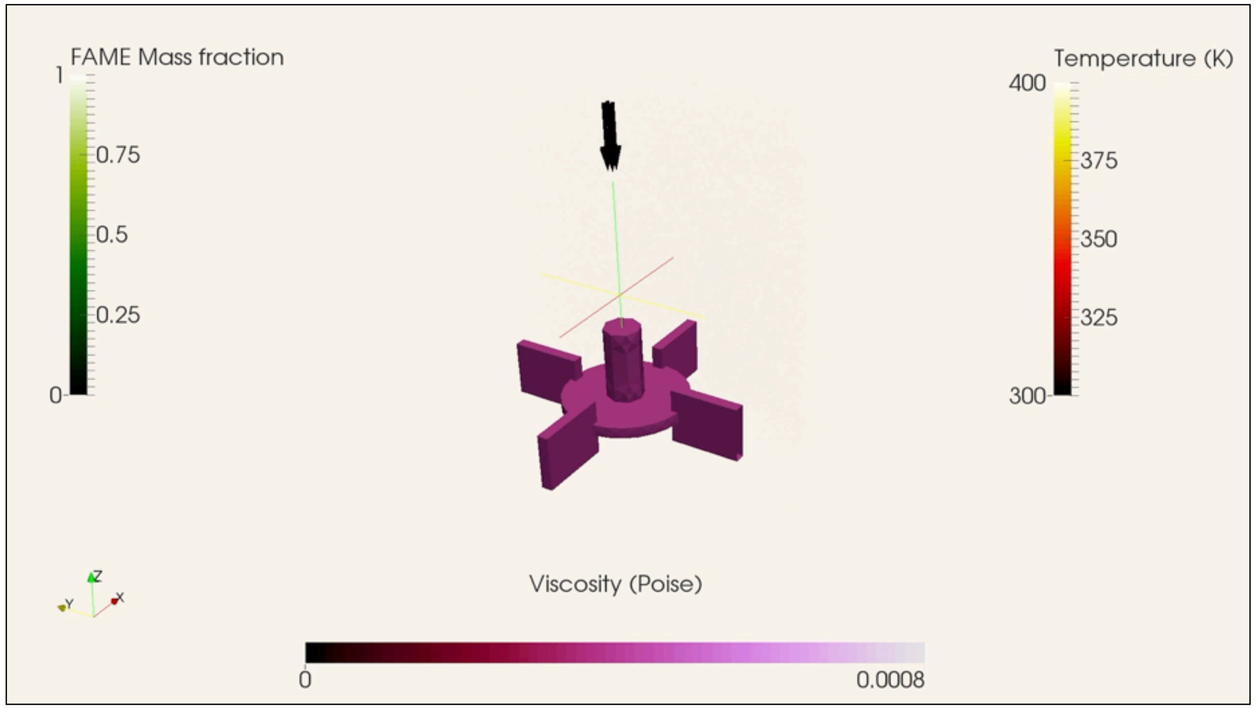


Guillaume Houzeaux, Raúl de la Cruz, Herbert Owen, and Mariano Vázquez. Parallel uniform mesh multiplication applied to a Navier- Stokes solver. *Computers and Fluids*

Alya

Parallel multi-physics code developed at BSC

Code features:



Born 2004

+- 700K code lines

+- 40 researchers

+- 10 organisations

Centralized SVN repository

Nightly test suites

One code, no multiple versions

Solvers in-house, no 3rd-party libraries (just METIS)

Main code architects: Guillaume Houzeaux and Mariano Vázquez

Lindgren (Sweden), Cray XE system at PDC, incompressible flow 12.288 CPU's (collaboration with Jing Gong from PDC)

Huygens, (The Netherlands), IBM power 6, incompressible flow, 2.128 CPU's

Jugene BG (Germany): 16.384 CPU's, incompressible flow (Prace project for Mesh multiplication) and, running first tests of FSI in collaboration with Paolo Crosetto (Julich)

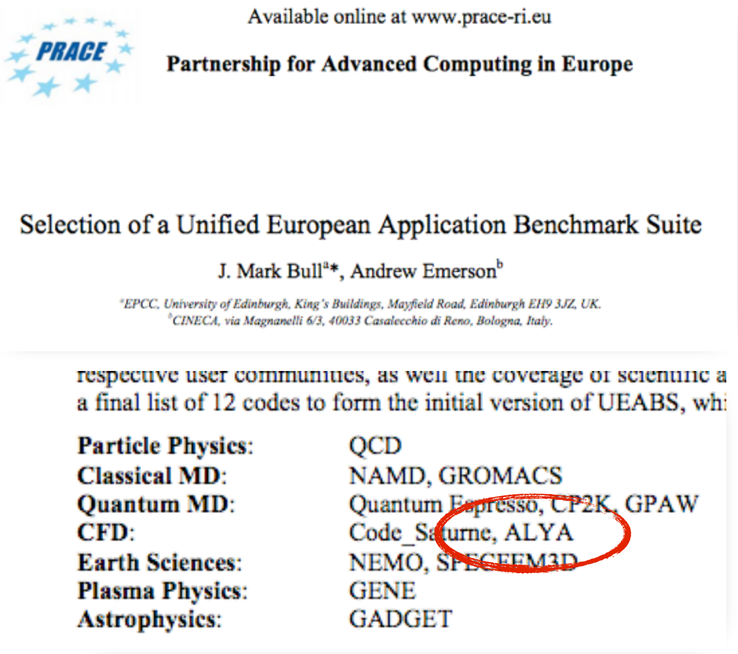
Fermi BG (Italy): 16.384 CPU's, incompressible flow + species transport + Lagrangian particles (Prace project for nose)

Curie Bullx (France): 22.528 CPU's, incompressible flow (collaboration with Jing Gong - PDC)

Marenostrum: 5.000 CPU's compressible flow, incompressible flow, thermal flow (scalability test)

superMUC (Germany): 125.000 CPU's, incompressible flow & combustion

NCSA Blue Waters (USA): 100.000 CPU's, incompressible flow & combustion, electromechanics cardiac coupling



Available online at www.prace-ri.eu

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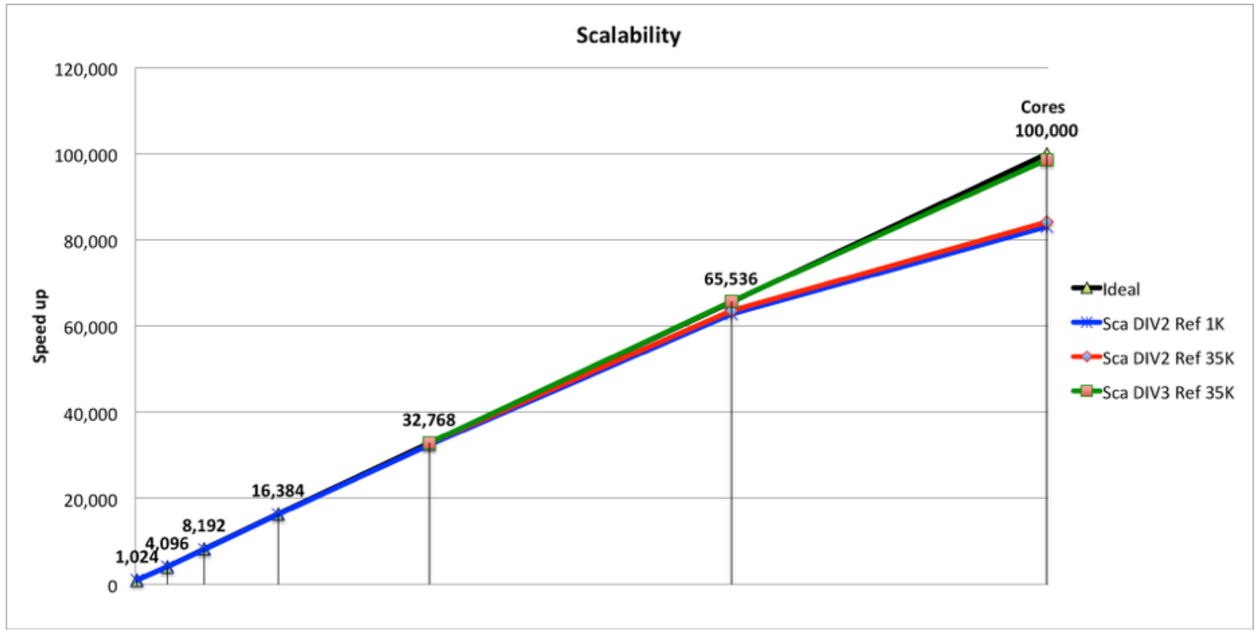
[b]CINECA, via Magnanelli 6/3, 40033 Casalecchio di Reno, Bologna, Italy.

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

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

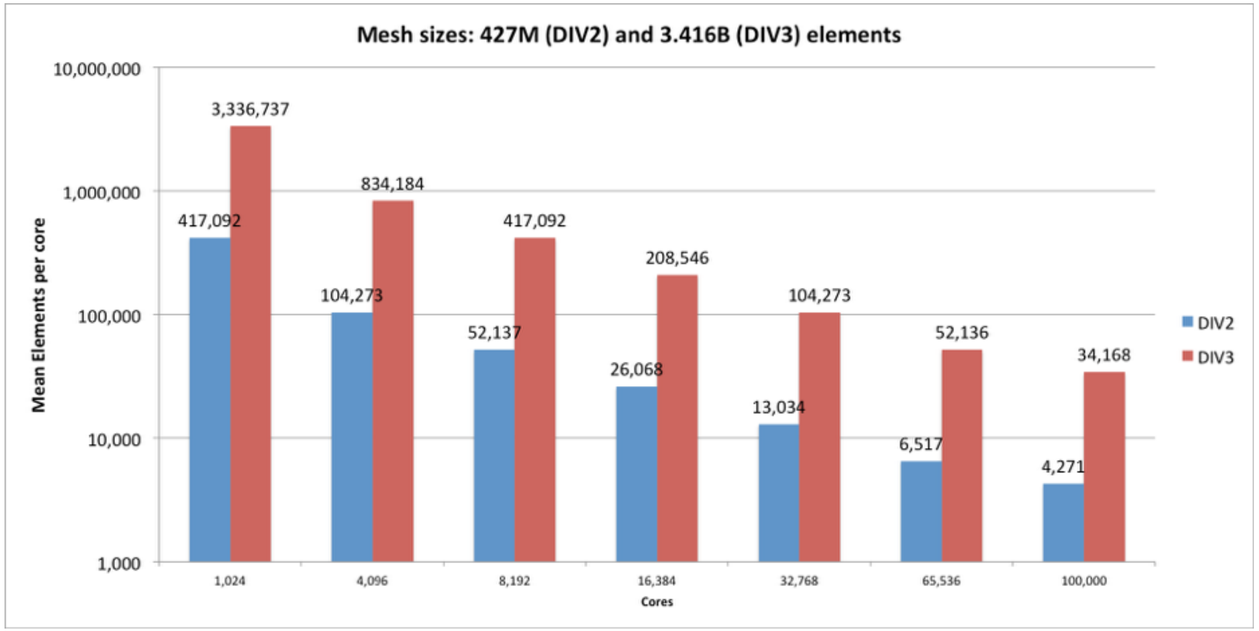


Multi-physics cardiac electromechanical model

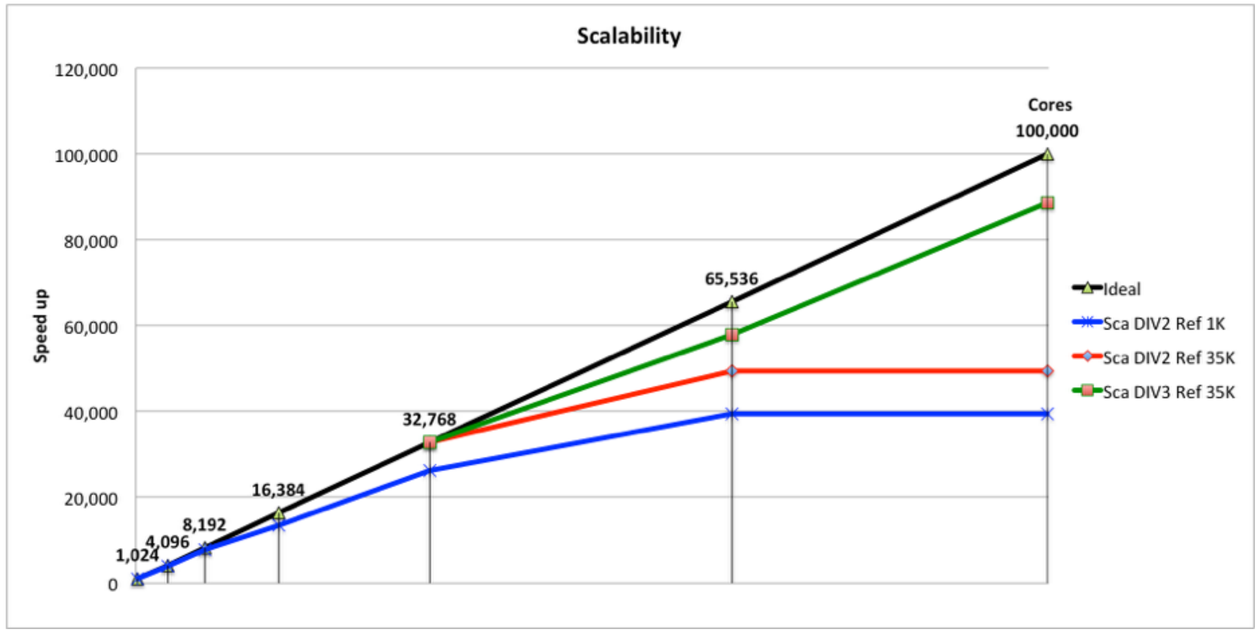
3.5B tetrahedra

Explicit solvers

100K cores Blue Waters



Collaboration project with Seid Koric NCSA



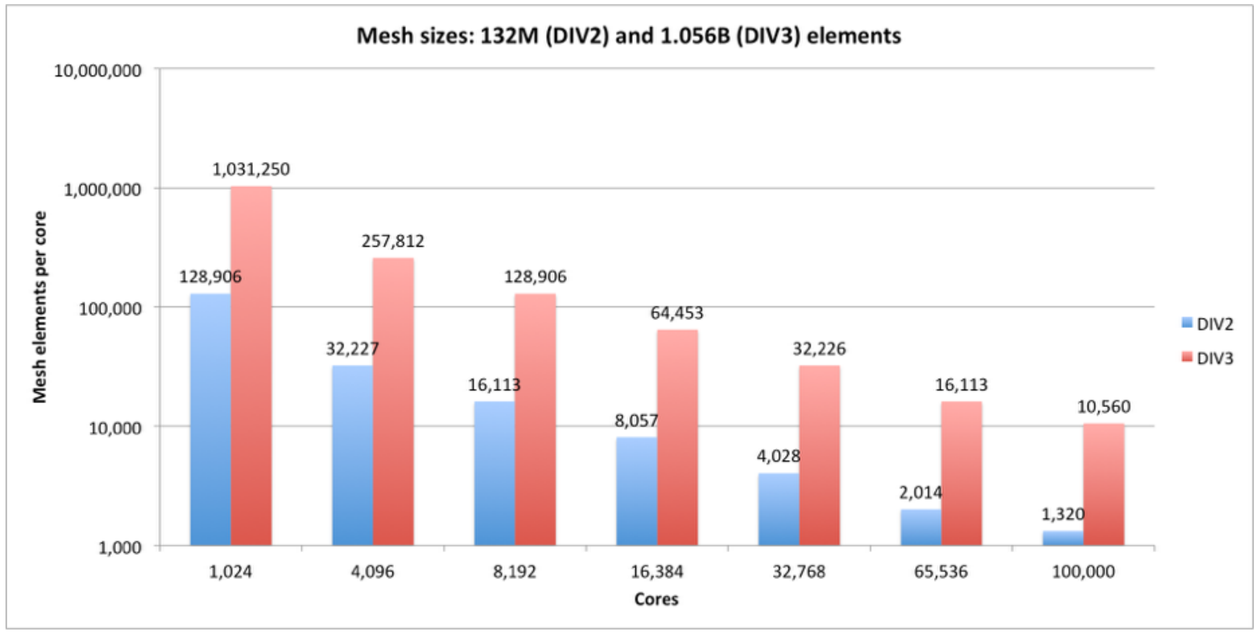
Multi-physics simulation of a kiln

Combustion - low Mach Navier Stokes

Implict solvers

4.2B tetrahedra

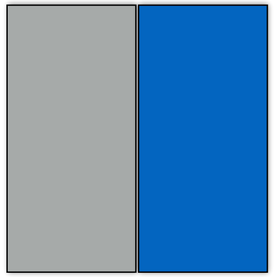
100K cores Blue Waters



Collaboration project with Seid Koric NCSA

Defining parallel multi-physics coupling

Very generally speaking and to fix ideas..



Contact domains:

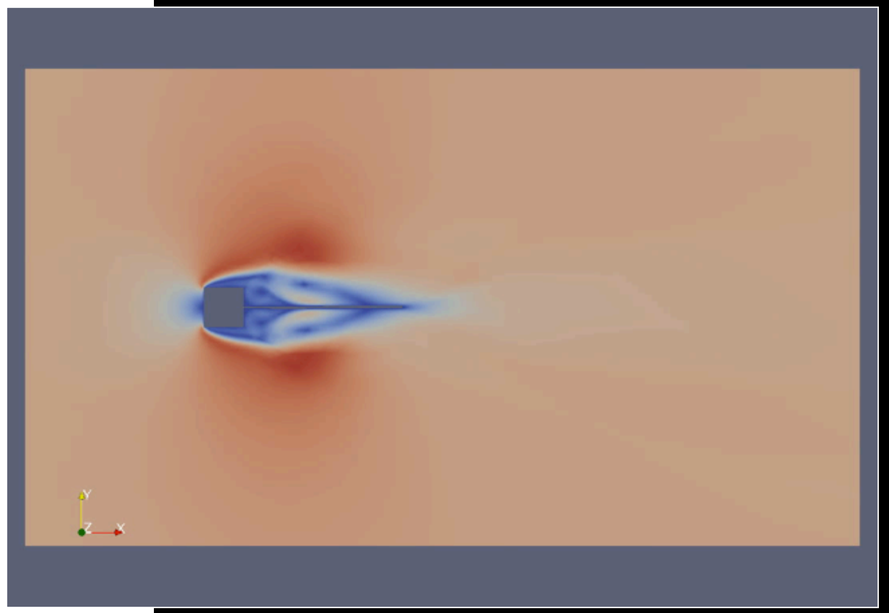
Fluid-structure interaction

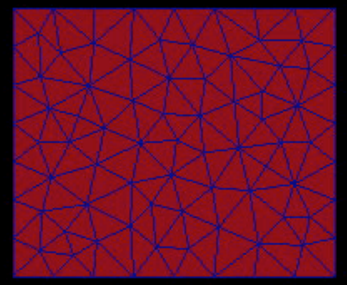
Contact and impact problems

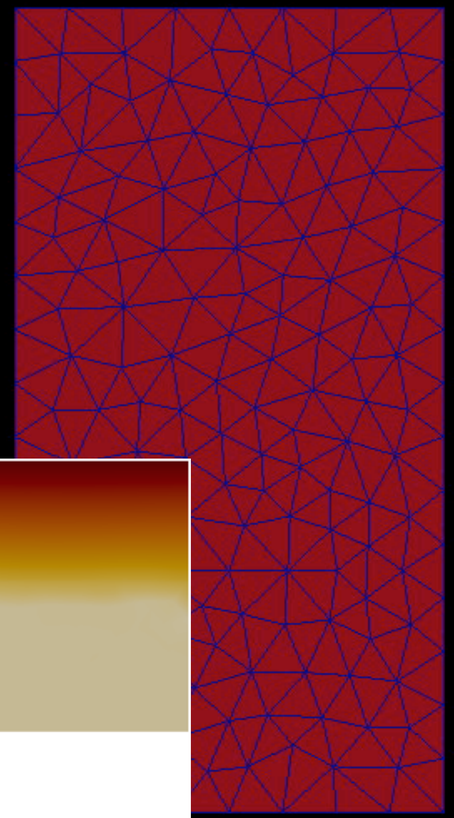
N-bodies collisions

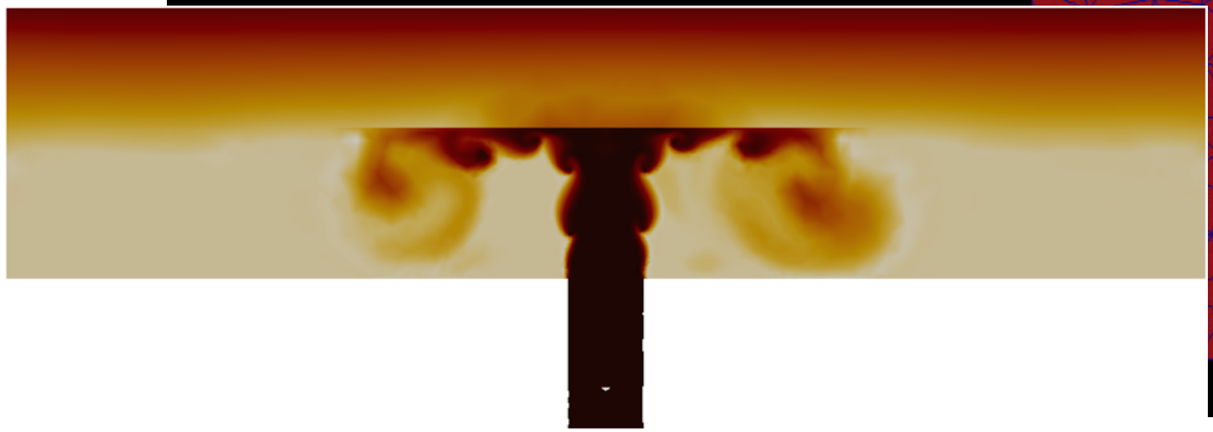
Heat transfer

Meshes can/cannot coincide

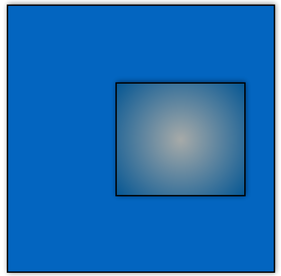








Very generally speaking and to fix ideas...



Overlapping domains:

Overset meshes and Chimera

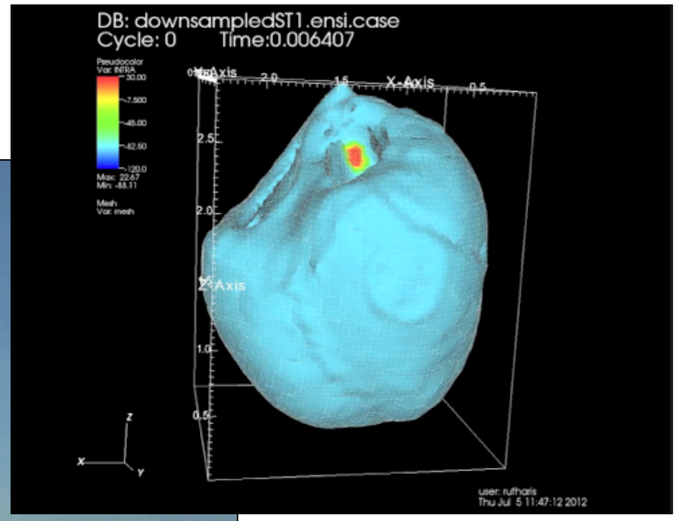
Electromechanical cardiac model

RANS modelled turbulence

Multi-scale problems

Particles and immersed bodies

Meshes can/cannot coincide



Issues

Coupling connectivity among MPI tasks

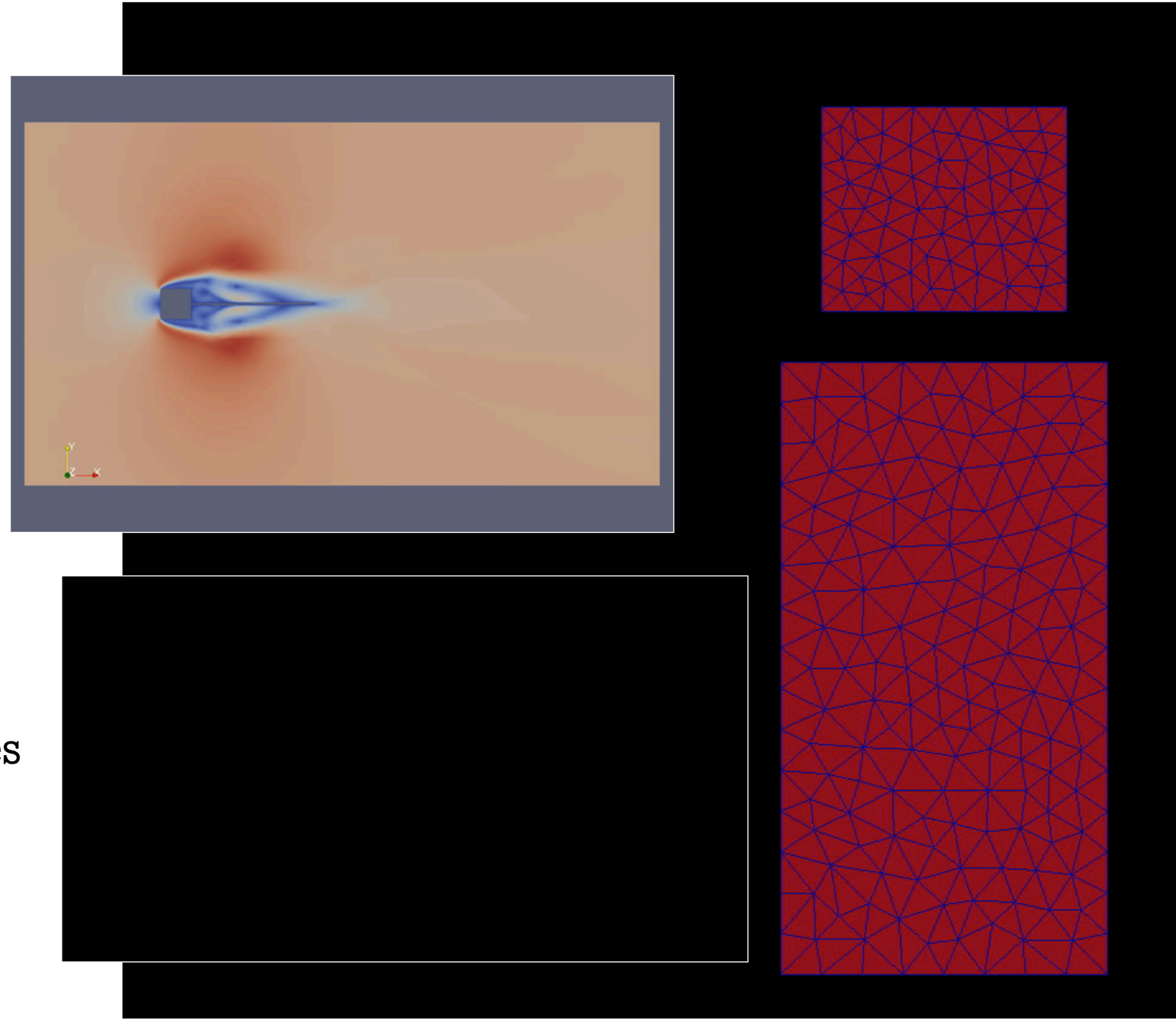
Numerically stable coupling algorithms

Preconditioners for the coupled scheme

Time-scale disparity

Synchronous/Asynchronous schemes

Coupling different codes (multi-codes)

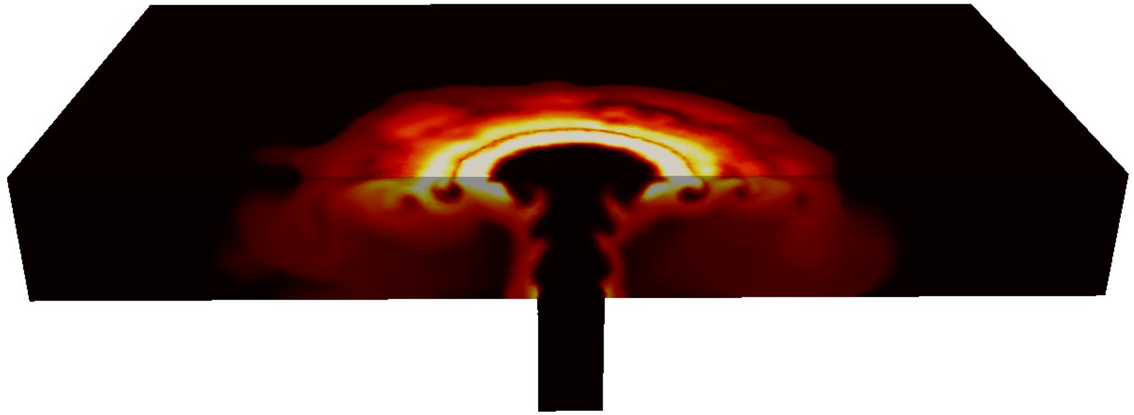


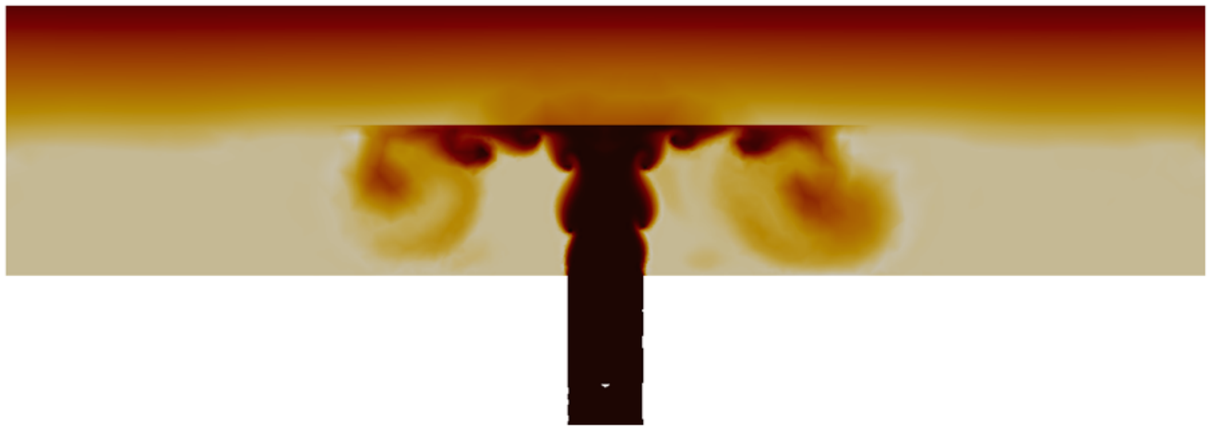
Alya

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)

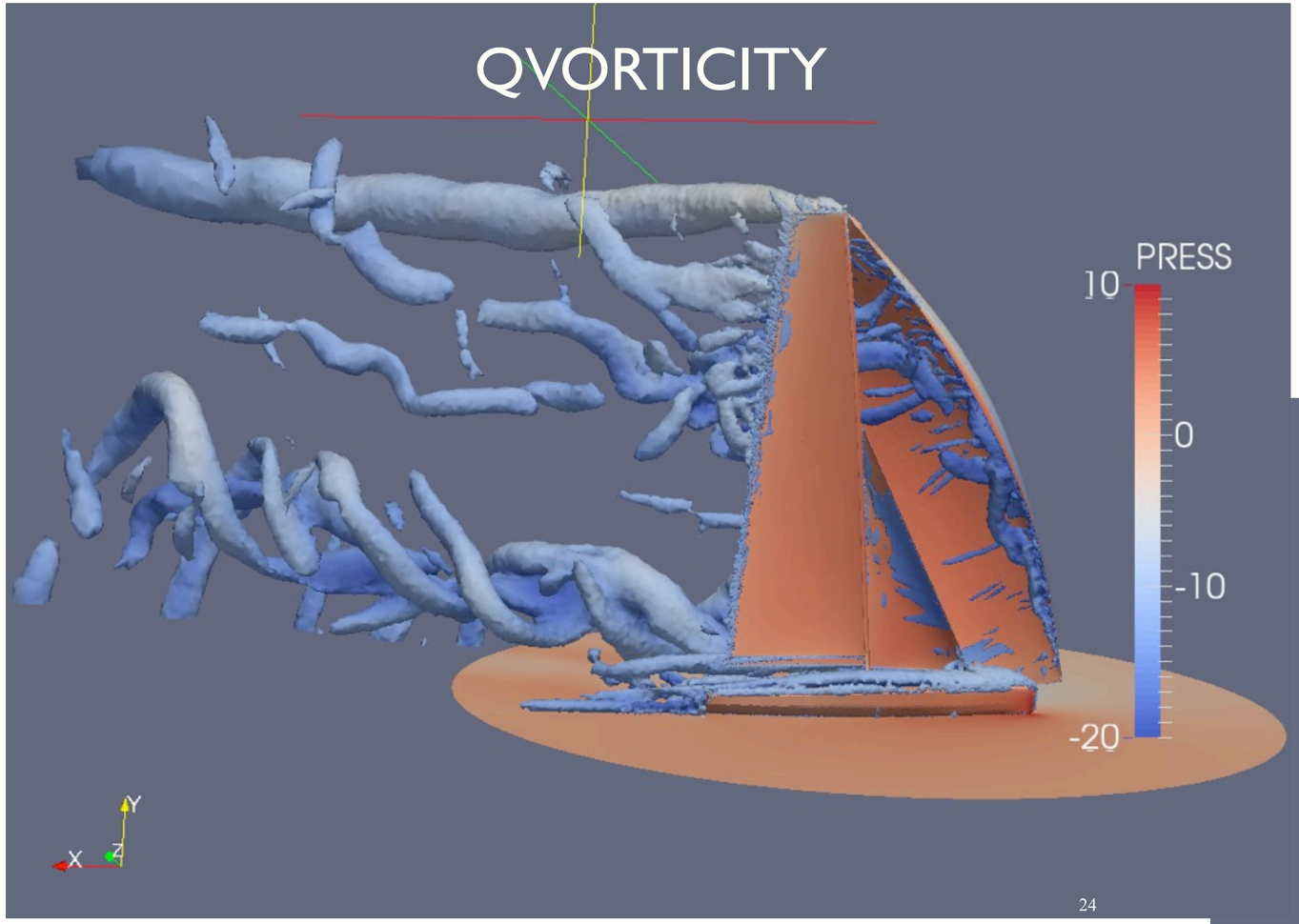


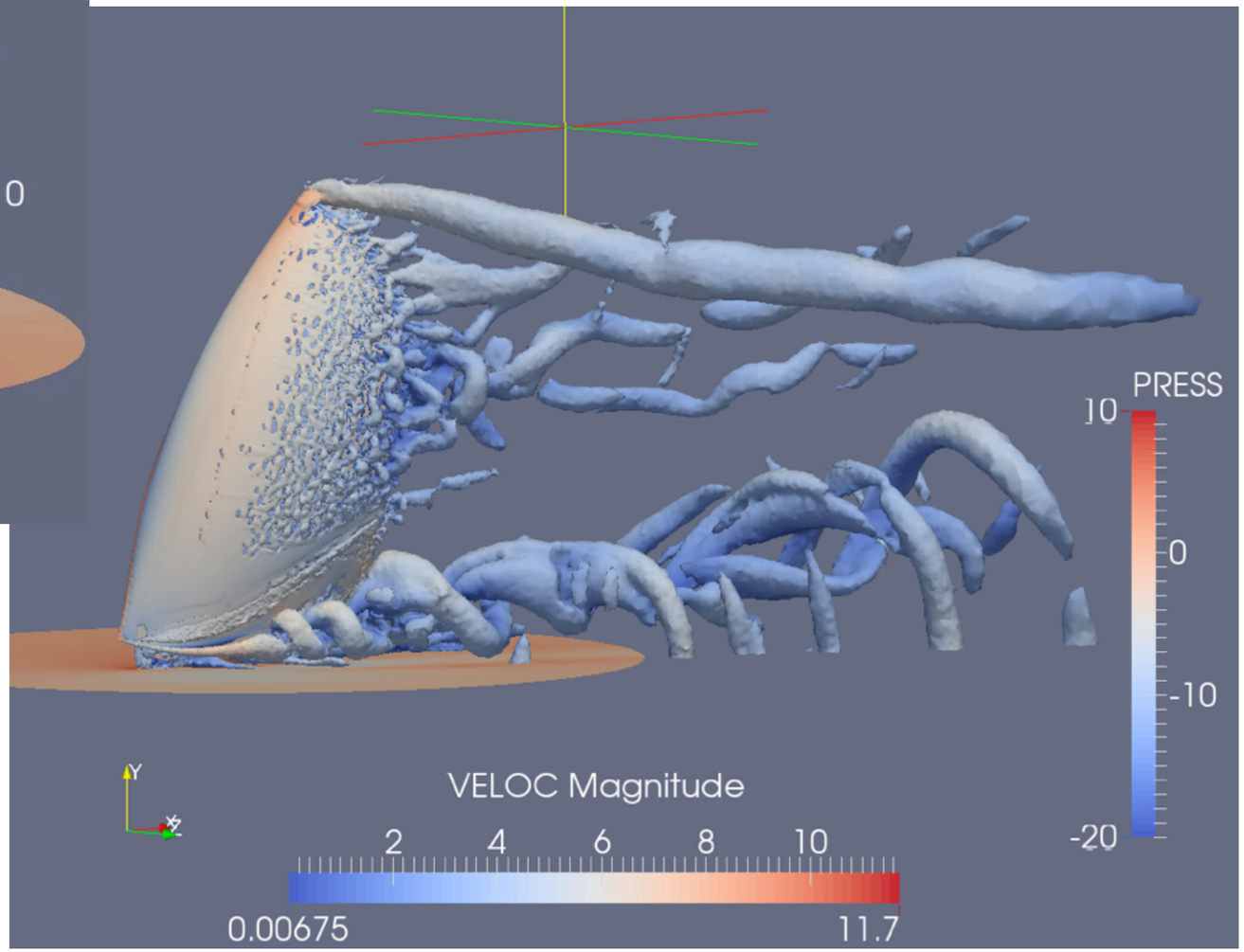


Simulations for Industry

Aerodynamics of vehicles

LES TURBULENCE MODELING FOR RACE BOAT SAILS





BASIC RUN DATA

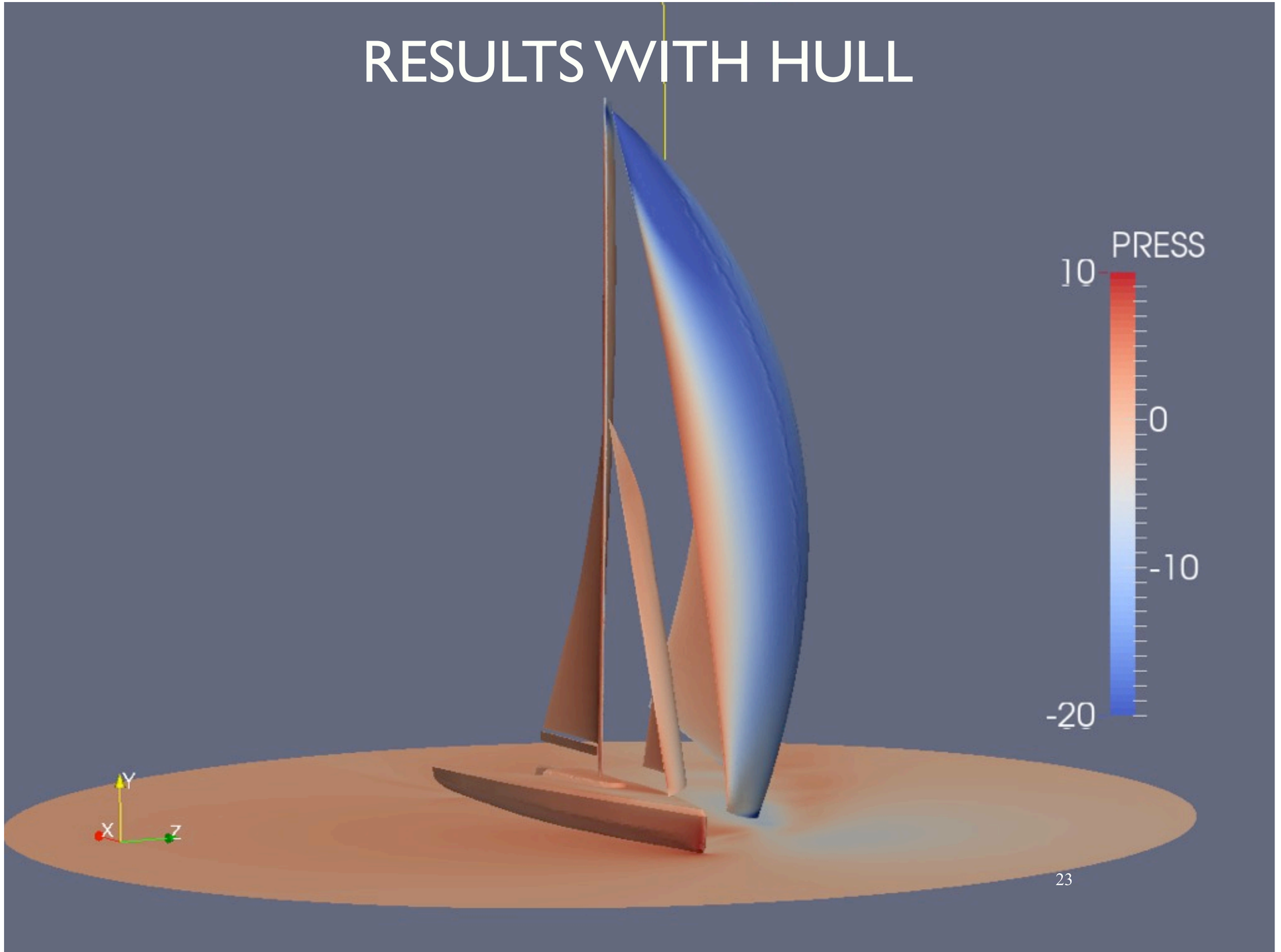
MESH: 6M Nodes & 33M Elements
Tetrahedras, prisms and pyramids

TIME STEP SIZE = 0.005 sec.

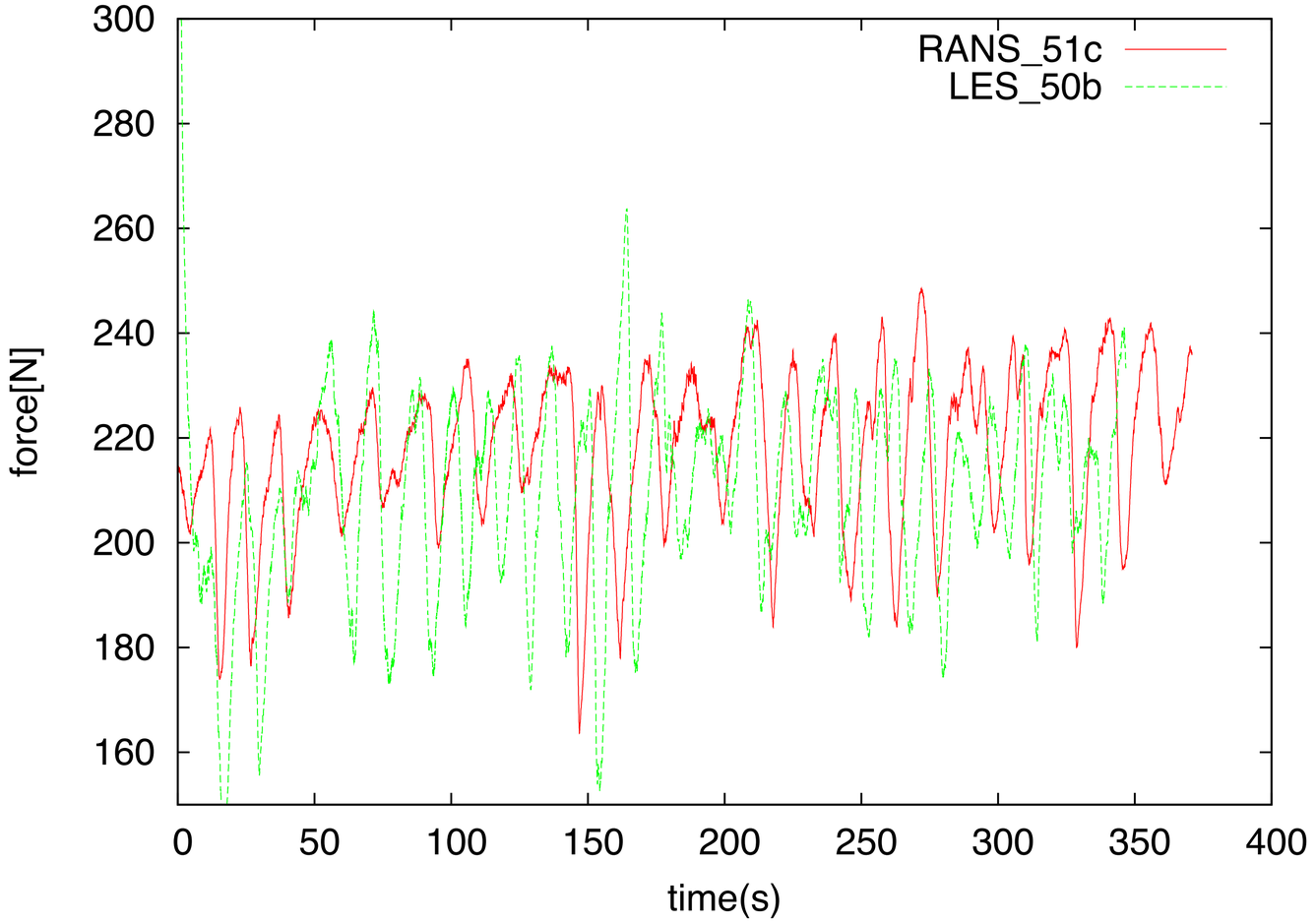
NUMERICAL METHOD: Variational Multiscale Stabilized Finite Element Method implemented in the code ALYA

LES MODEL: WALE by Nicoud

RESULTS WITH HULL



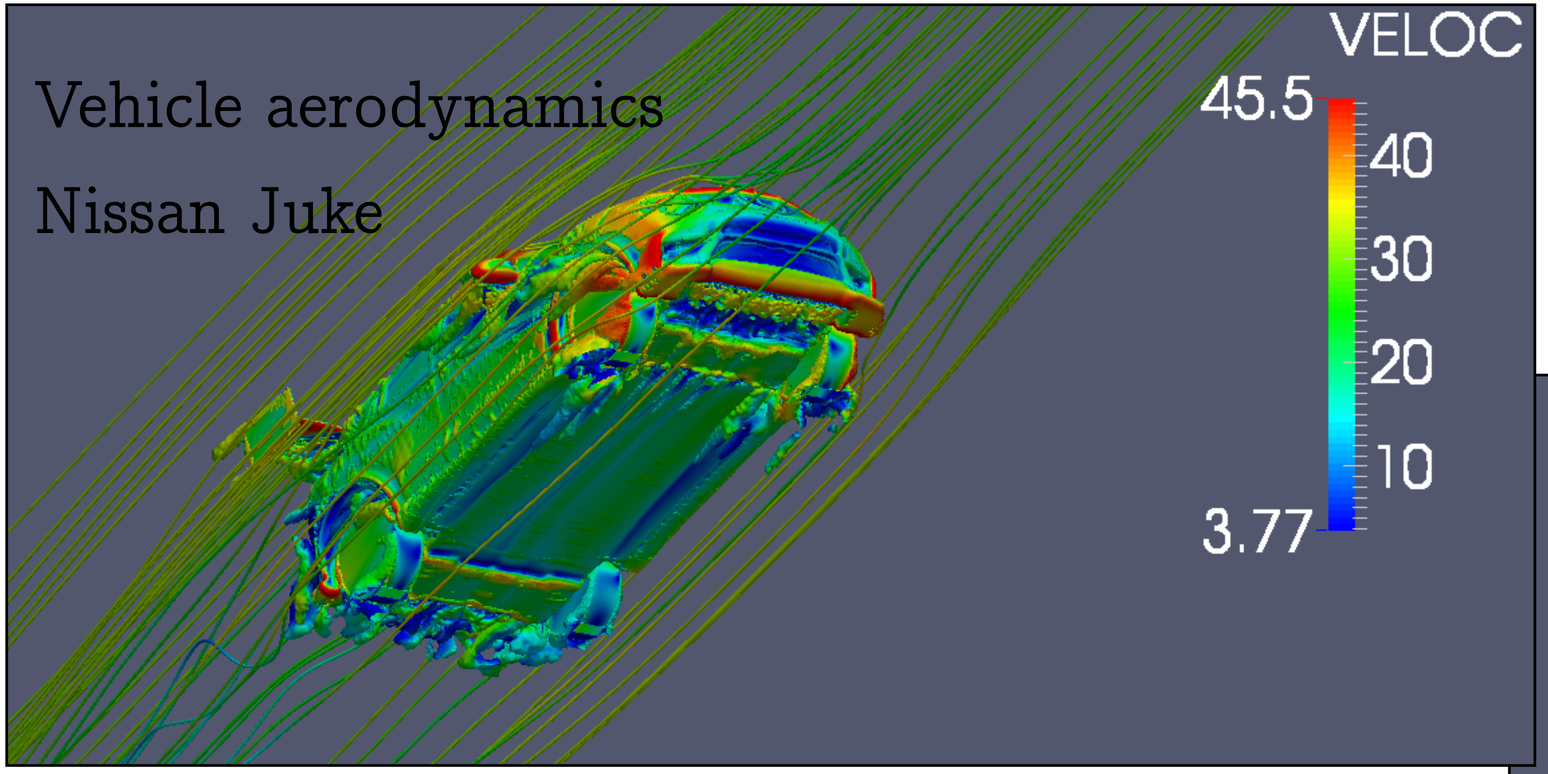
Forces on the sails



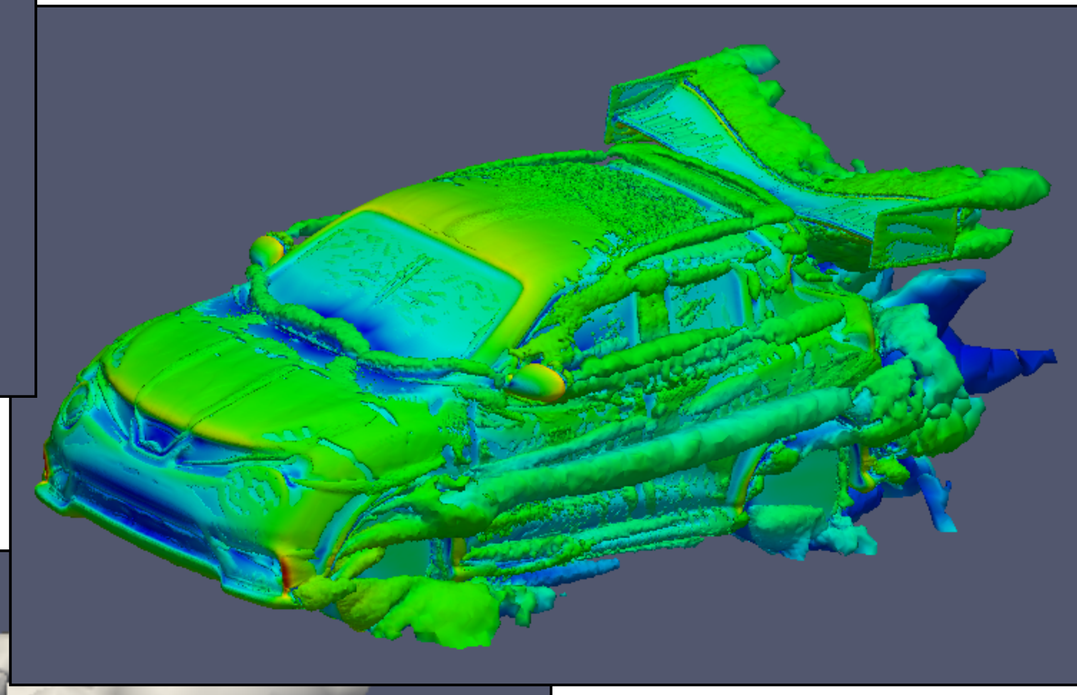
Main

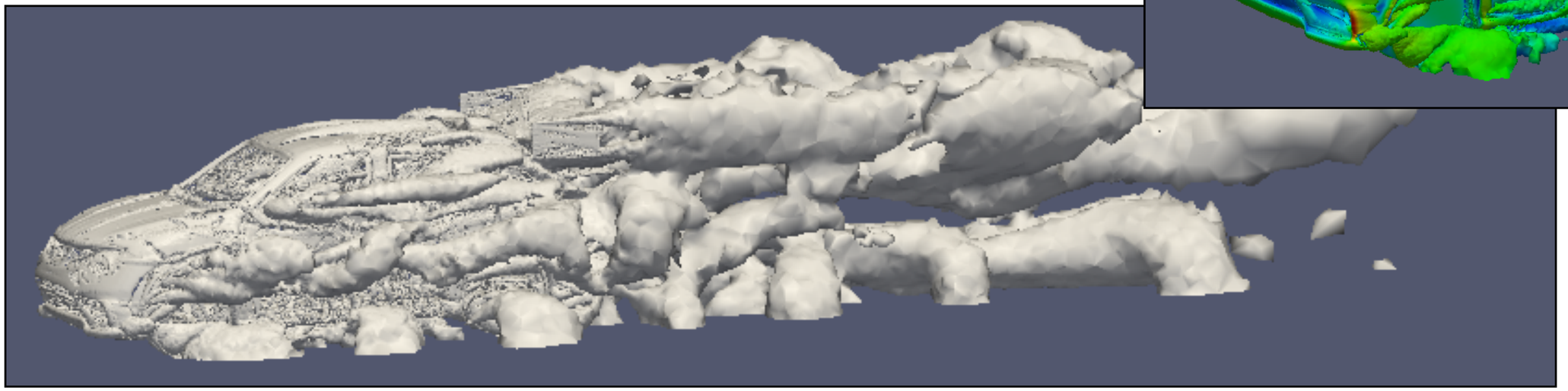
Vehicle aerodynamics

Nissan Juke



Spoiler force





Multi-physics:

Chemical reactions and Combustion

Motivation

Compressible flow

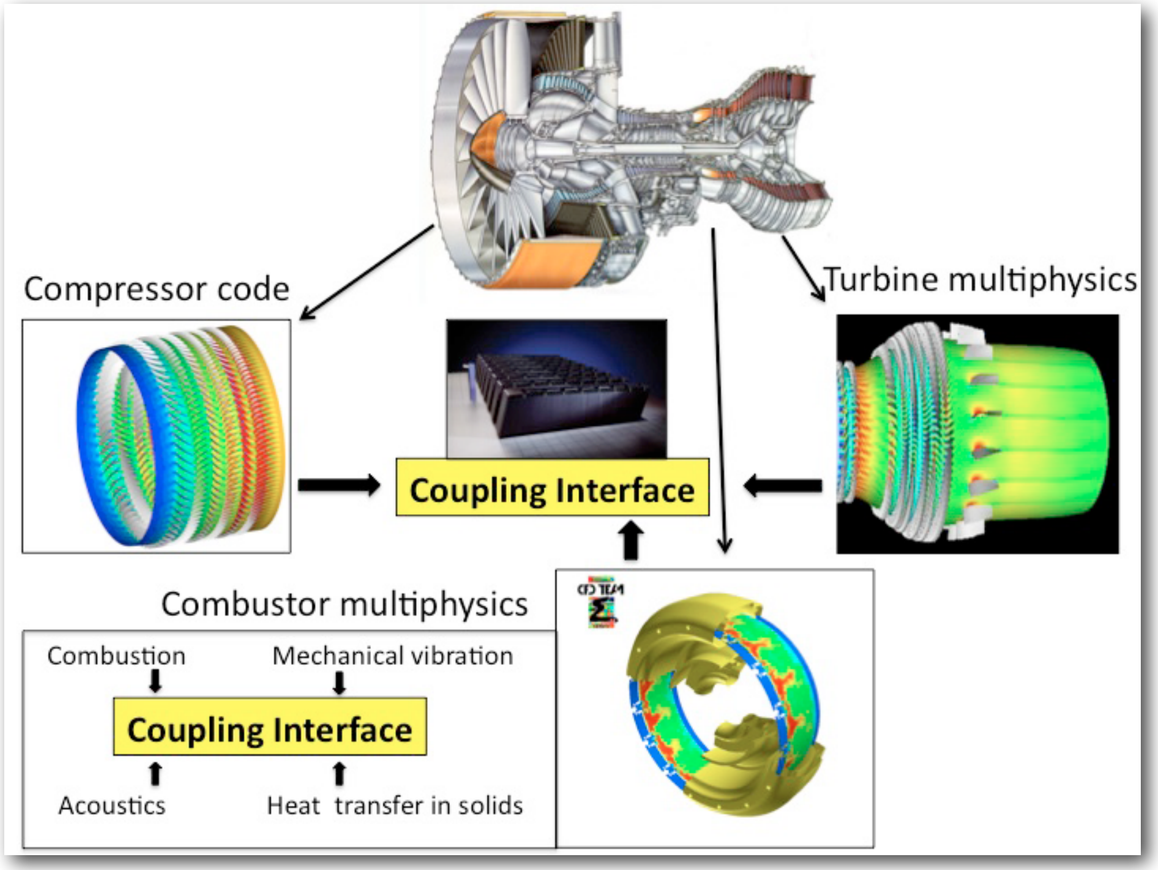
Turbulence

Multi-species flow

Combustion

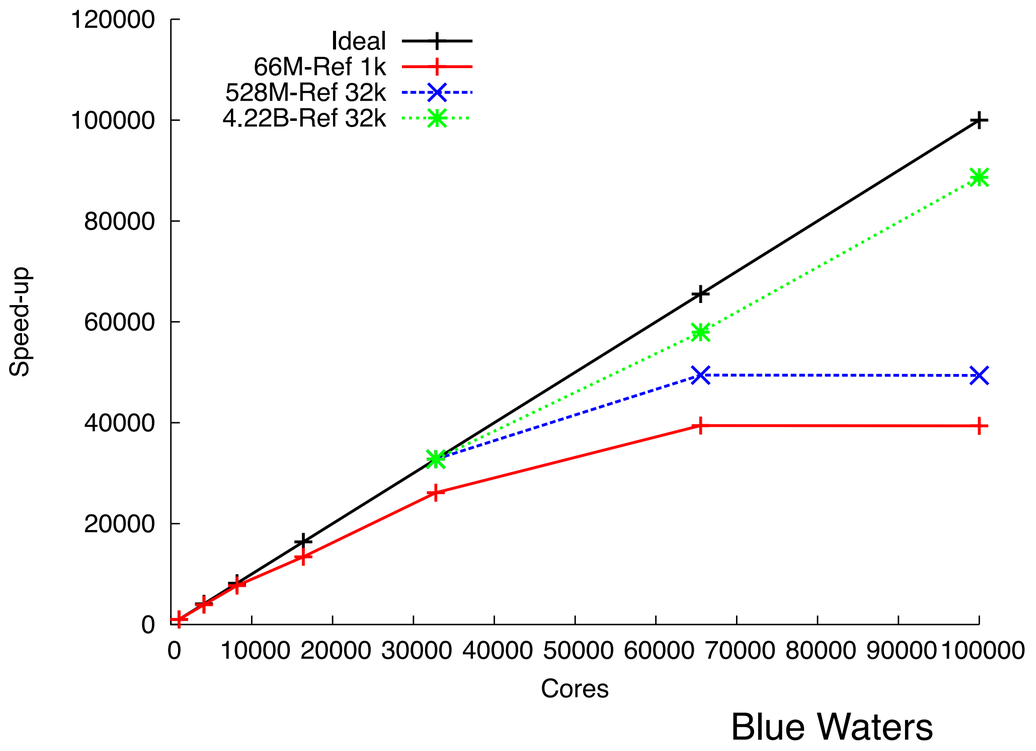
Heat transfer

Aeroelasticity

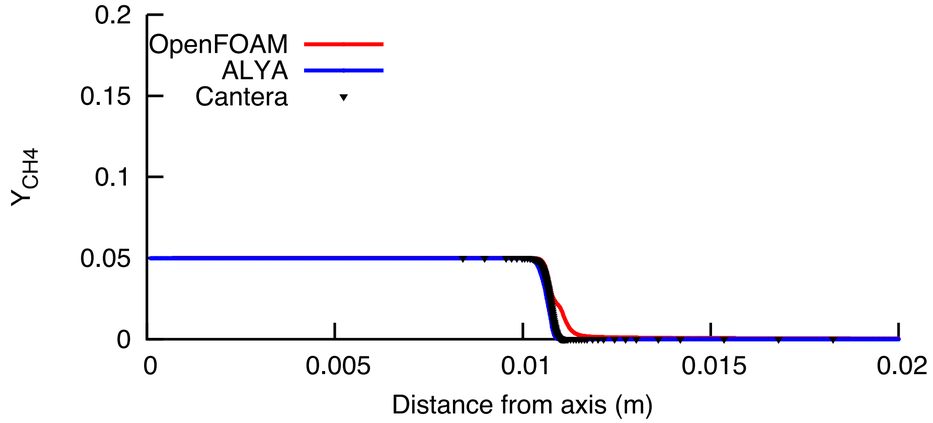


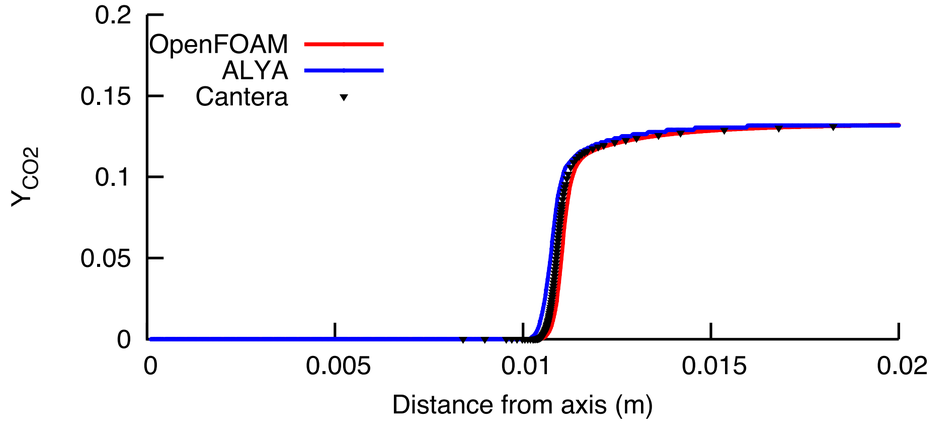
Modelling approach summary

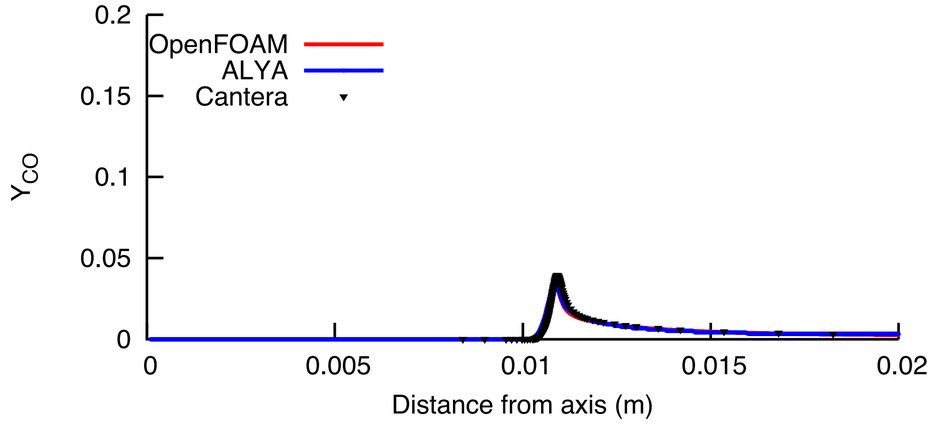
- Low-Mach/compressible
- Finite-rate kinetics:
  - Dynamic Thickened Flame Model
- Tabulated chemistry
  - CFI combustion model (FGM-based)
  - Manifold $\phi\left(\widetilde{c}, \widetilde{c''^2}, \widetilde{f}, \widetilde{f''^2}, h\right)$
- Premixed/Non-premixed & partially premixed combustion
- RANS/LES formulation
- Conjugate-heat transfer (CHT) coupling (cooling, heat losses, thermal stresses)

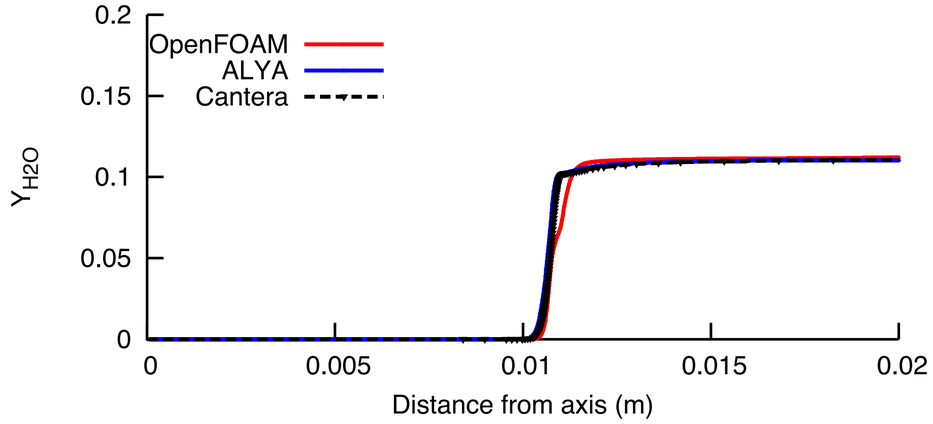


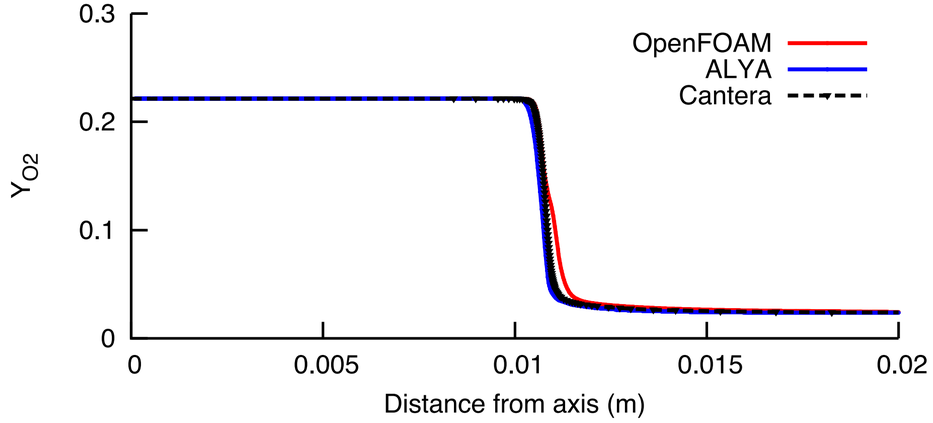
VALIDATION OF 1D LAMINAR FLAME AGAINST OPENFOAM

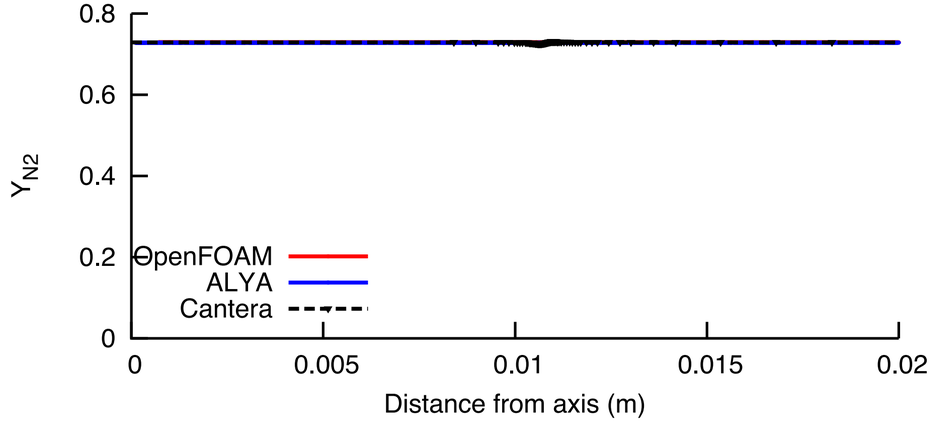






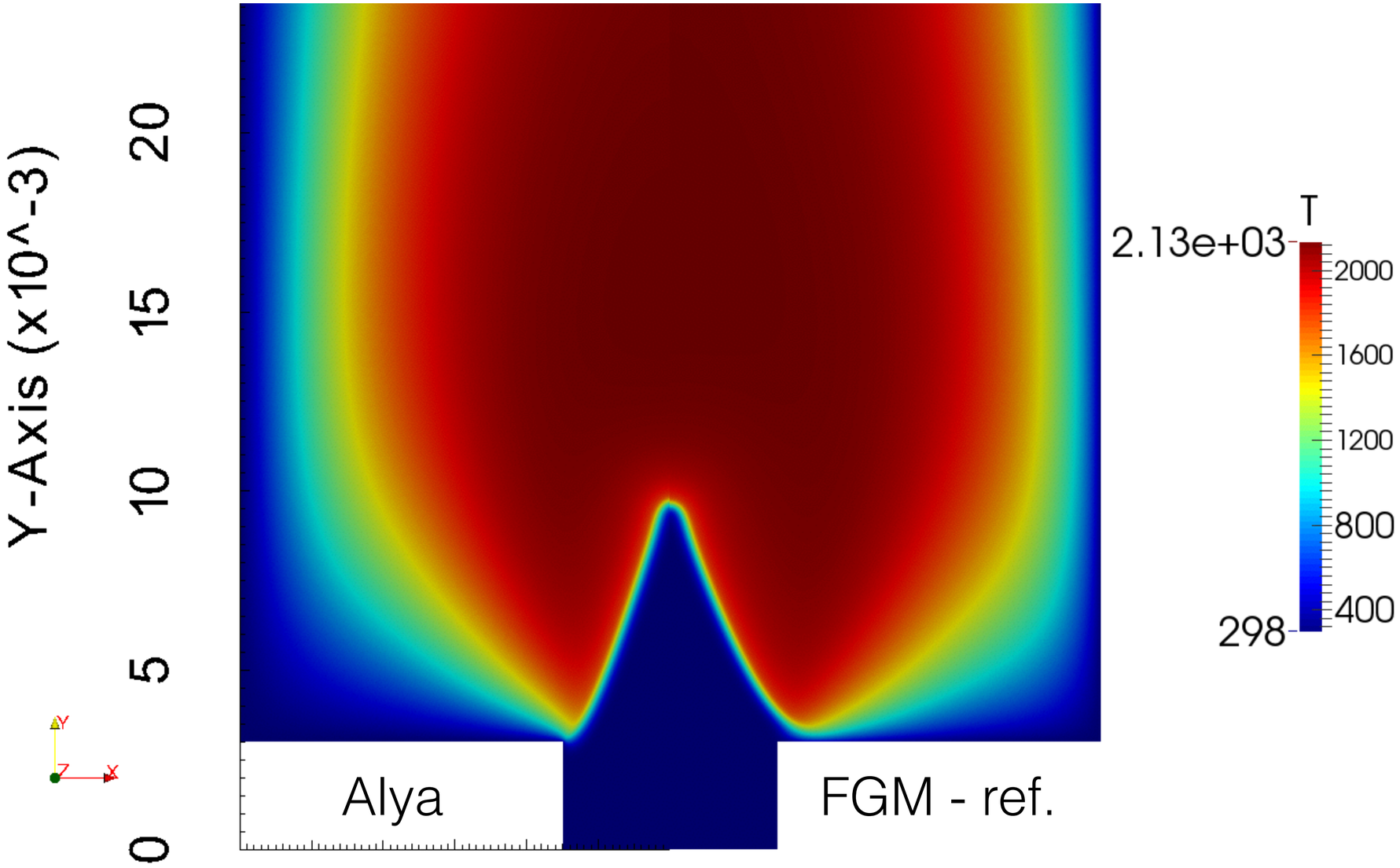




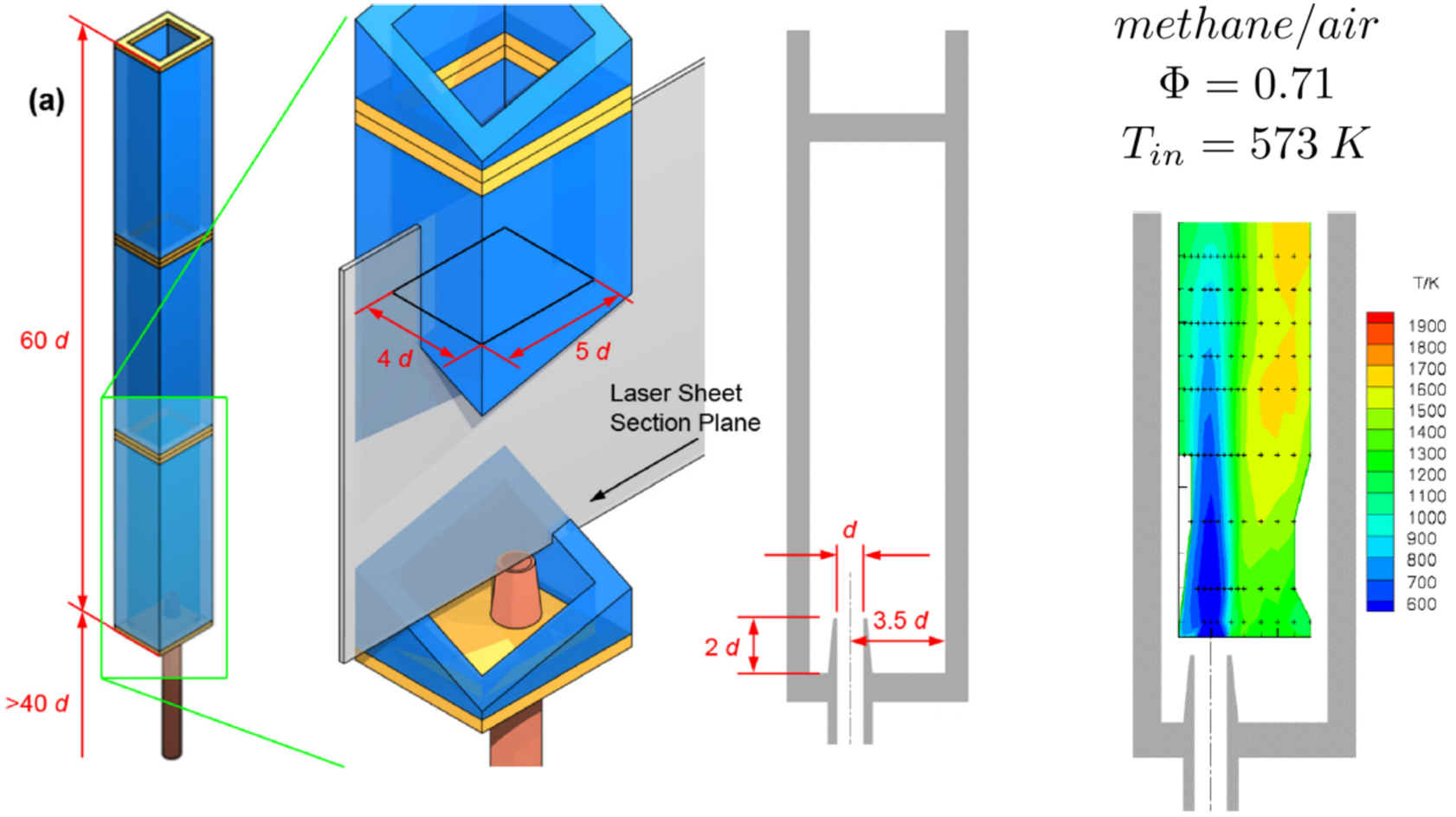


2D LAMINAR FLAME

2D bunsen flame: T=298K, ER=0.9, p=1bar, Le=1

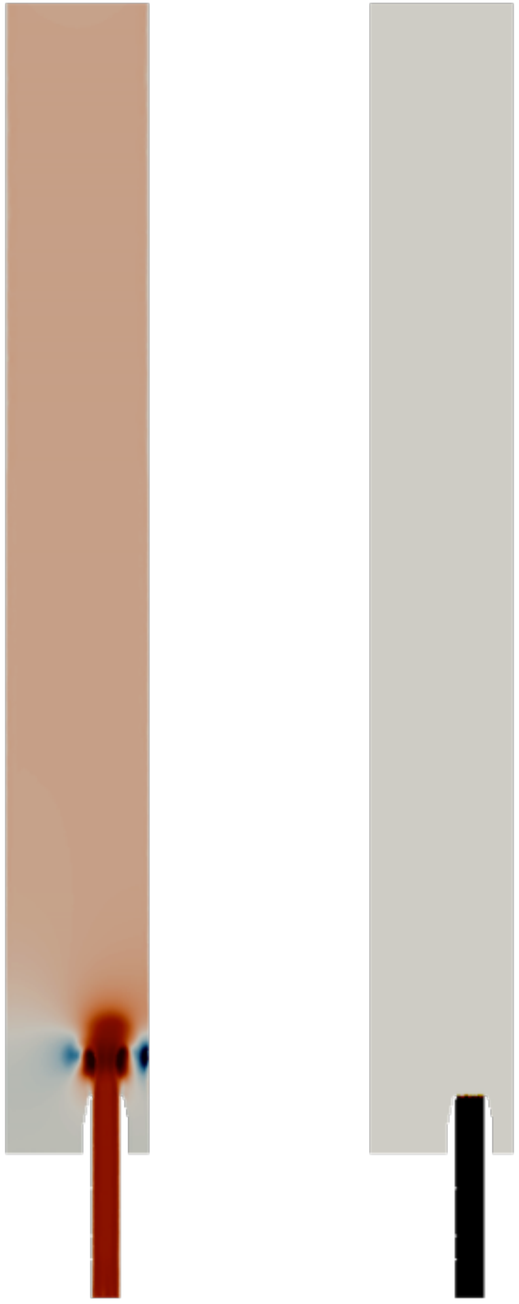


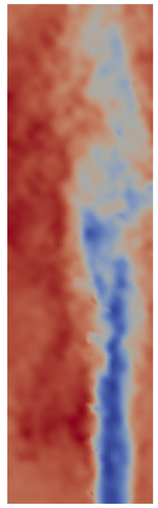
FLOX® combustor - DLR **Turbulent Flame**



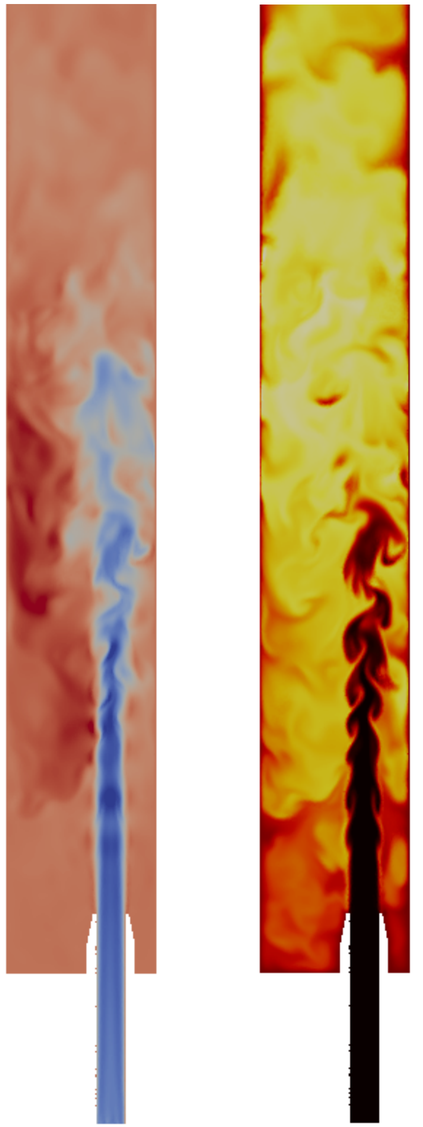
O. Lammel et al., *J. Eng. Gas Turbines Power,* 2012

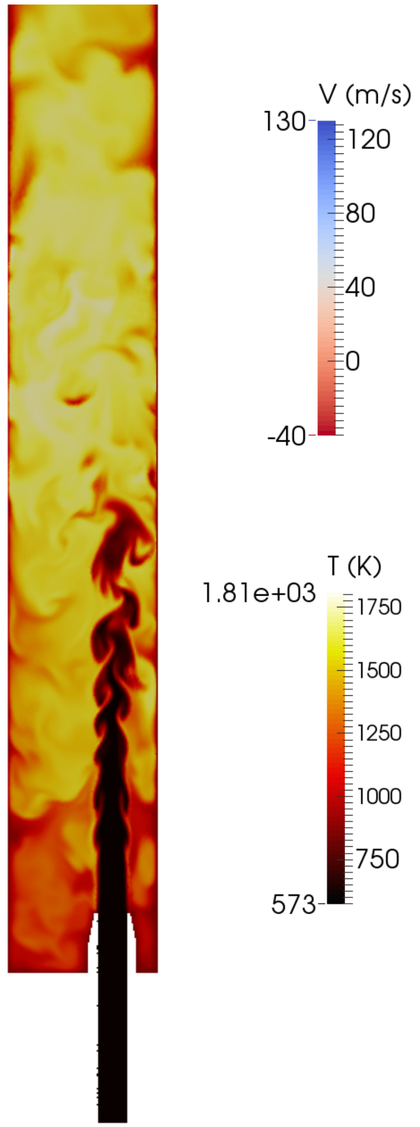
FLOX® combustor - DLR





Experiments

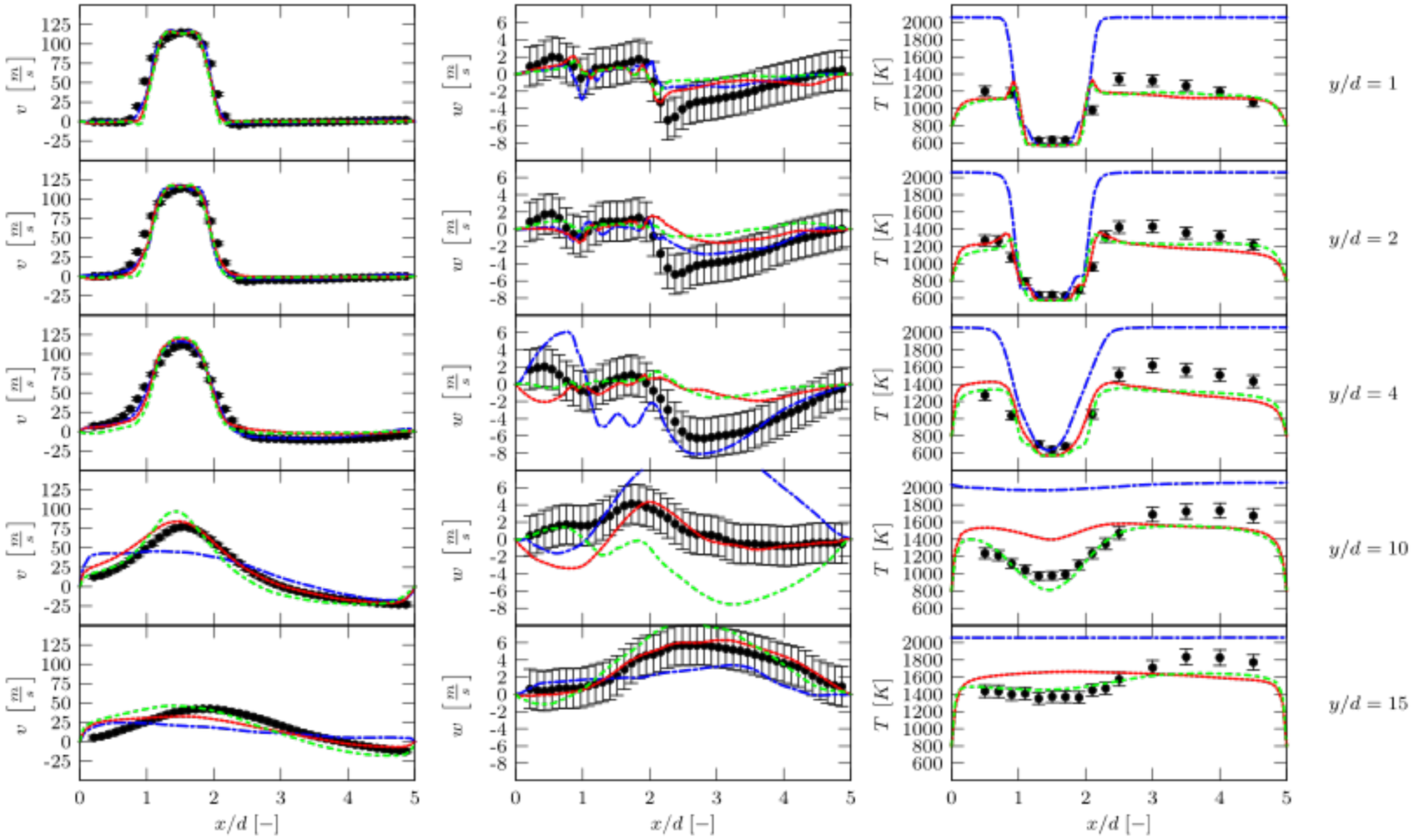




Alya - LES-CFI Combustion Model

FLOX® combustor - DLR

Validation LES

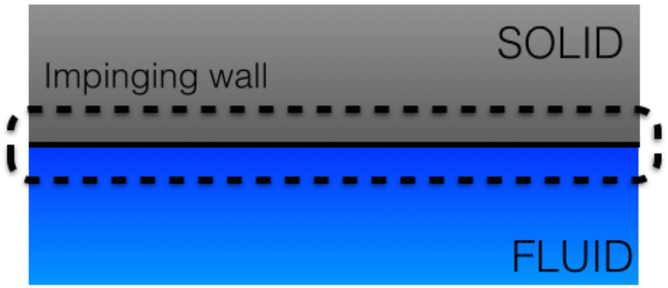


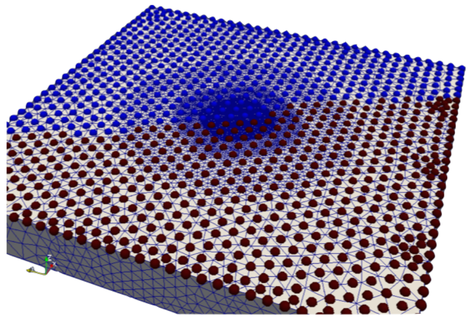
Profiles of time-averaged axial and transversal velocity and temperature for the LES simulations (dots: experiments, red: non-adiabatic, green: non-adiabatic with heat loss in chemistry).

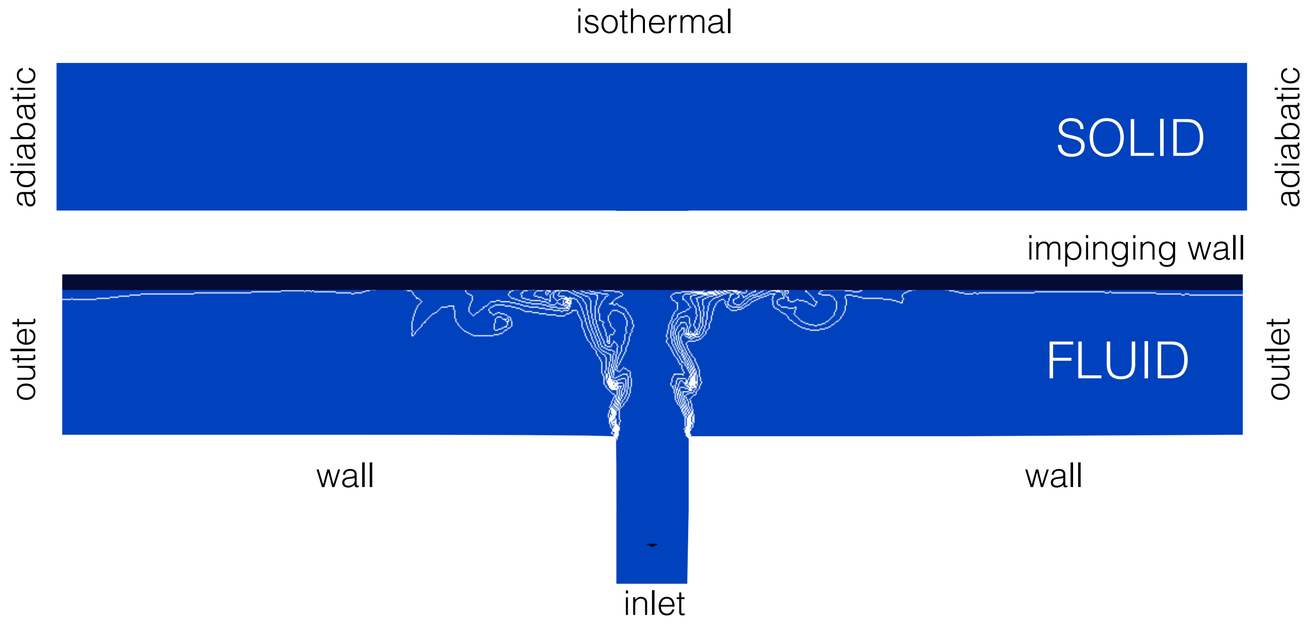
Turbulent flames

Impinging flames with conjugate-heat transfer

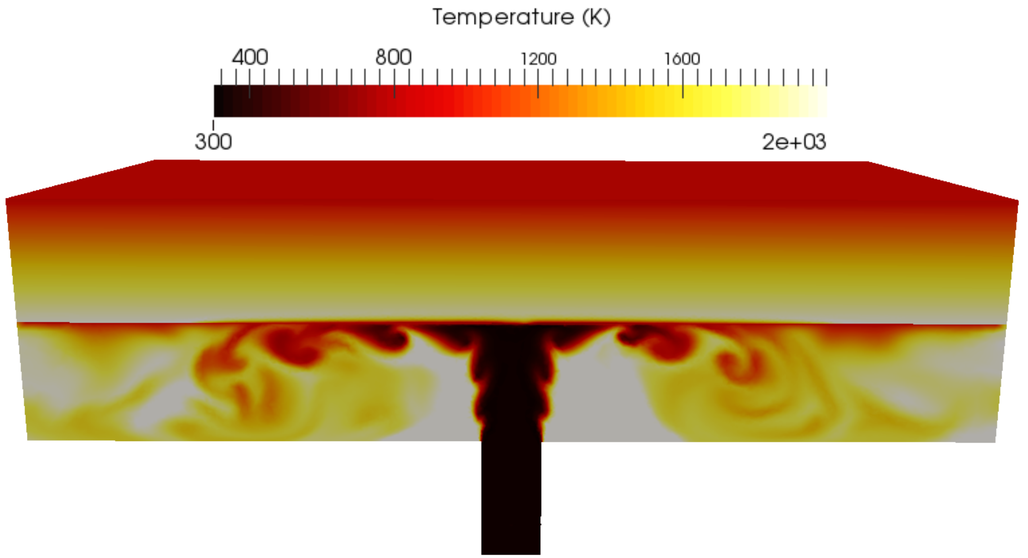
Configuration setup

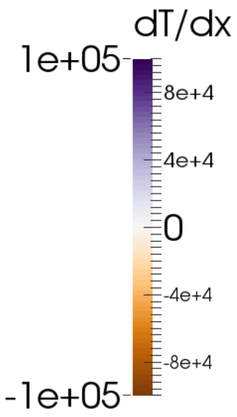


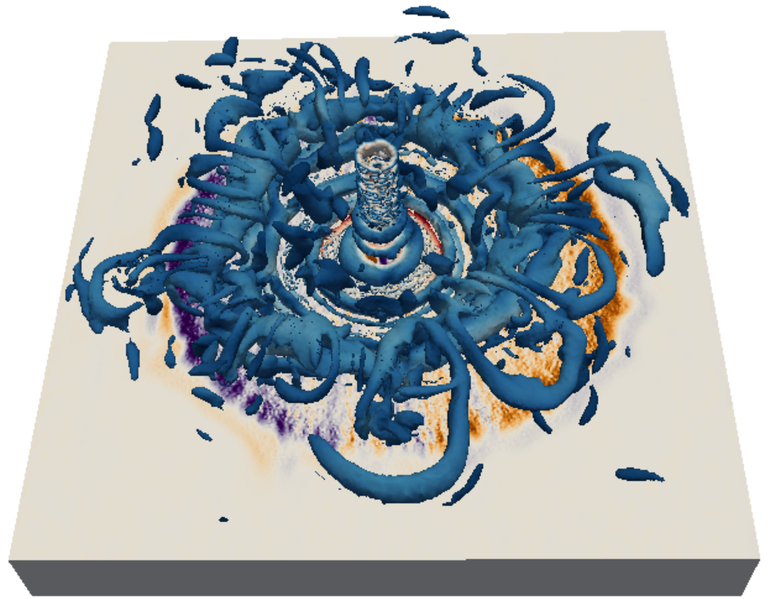




LES-CHT coupling for an impinging flame







(Ongoing work)

Turbulent flames

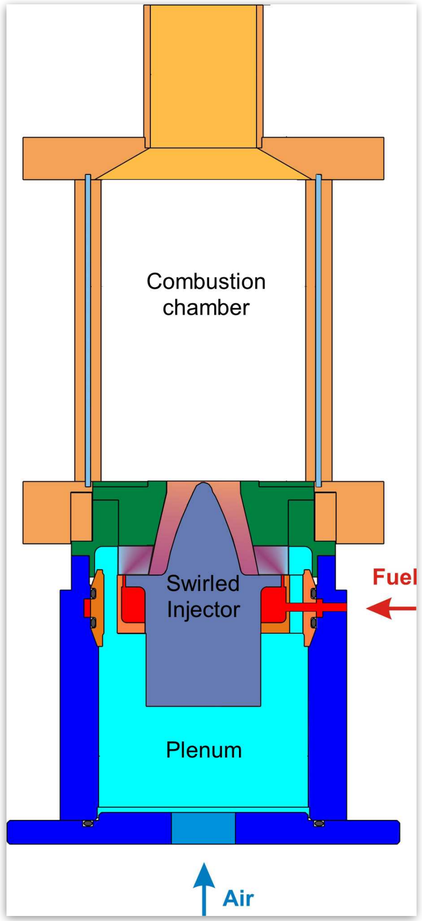
PREdiction and **C**ontrol of **C**ombustion **INSTA**bilities in Industrial Gas Turbines (**PRECCINSTA**)

Collaboration with:
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*
B. Cuenot and L.Y. Giquel, *Combustion Group, CERFACS*

UNIVERSITY OF TWENTE.

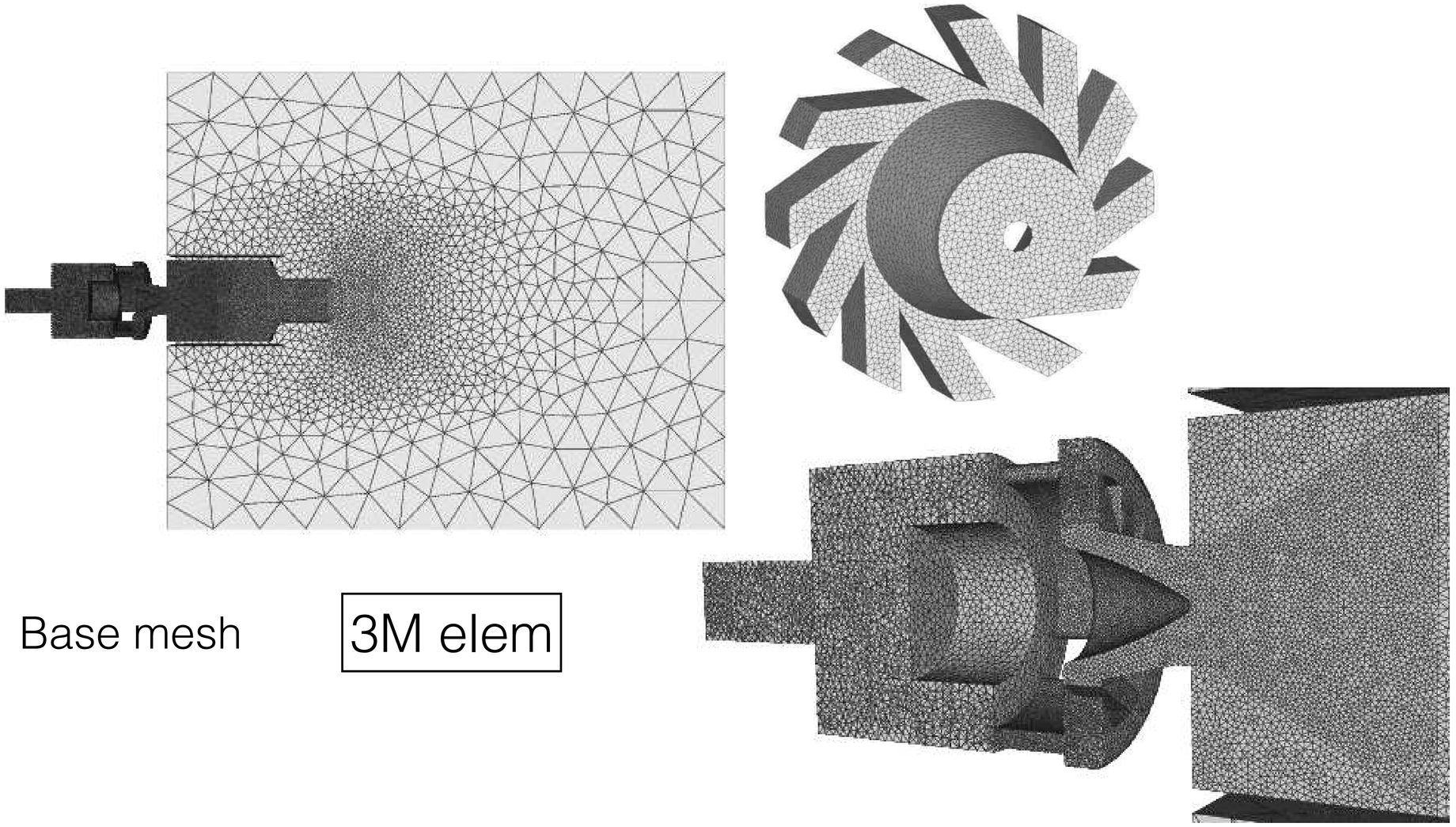
PRECCINSTA - DLR

Flow configuration



PRECCINSTA - DLR

Mesh

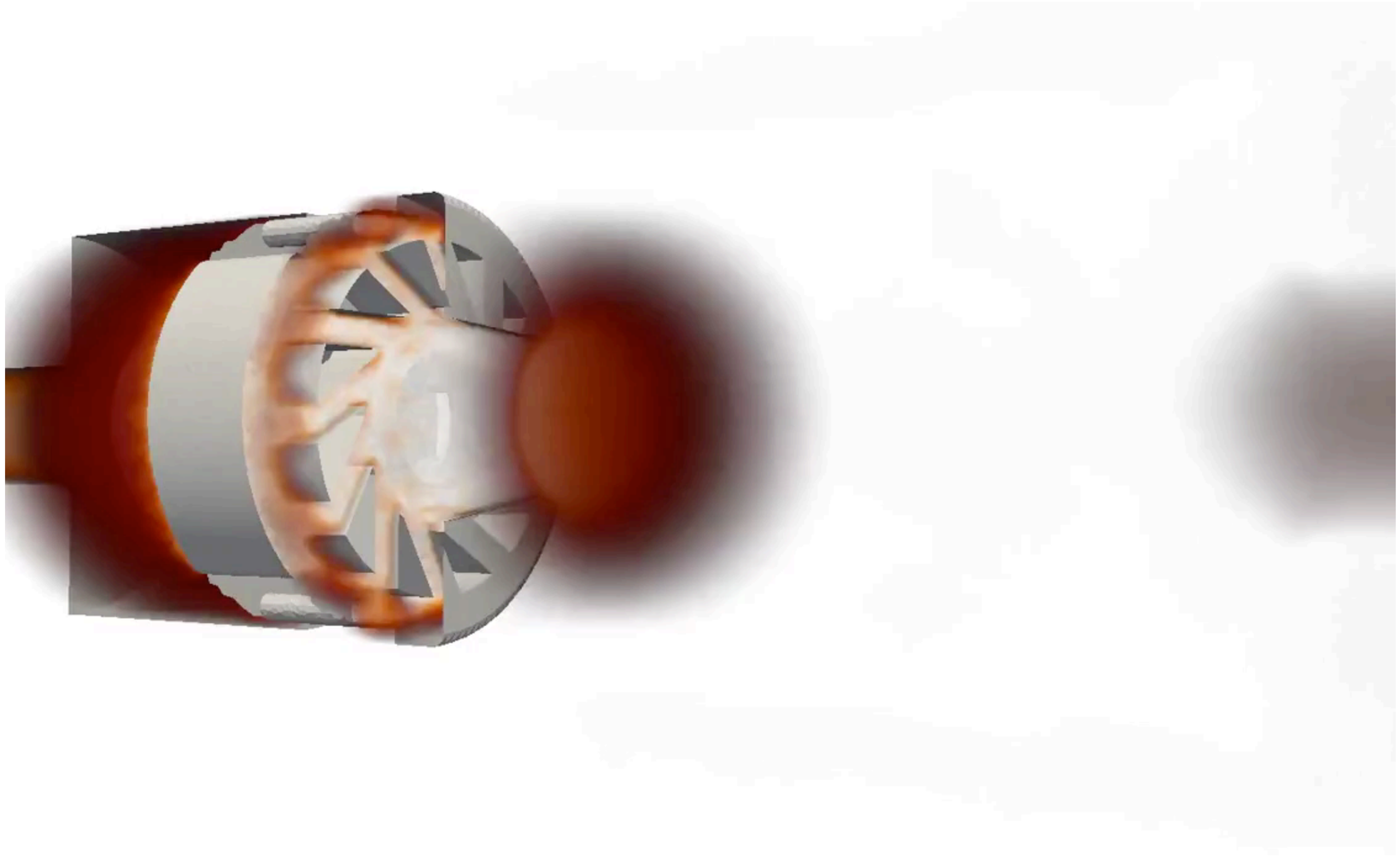


Base mesh

3M elem

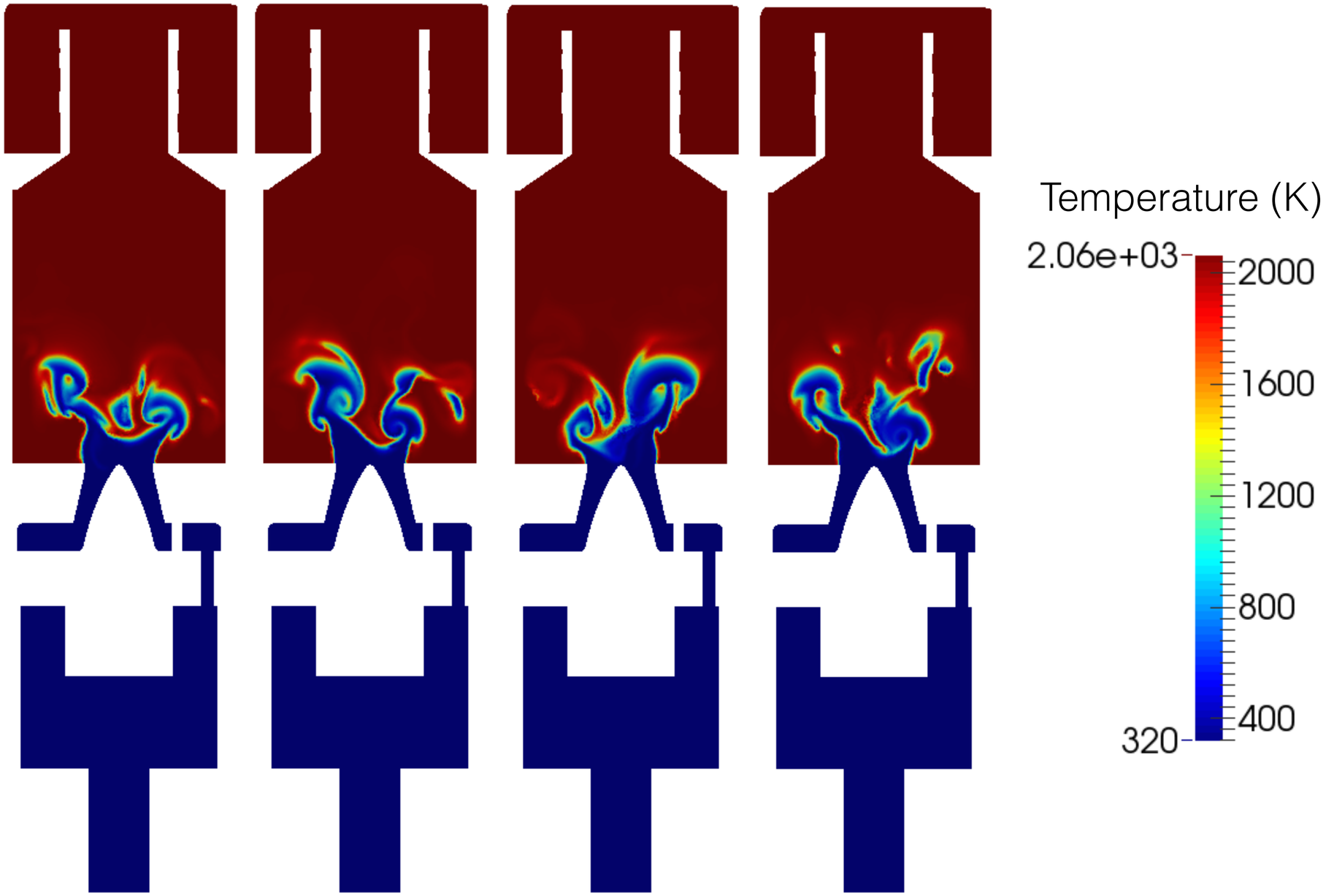
PRECCINSTA - DLR

Alya - LES



PRECCINSTA - DLR

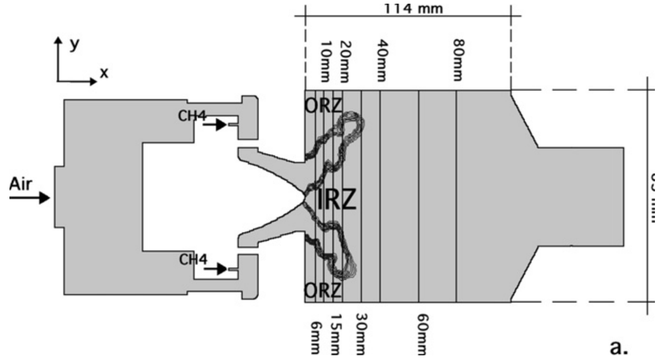
Alya - LES

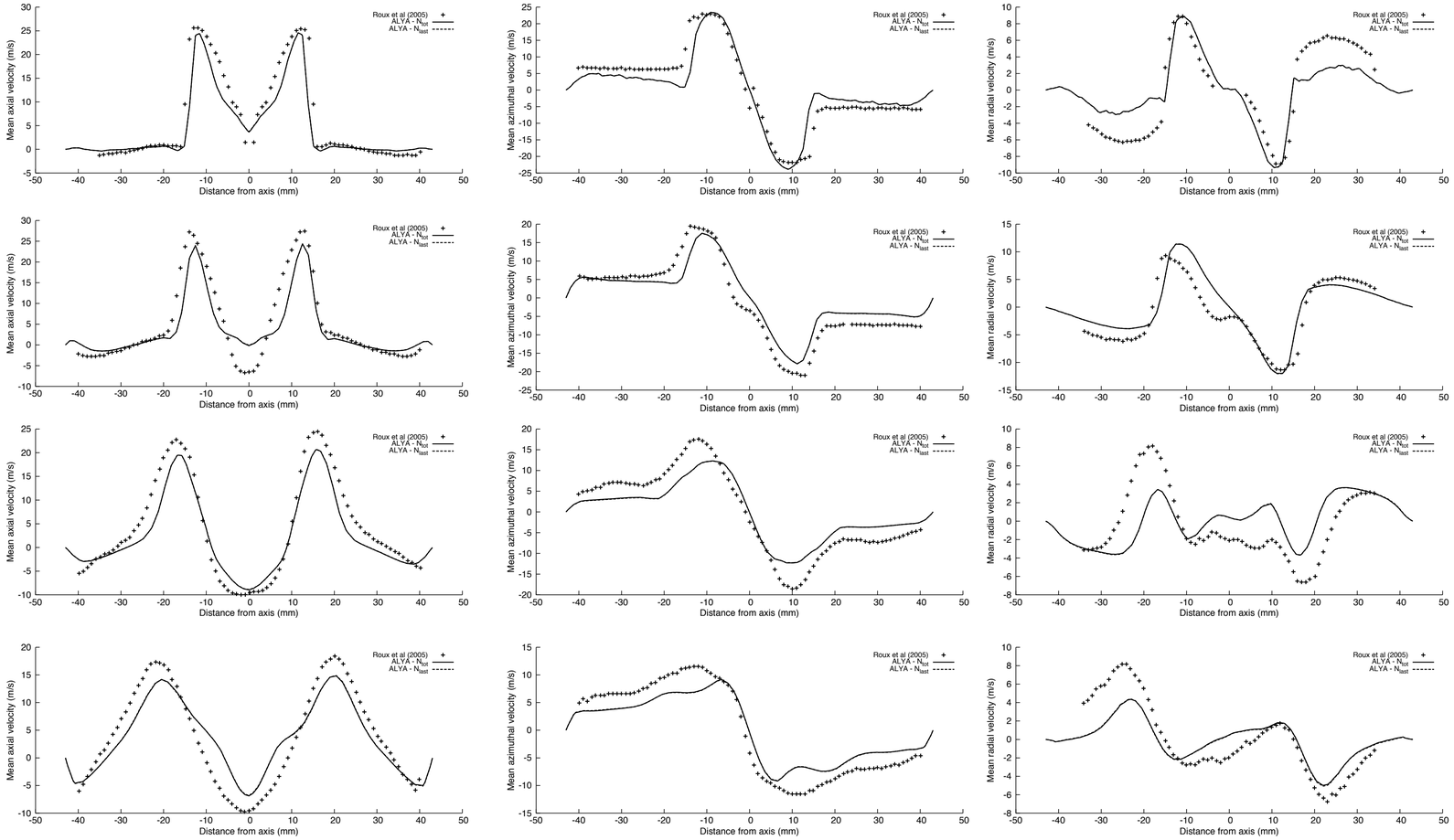


PRECCINSTA - DLR

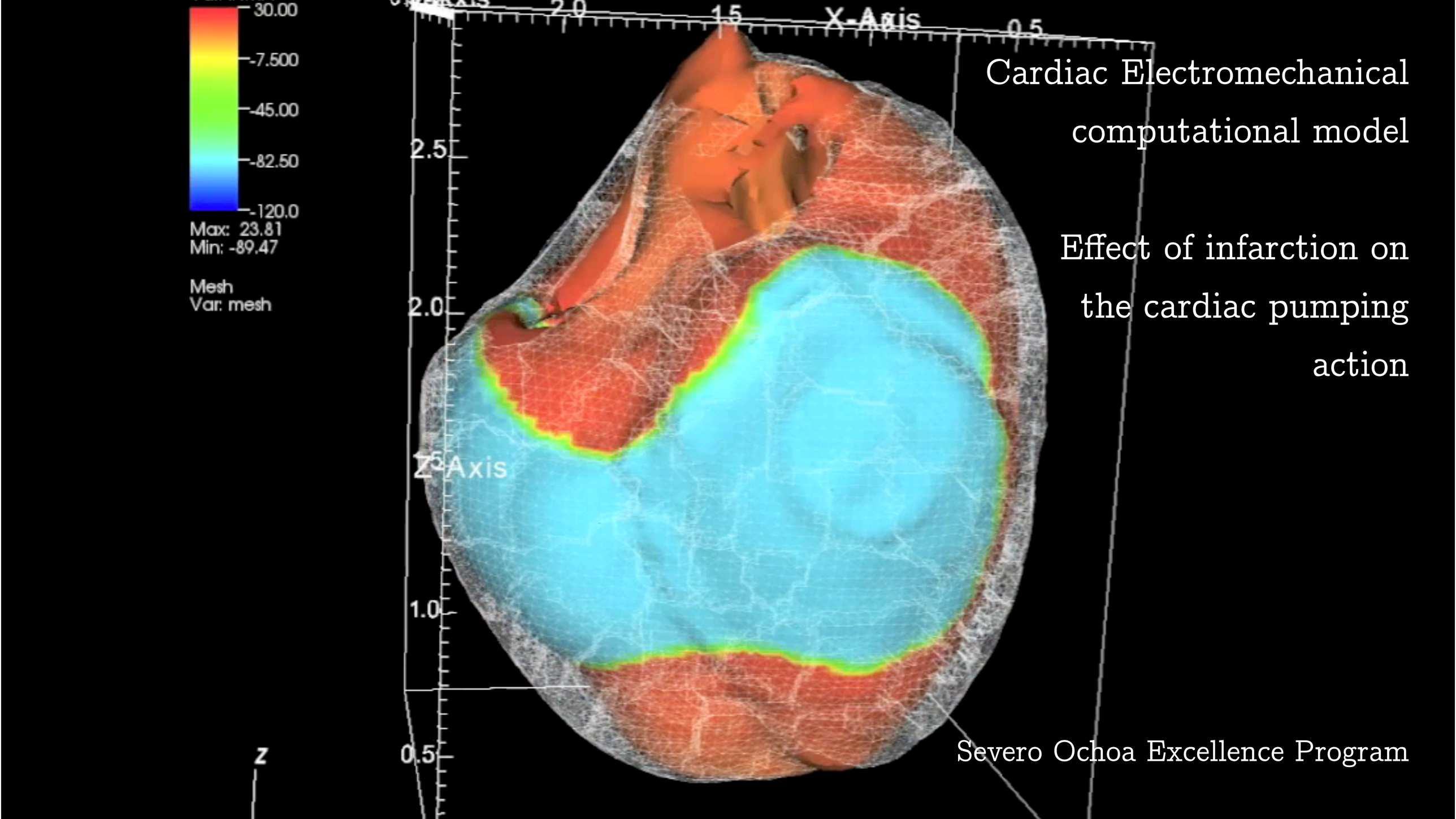
Alya - LES vs Experiments

Mean velocity





Simulations for Biomedical Research

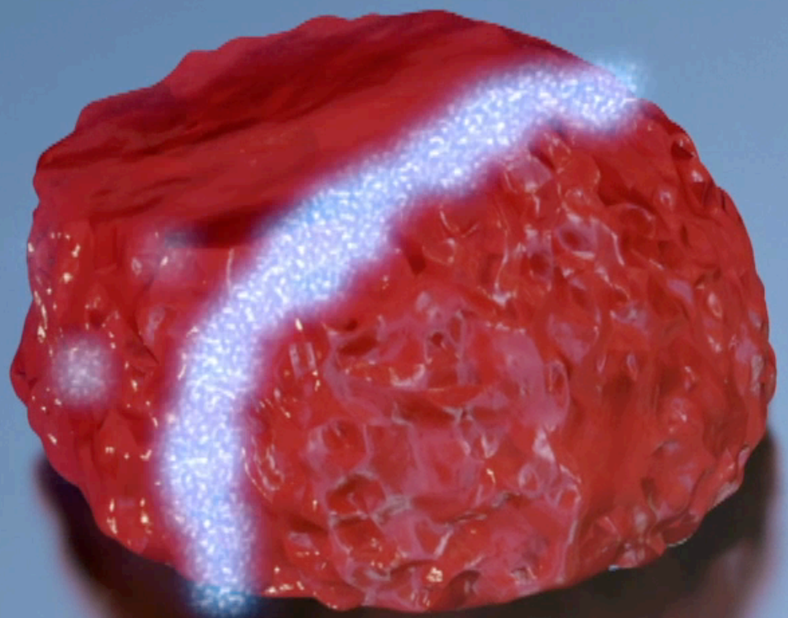


Cardiac Electromechanical computational model

Effect of infarction on the cardiac pumping action

Severo Ochoa Excellence Program

Effect of Quinidine in heart tissue
(simulated with Alya)

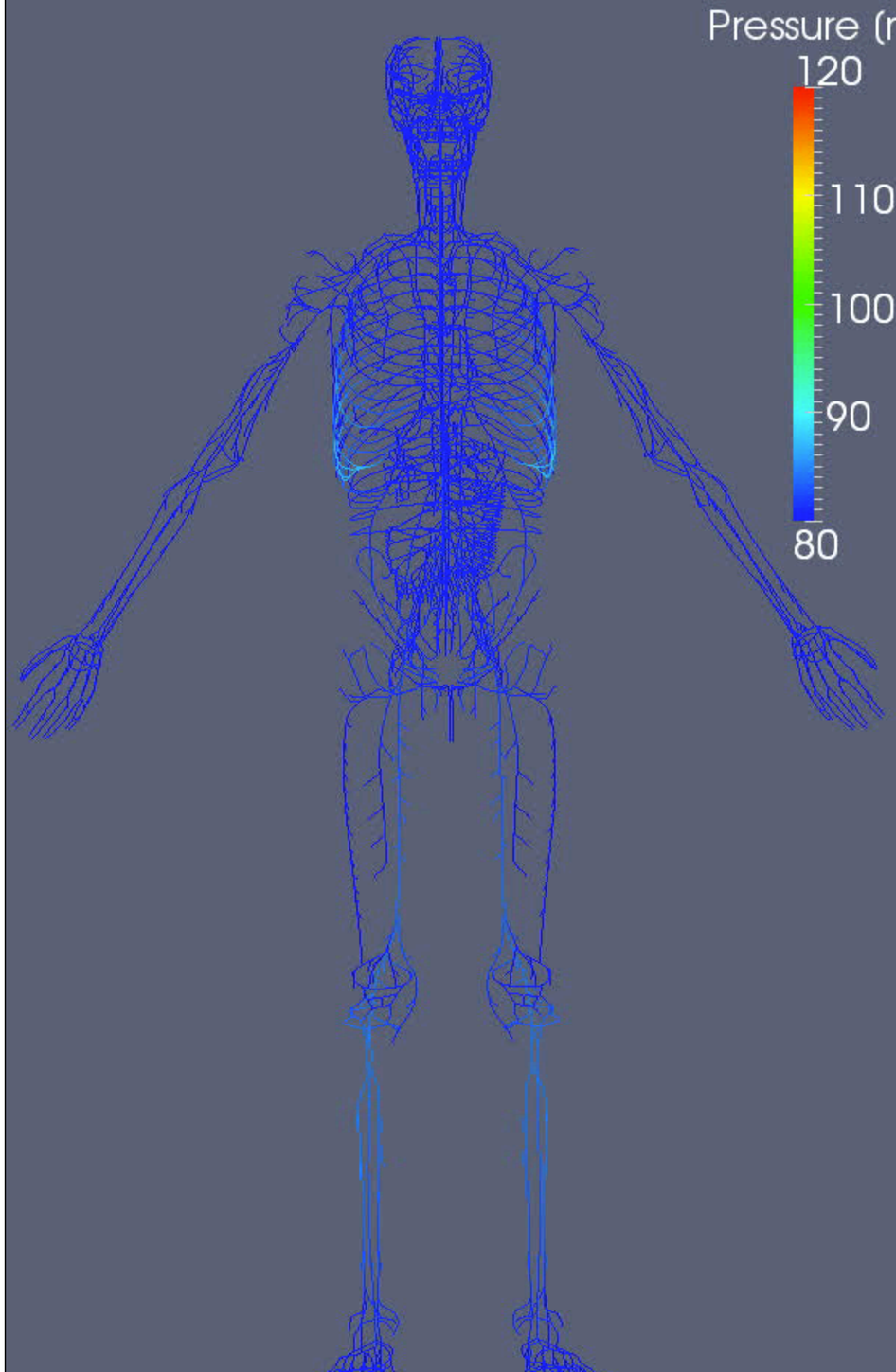


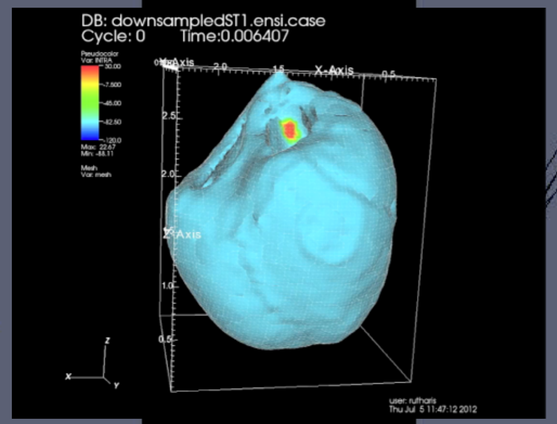
Brugada
S2-316

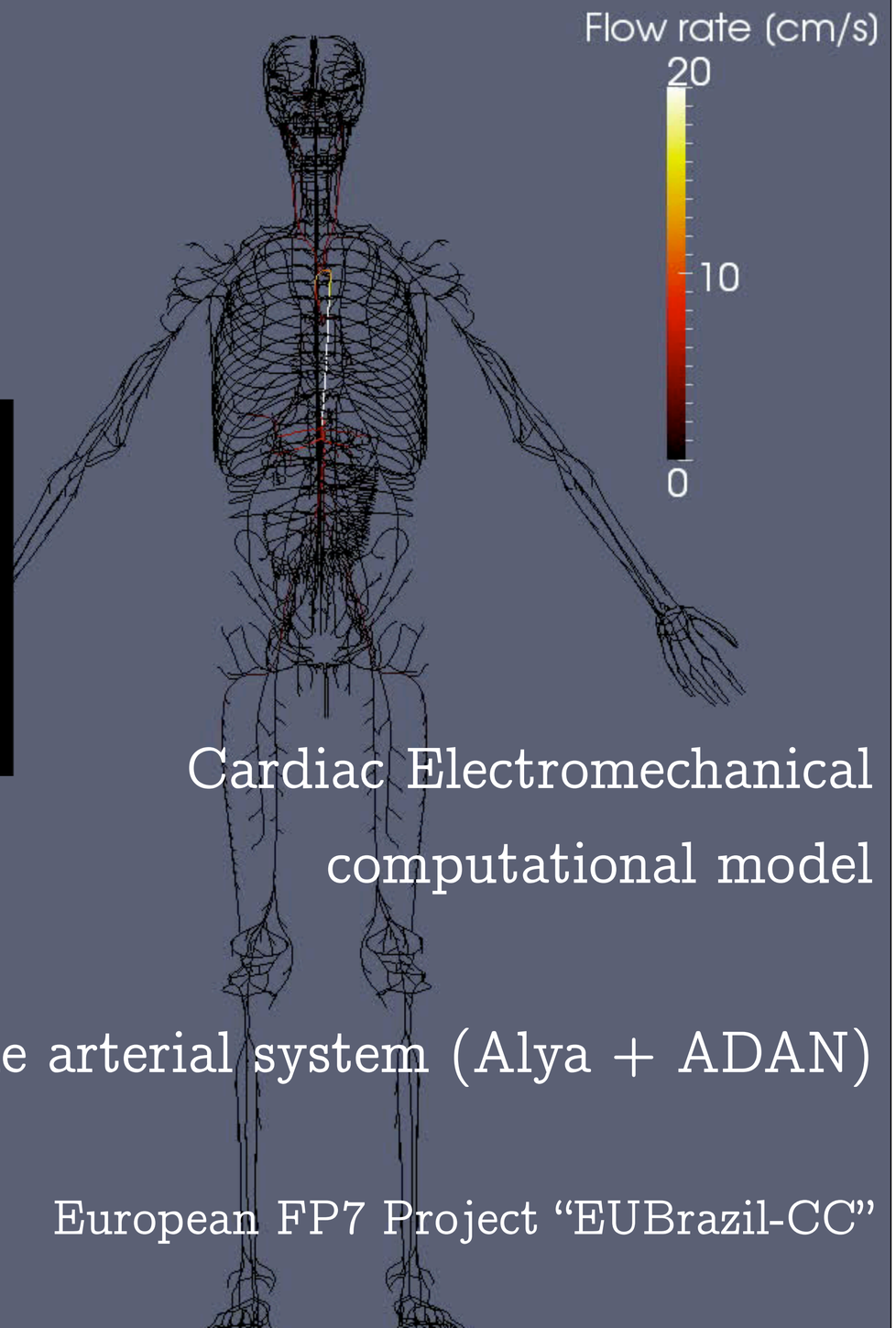
Cardiac Electromechanical
computational model

Anti-arrhythmic drugs action

Severo Ochoa Excellence Program







Cardiac Electromechanical computational model

Coupling with the arterial system (Alya + ADAN)

European FP7 Project “EUBrazil-CC”

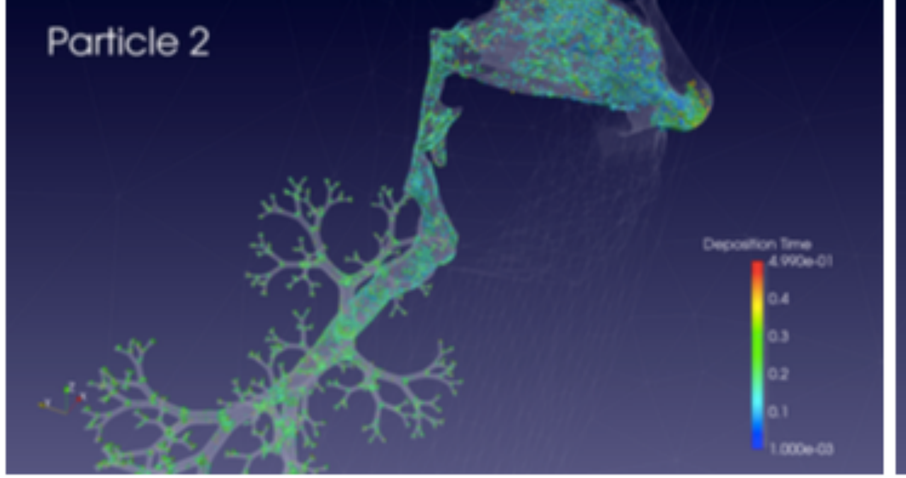
Respiratory system

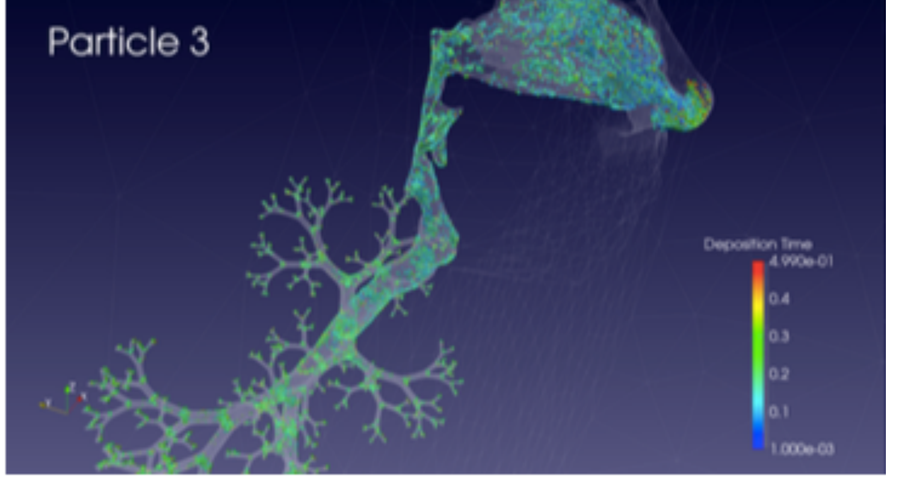
Drug delivery and massive particle tracking

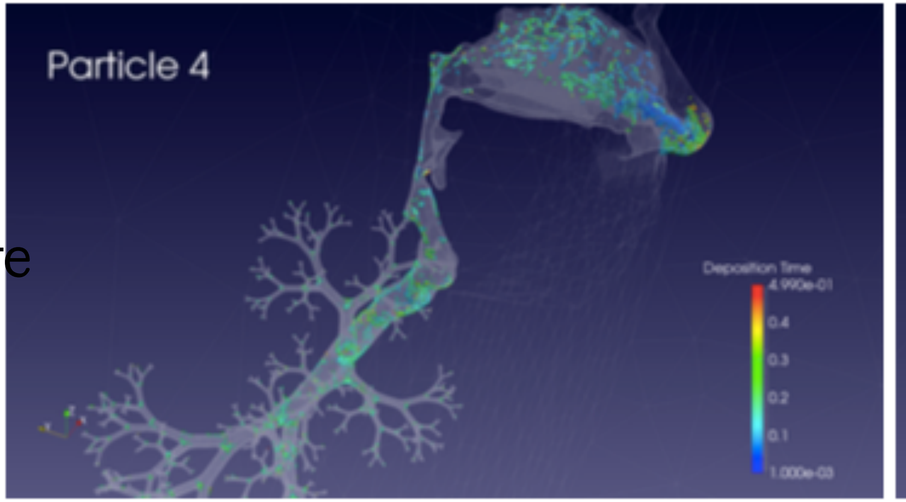
Respiratory system

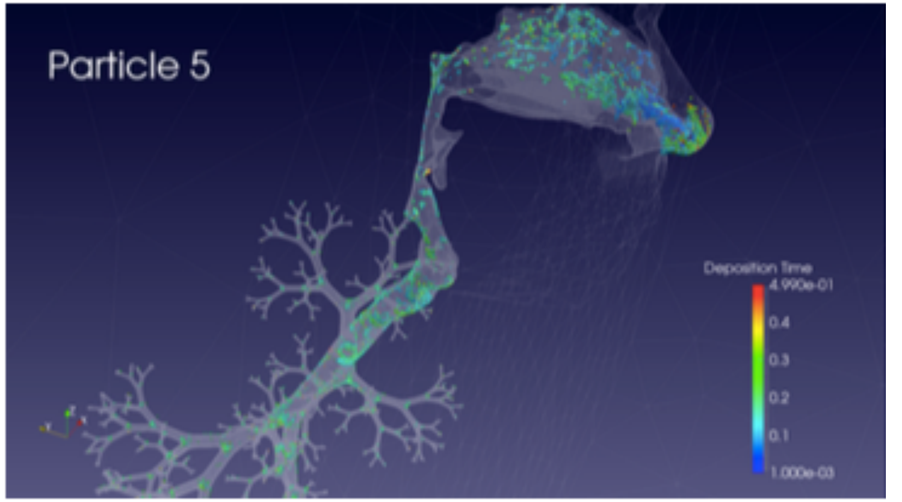
Drug delivery and massive particle tracking

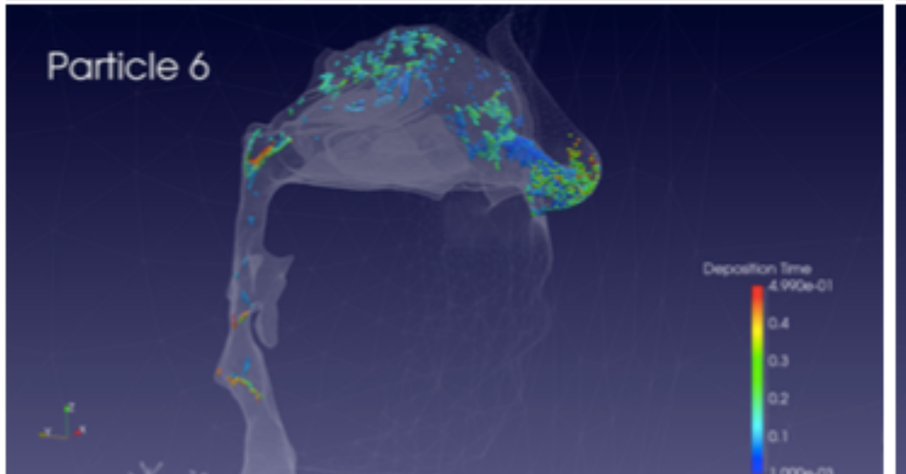
Particle deposition

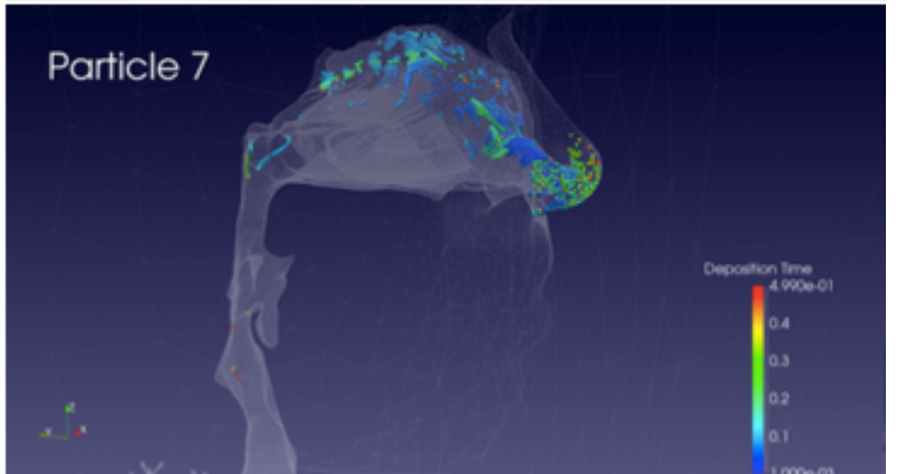










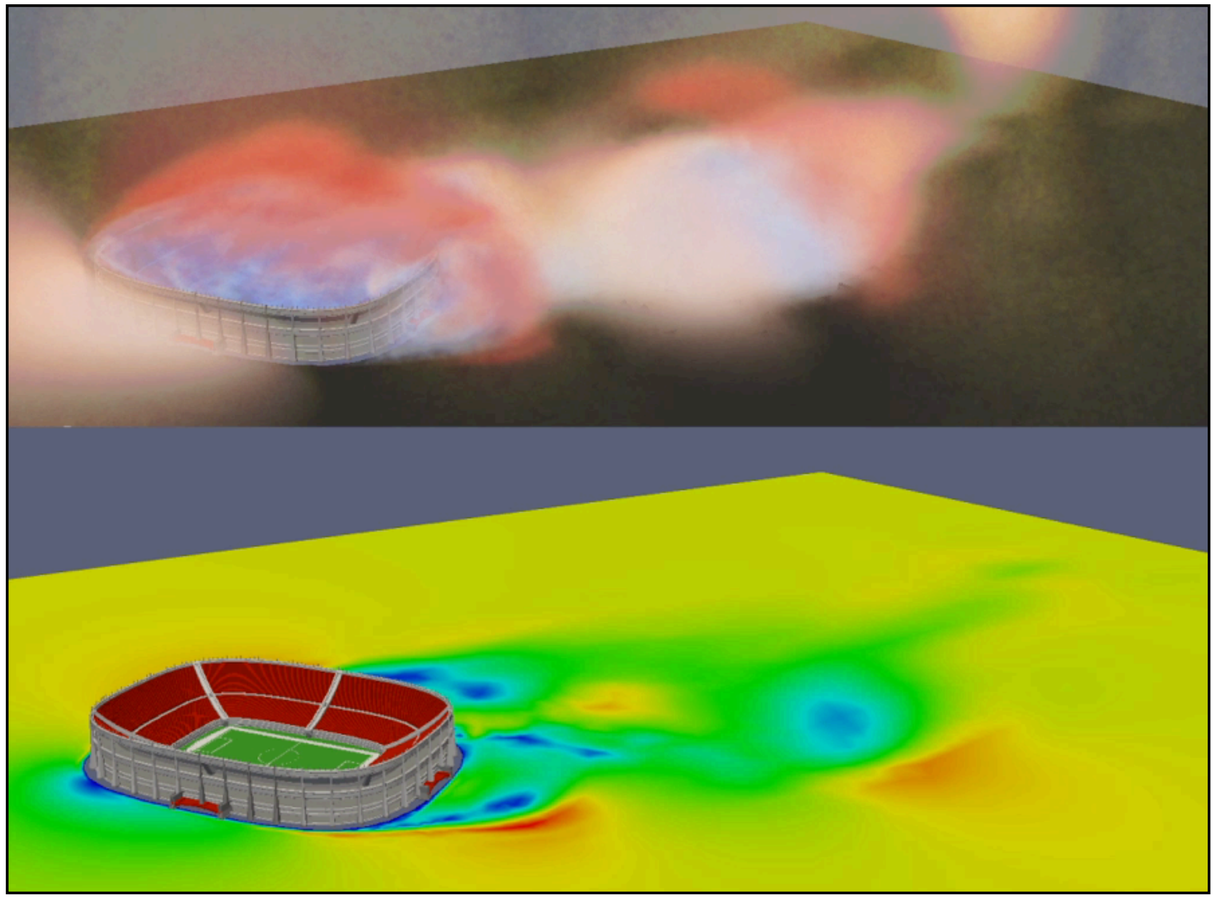


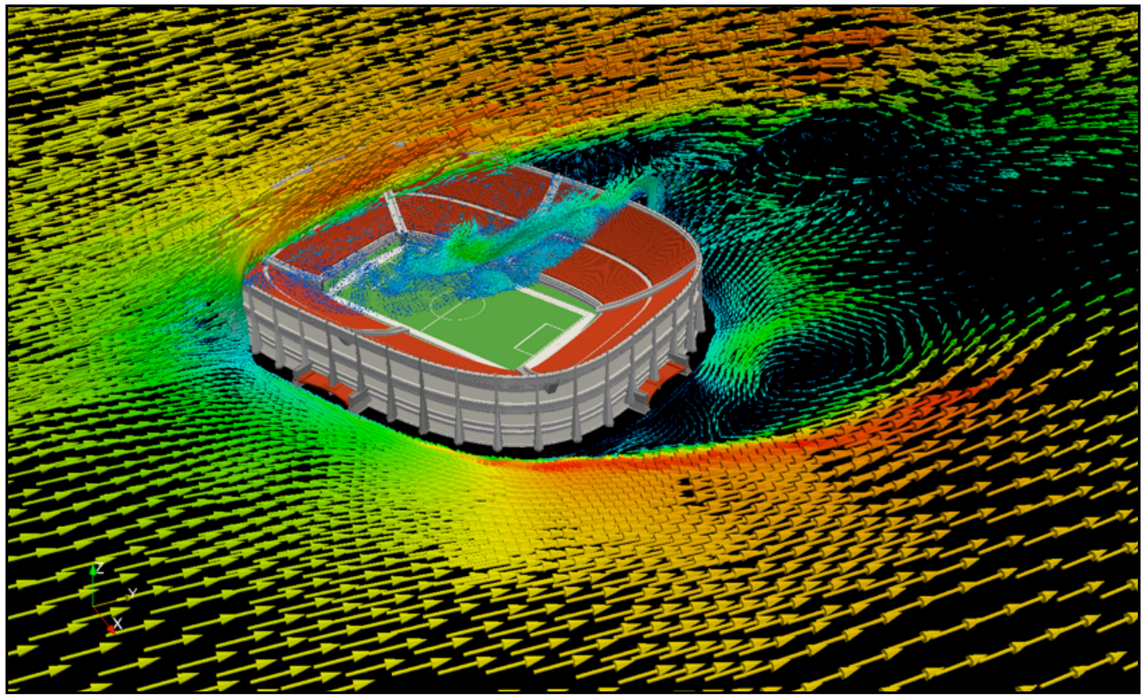
Simulations for Energy

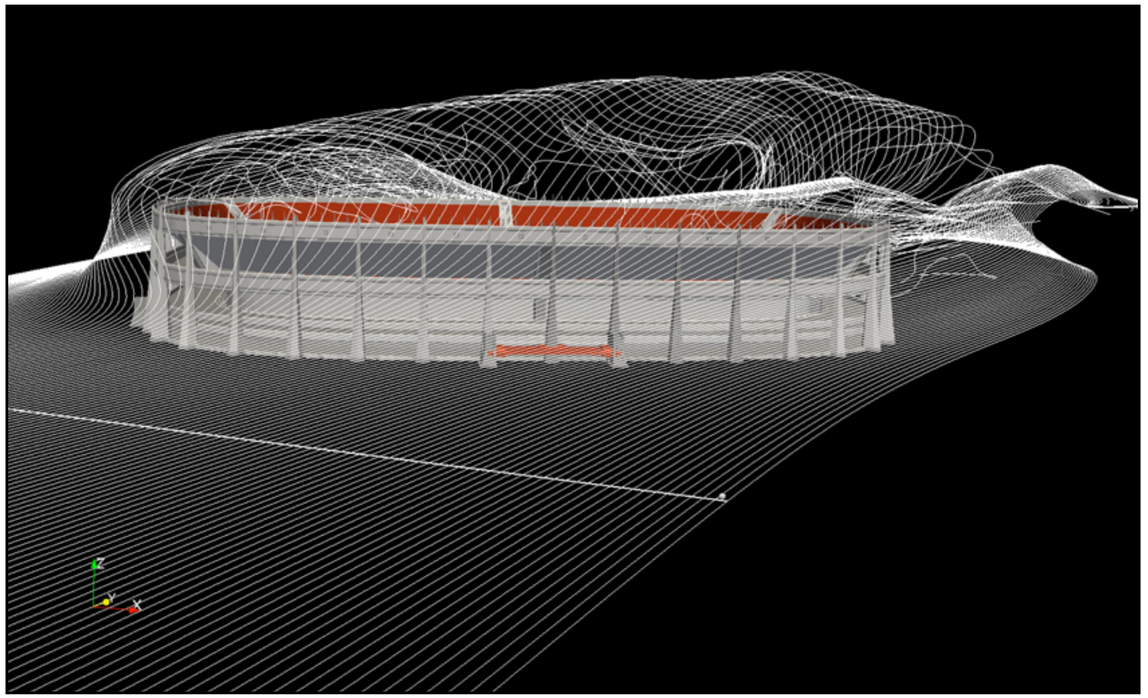
The wind and the environment

ATMOST Spanish project

Wind in urban environments







Partnership: IBERDROLA – BSC - CENER

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

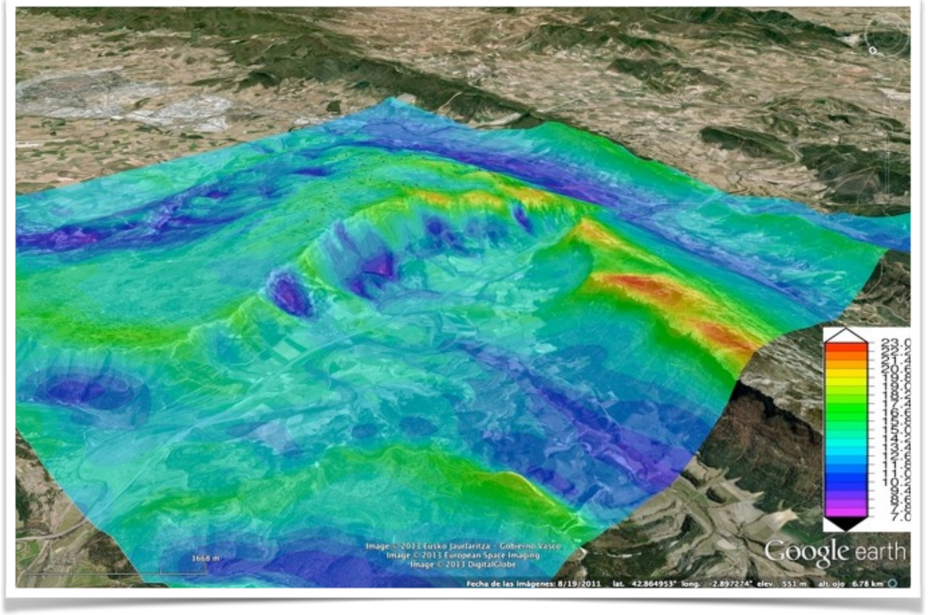
IBERDROLA

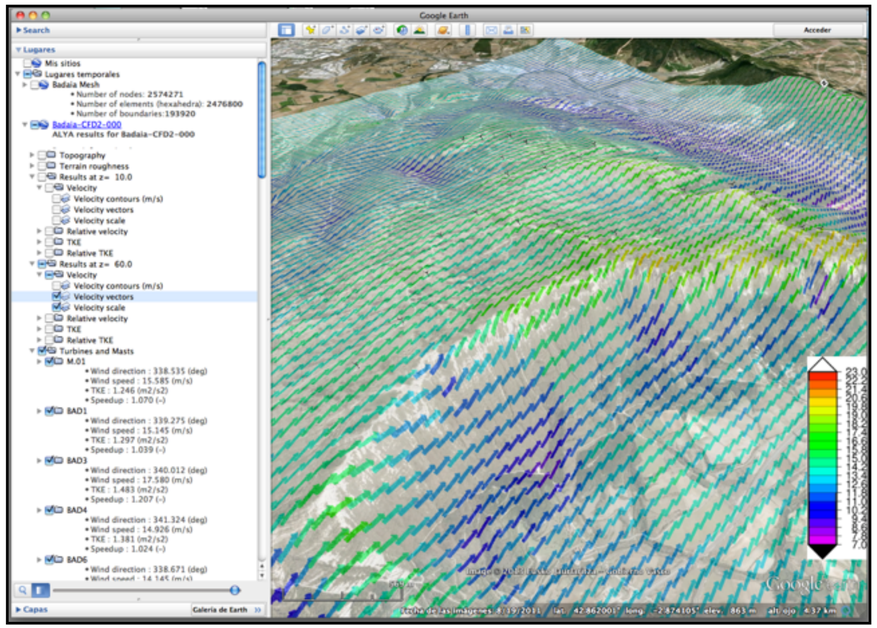
cener
centro nacional de energías renovables
FUNDACION CENER CIEMAT

Wind Energy Project objectives:

1. **Phase 1: wind farm planning**
   - Goal: to predict long-term wind farm production using CFD.
   - Mast measurements during a number of years (wind statistics).
   - Determine the optimal wind turbine positions to obtain the best profitability.

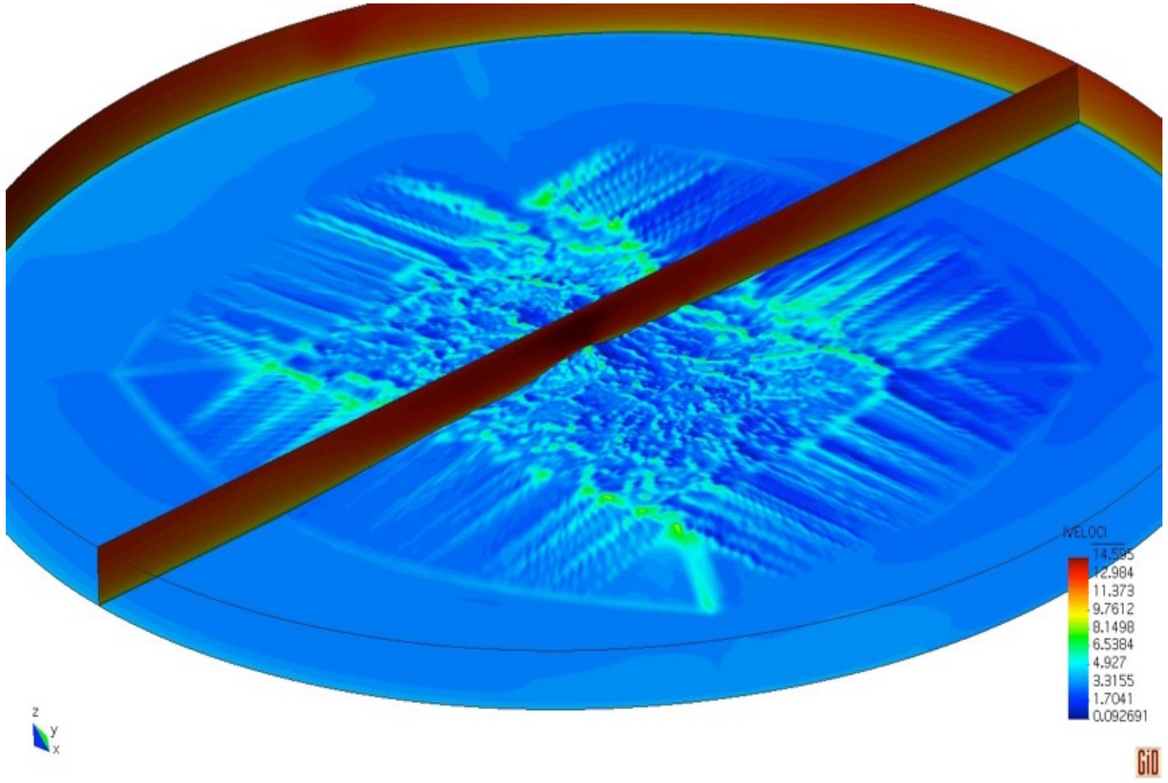
2. **Phase 2: wind farm exploitation**
   - Goal: to predict short-term wind farm production using CFD.
   - Downscaling from mesoscale NWP models (model chain).

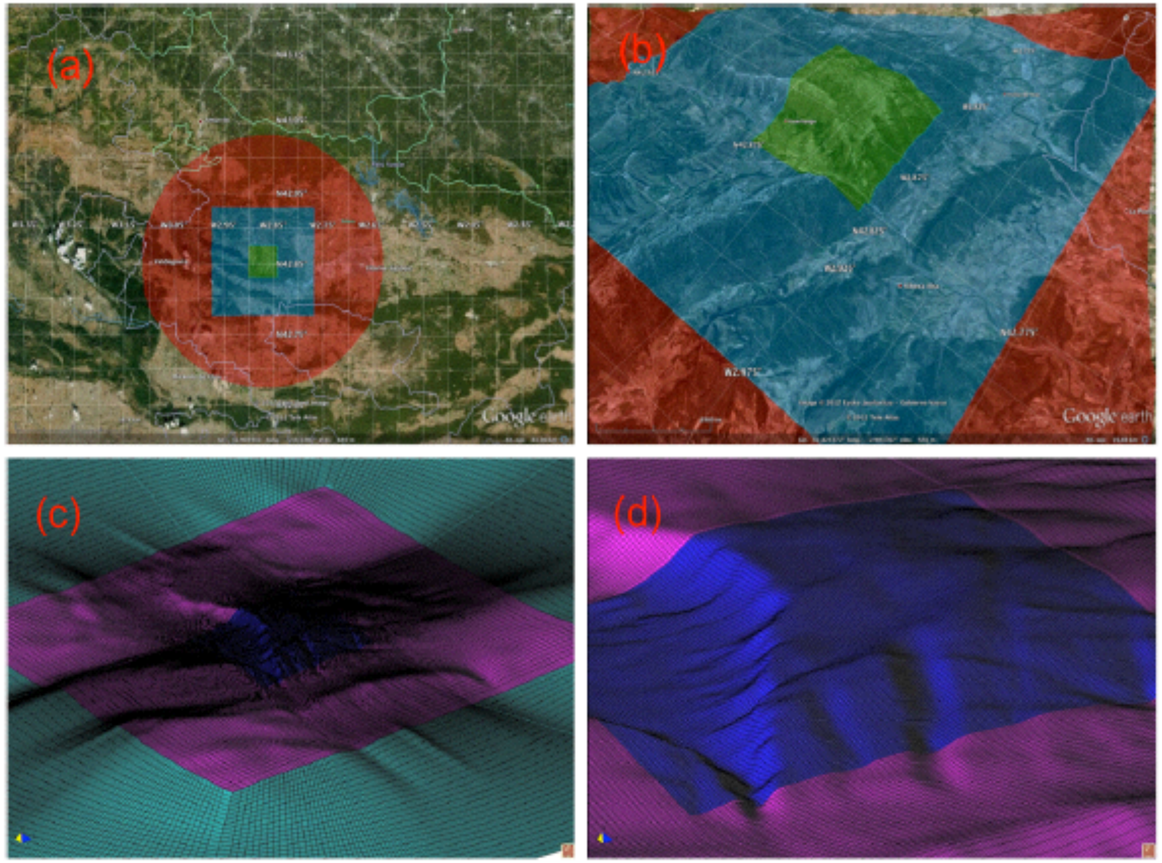




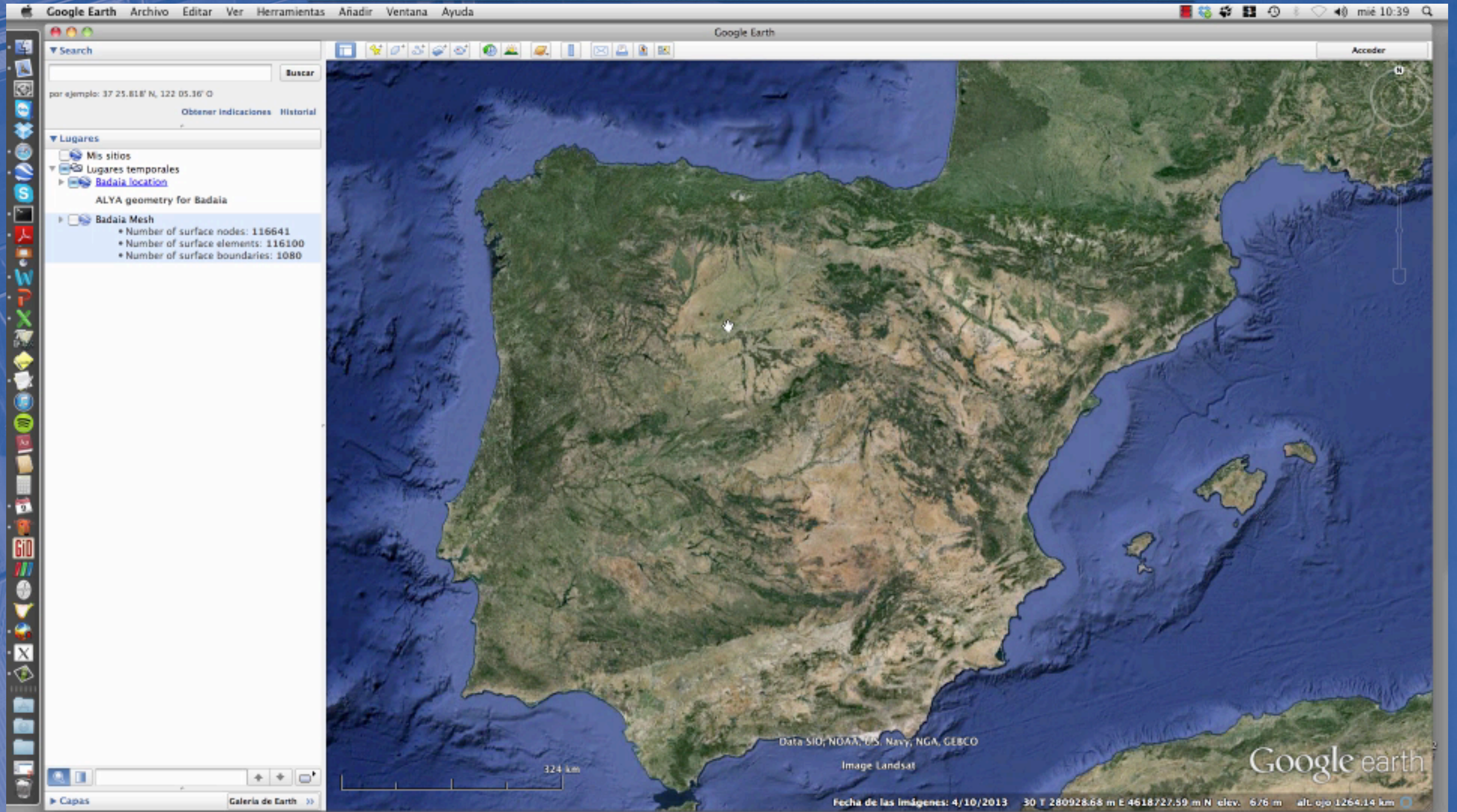
CFDWind: high resolution wind modelling

- Solution of the RANS equations coupled with a κ-ε length-limited turbulence model;
- Horizontal mesh resolution ~10s of meters.
- Coriolis, canopy, thermal coupling, actuator disc.





PreProcess in Google Earth Before Meshing



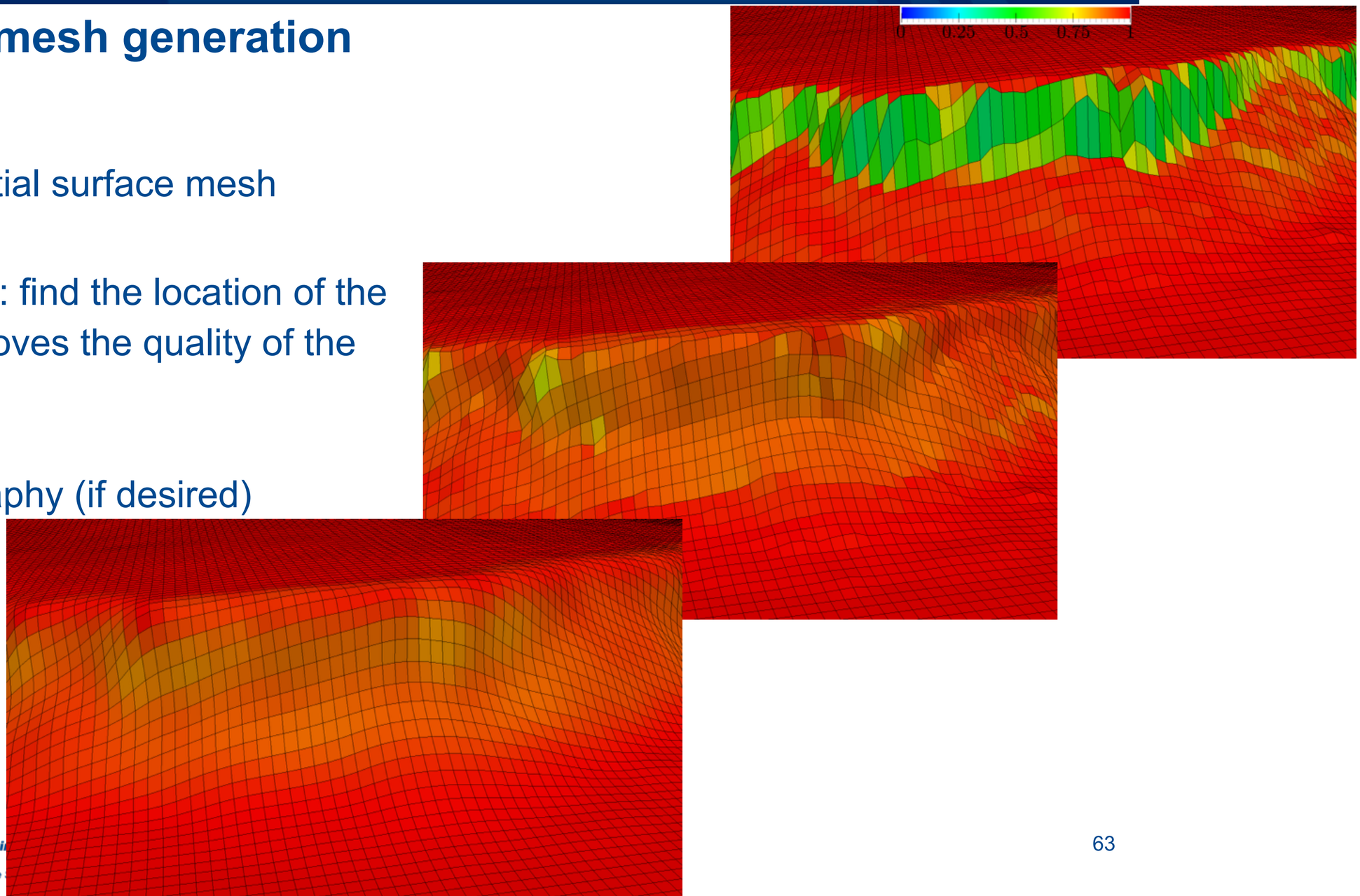
Optimization of the surface mesh

Topography mesh generation procedure

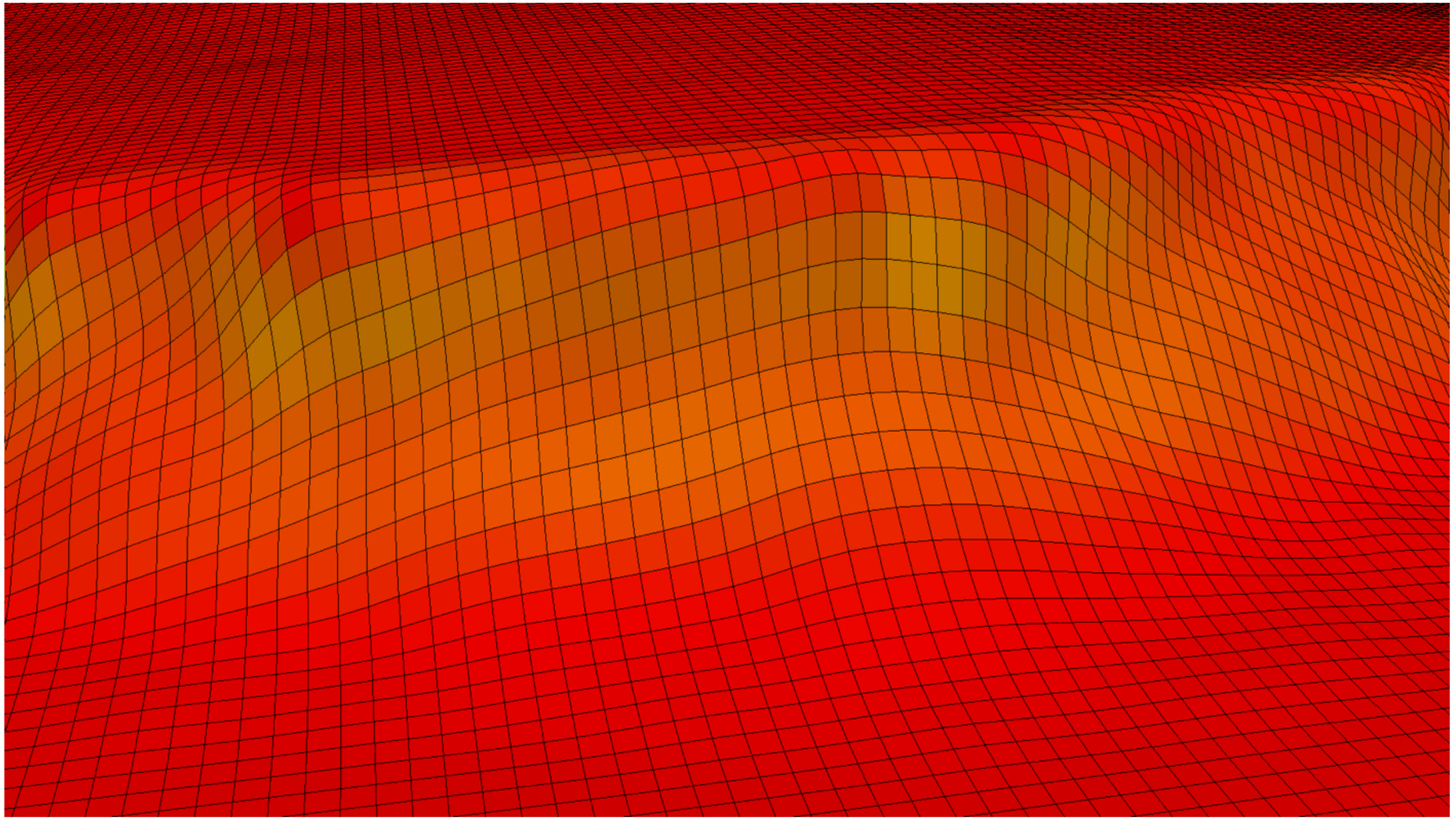
1. Generate an initial surface mesh

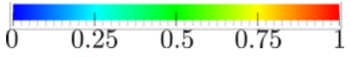
2. **Optimize mesh**: find the location of the nodes that improves the quality of the elements

3. Smooth topography (if desired)



Optimization of the surface mesh





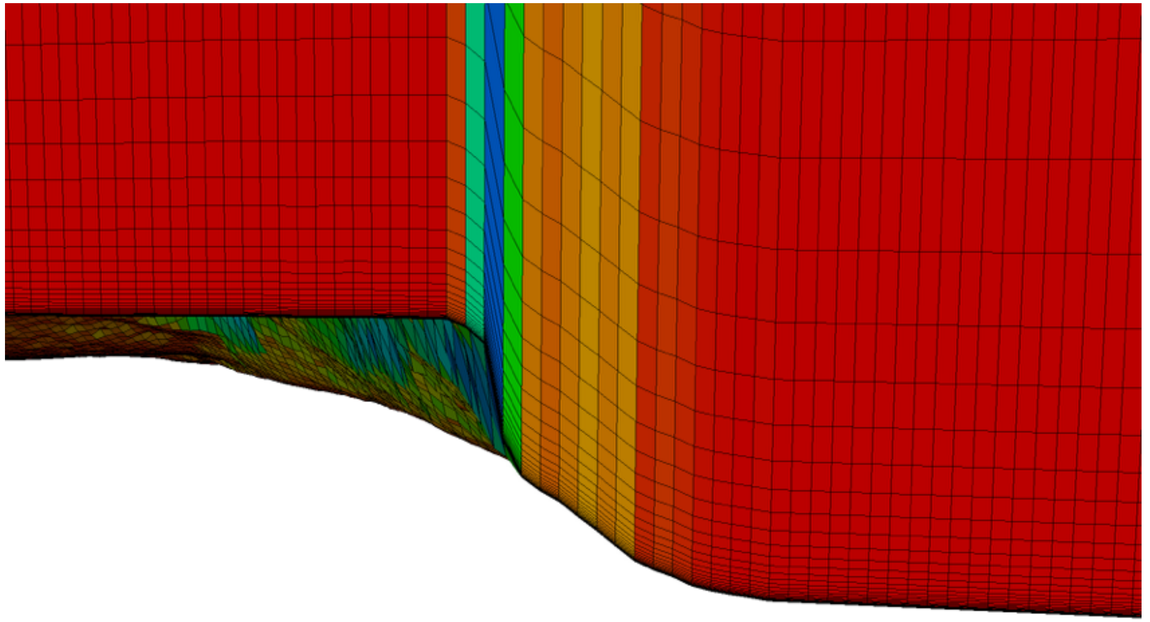
Mesh with initial topography

Optimized mesh

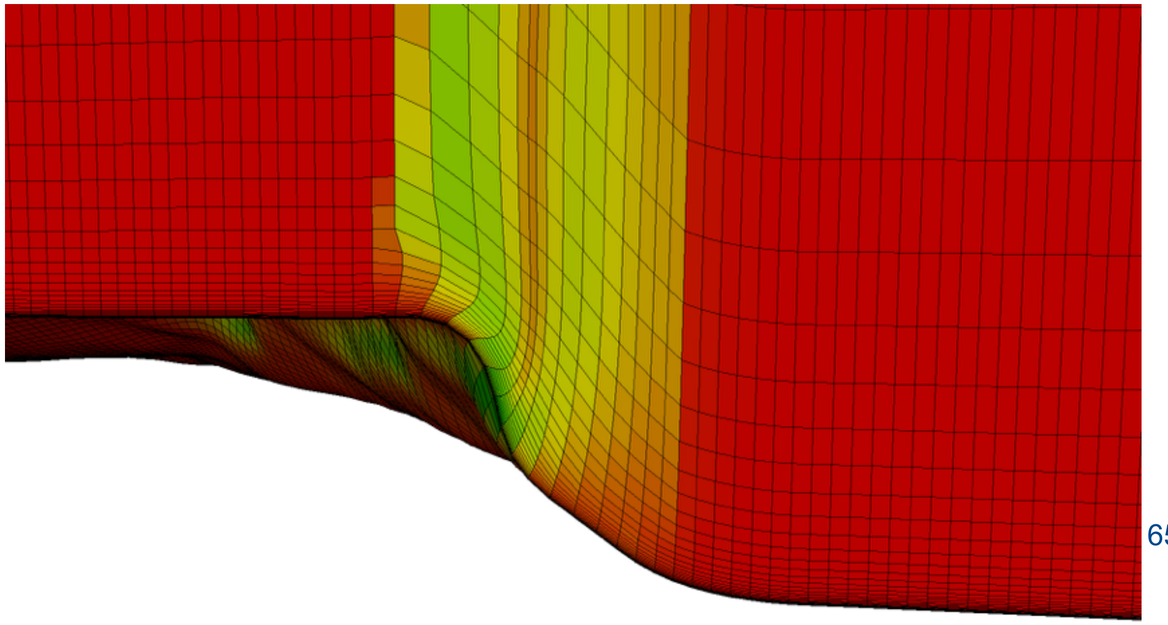
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Update 2: volume mesh generation algorithm

Mesh generation extruding in vertical direction

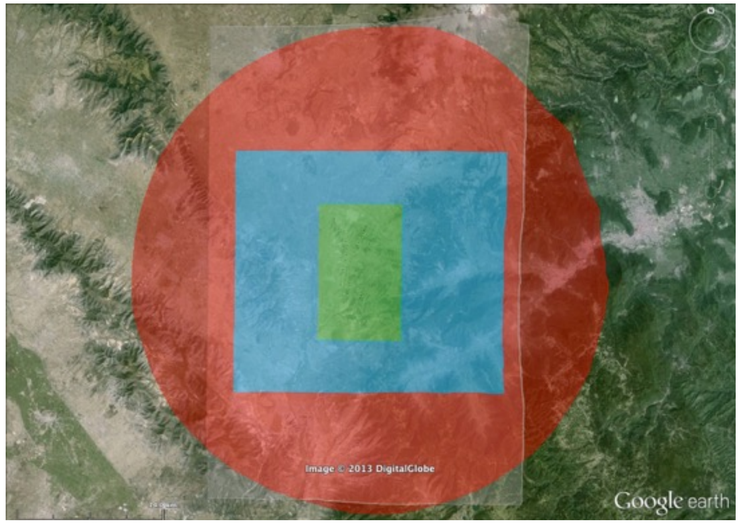


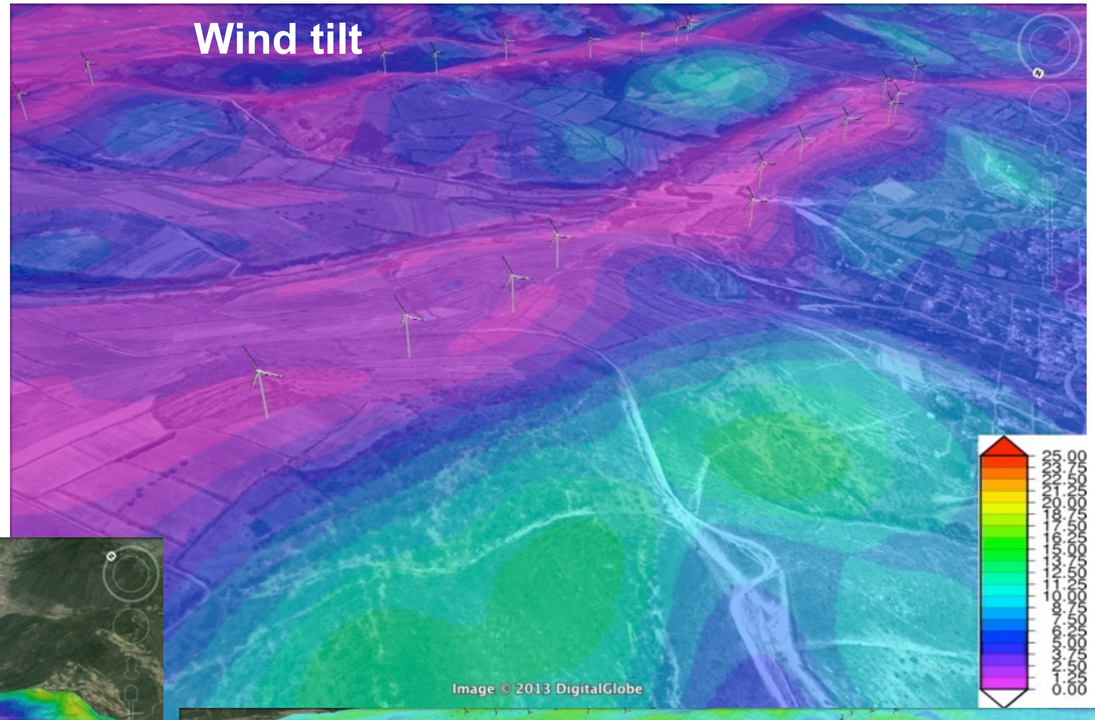
Mesh generation using the 3d optimization approach

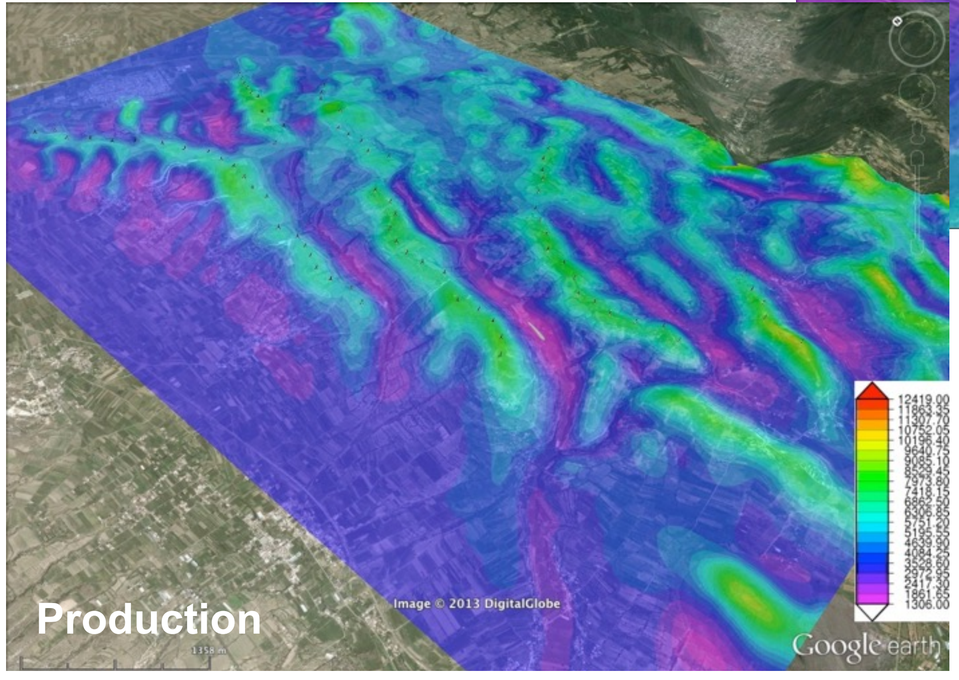


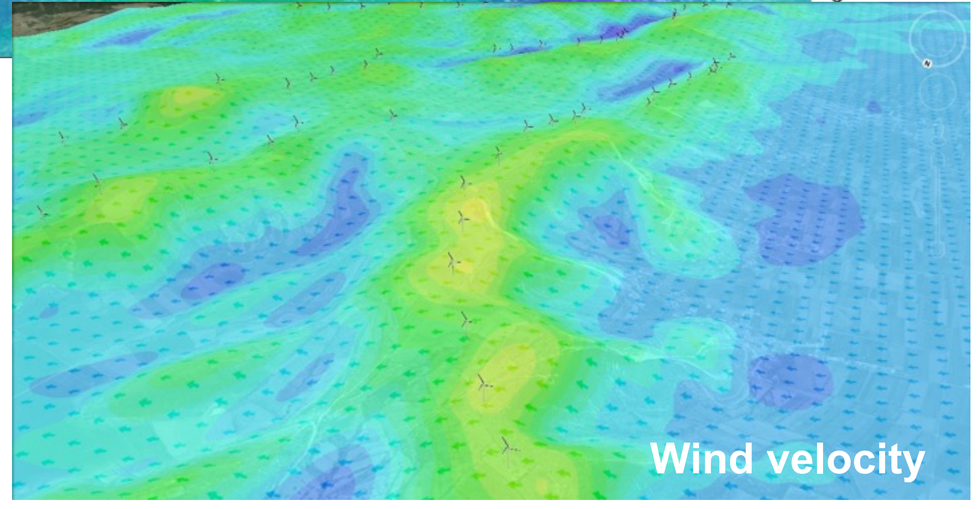
CFDWind: high resolution wind modelling

- Tailored post-process in Google Earth.

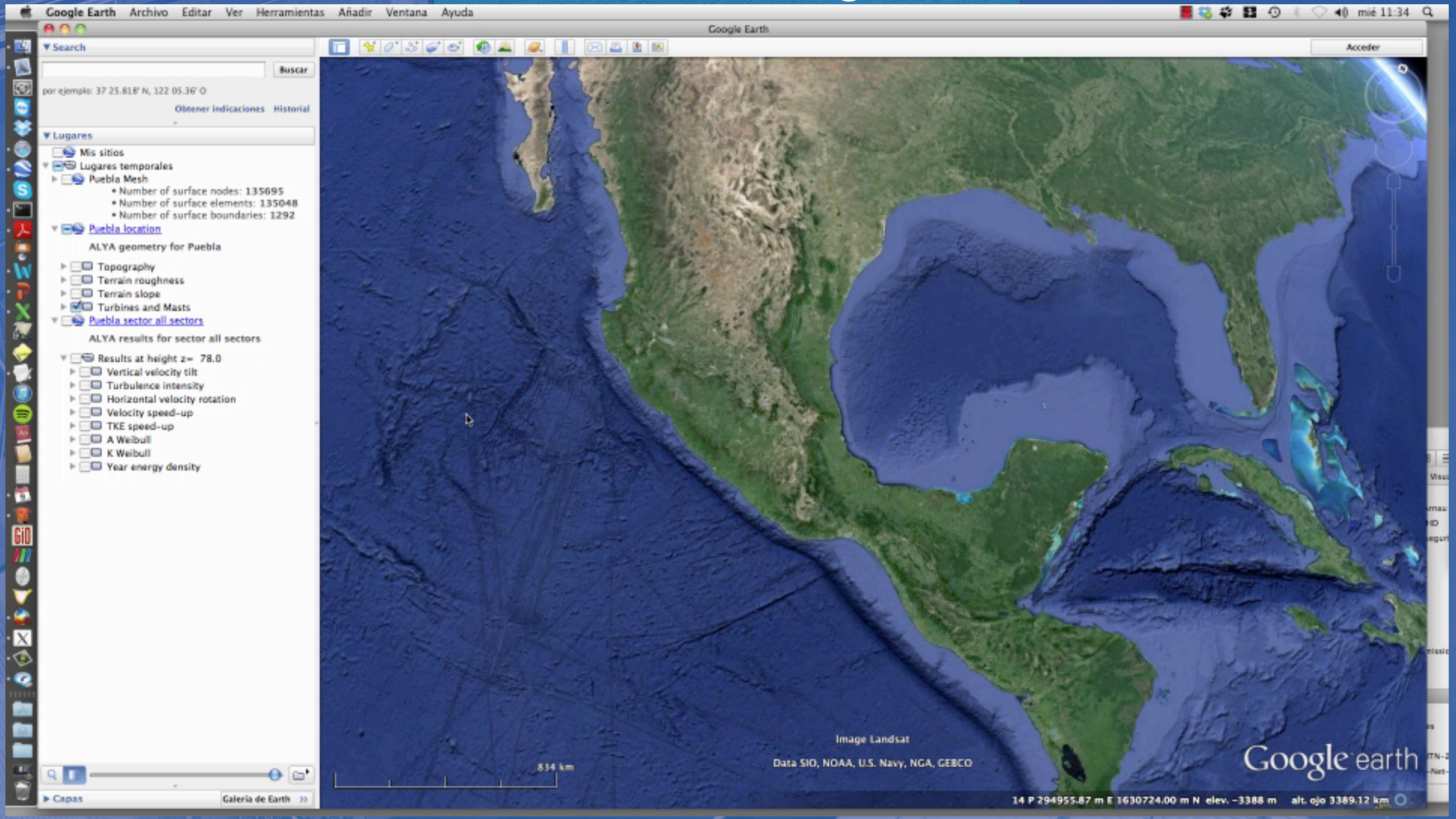






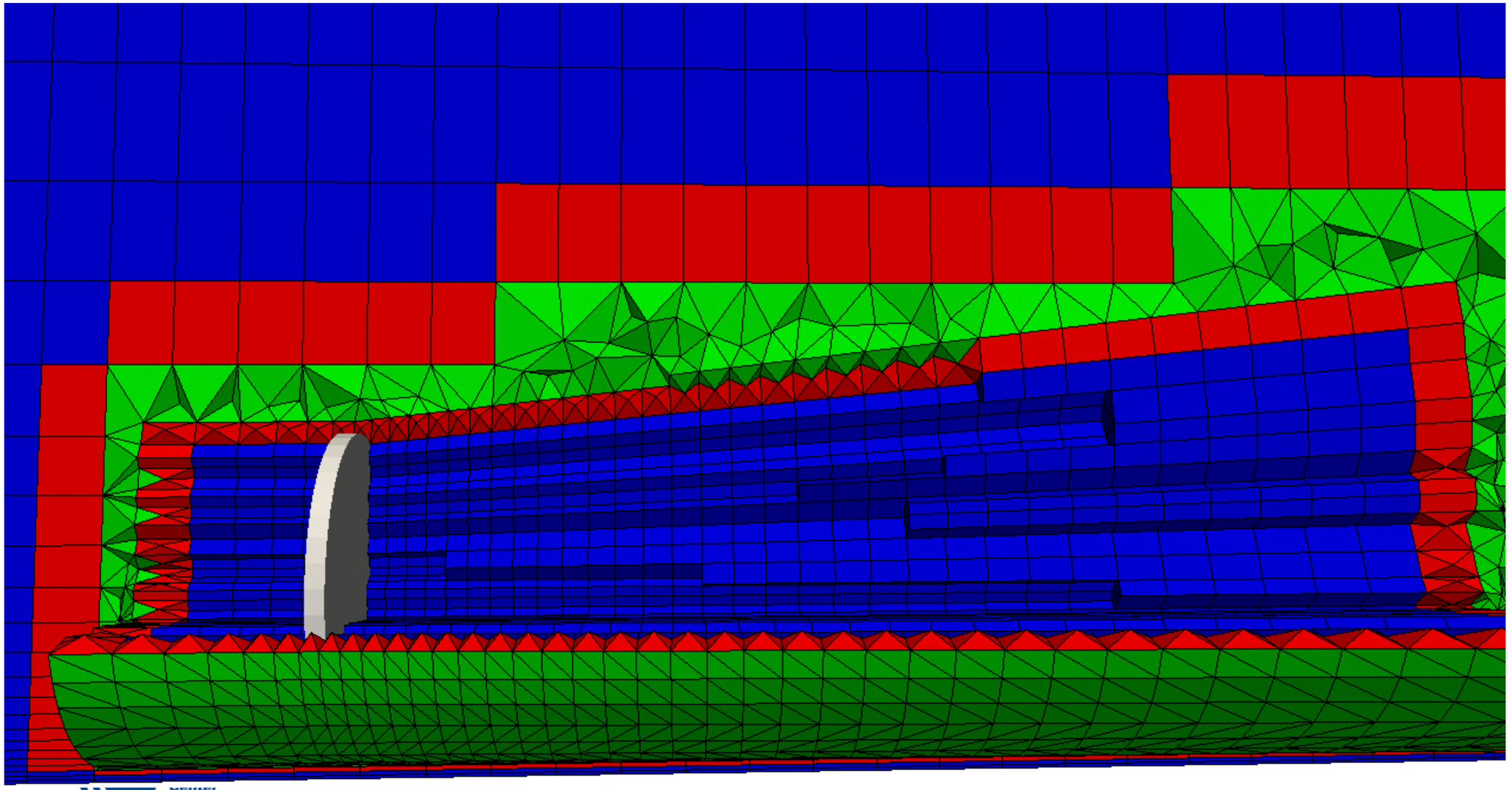


PostProcess in Google Earth

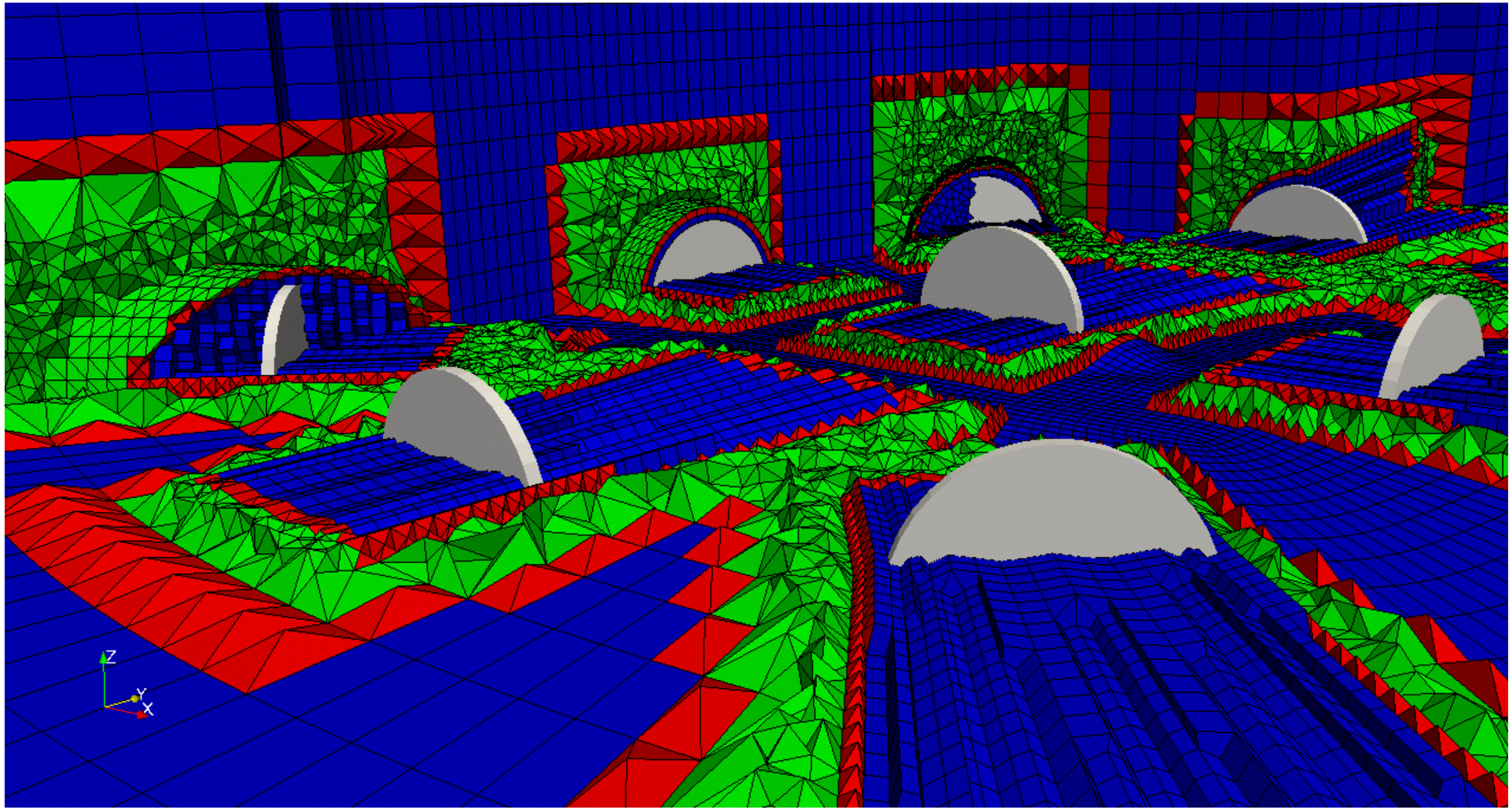


Actuator Disc

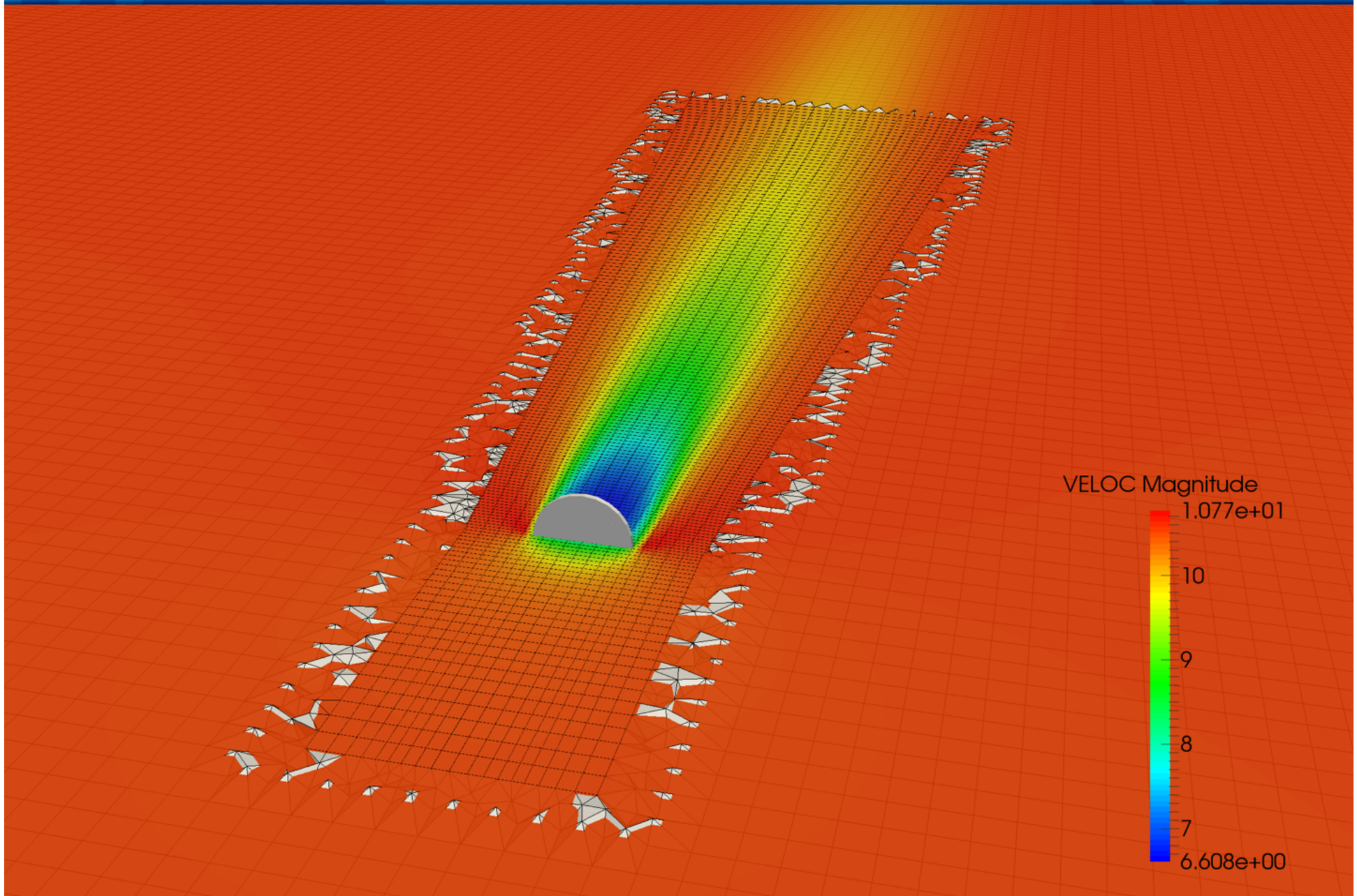
Hybrid conformal mesh generation procedure



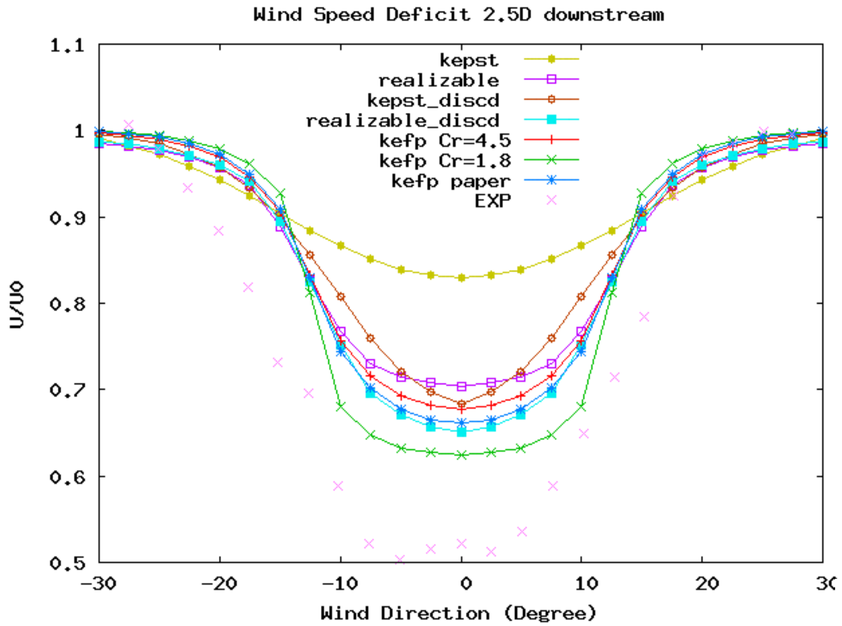
Examples: several discs

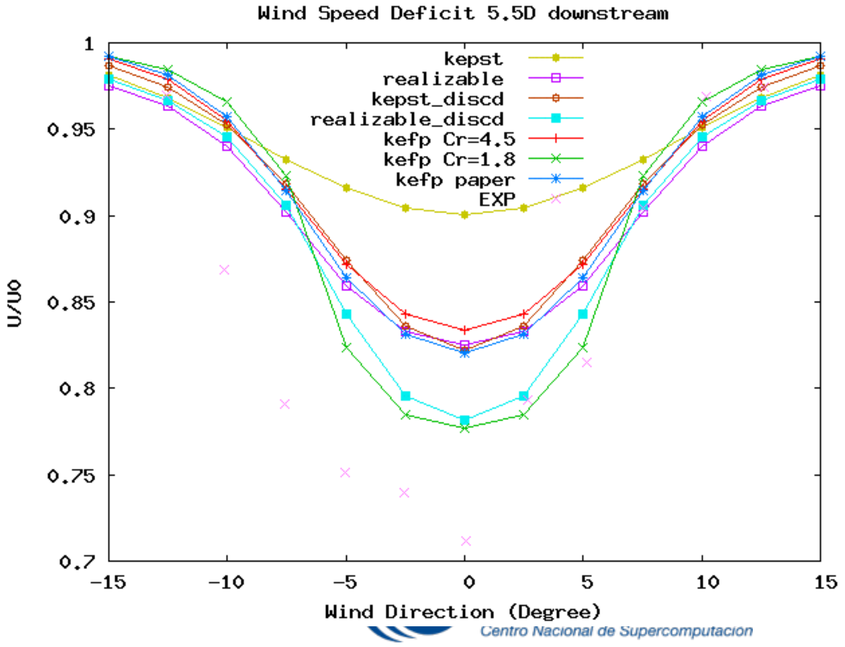


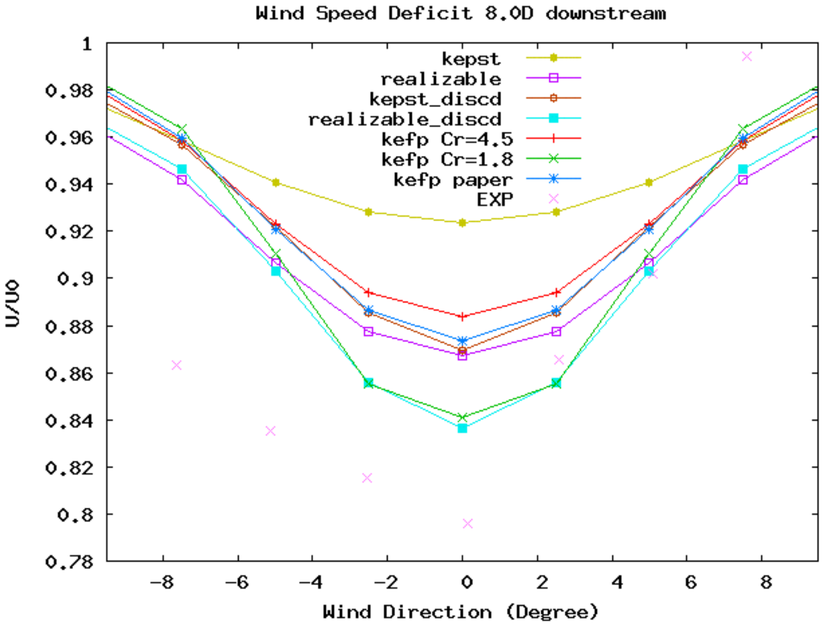
VALIDATION



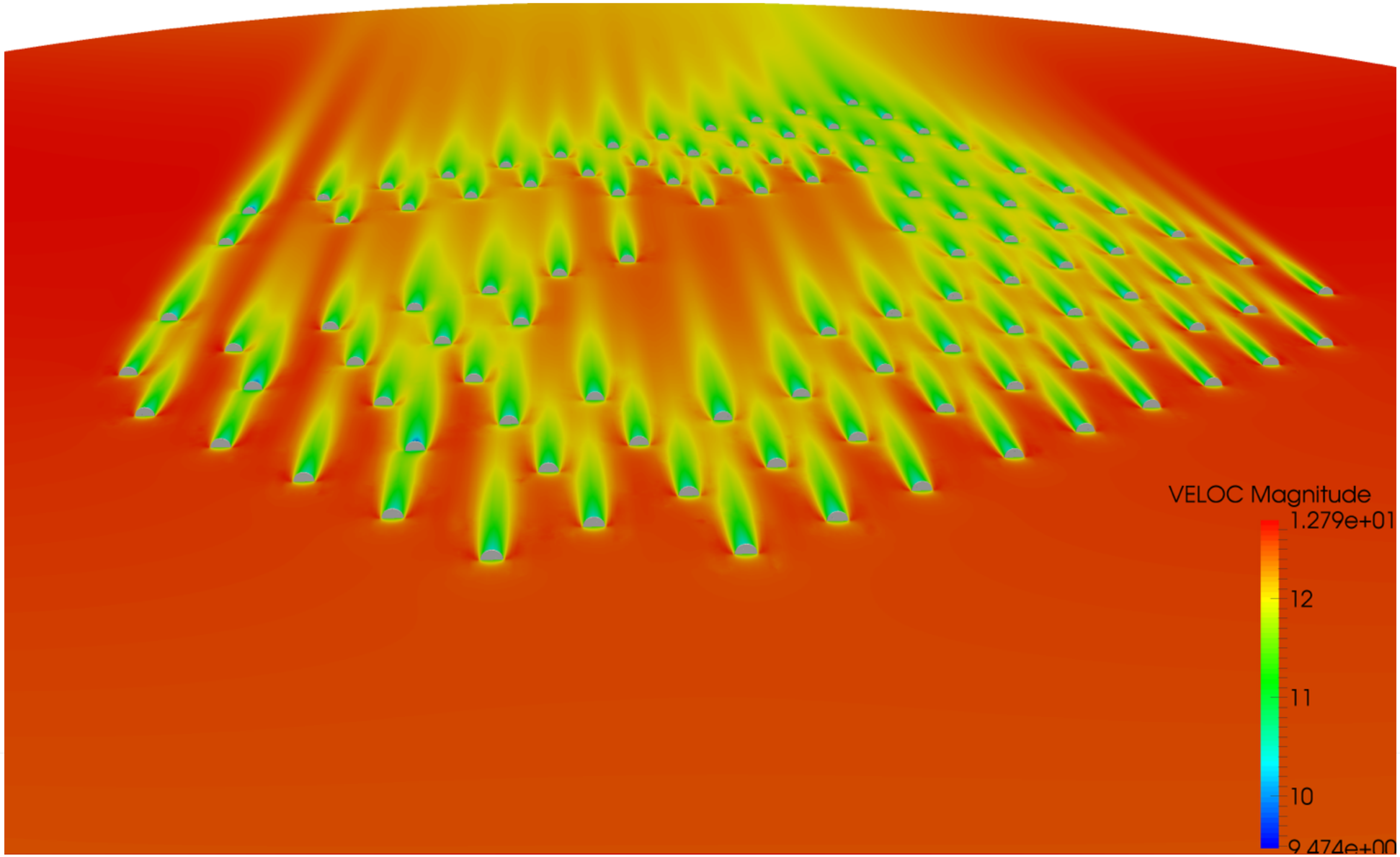
VALIDATION (SEXBIERUM)



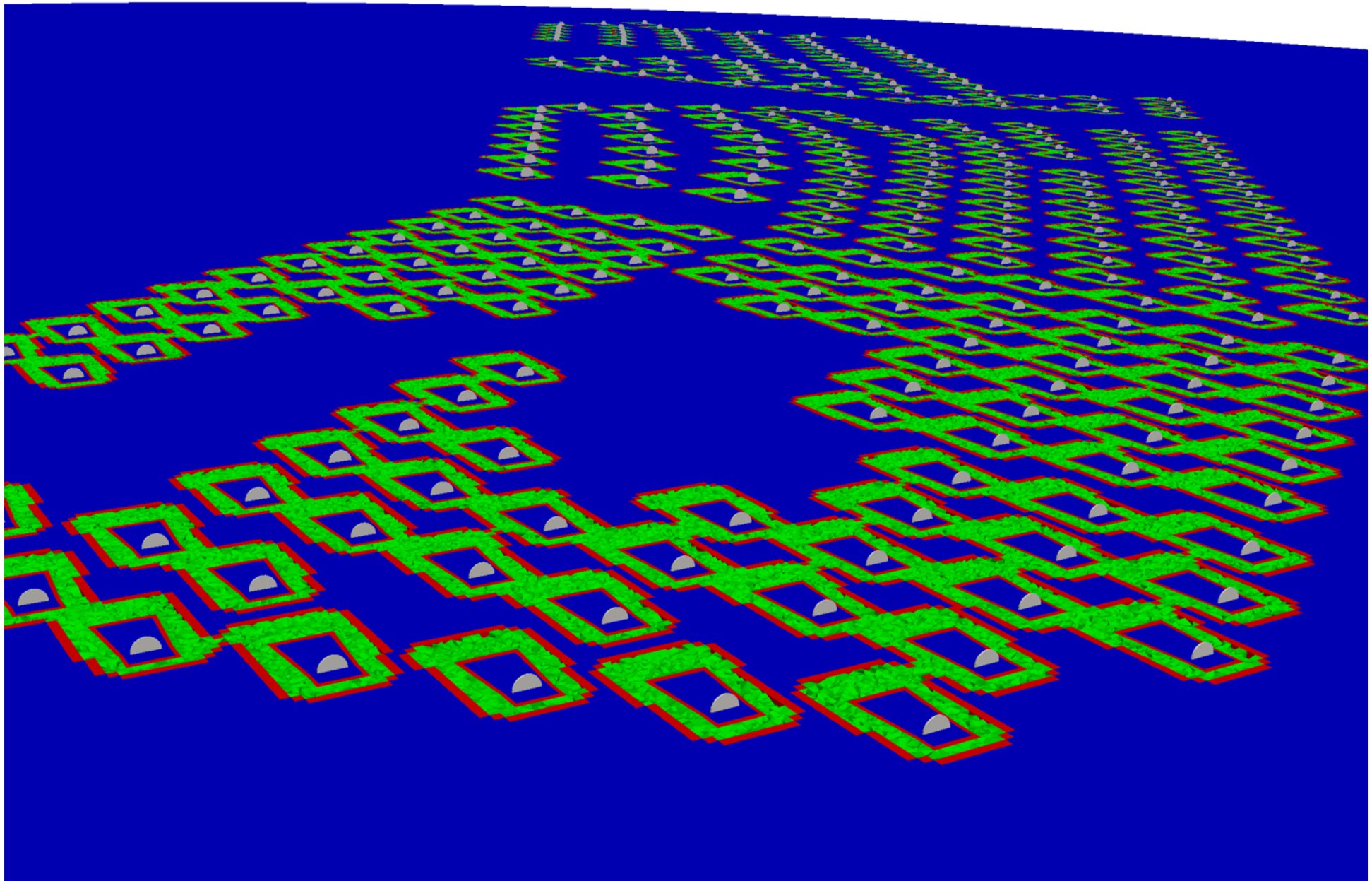




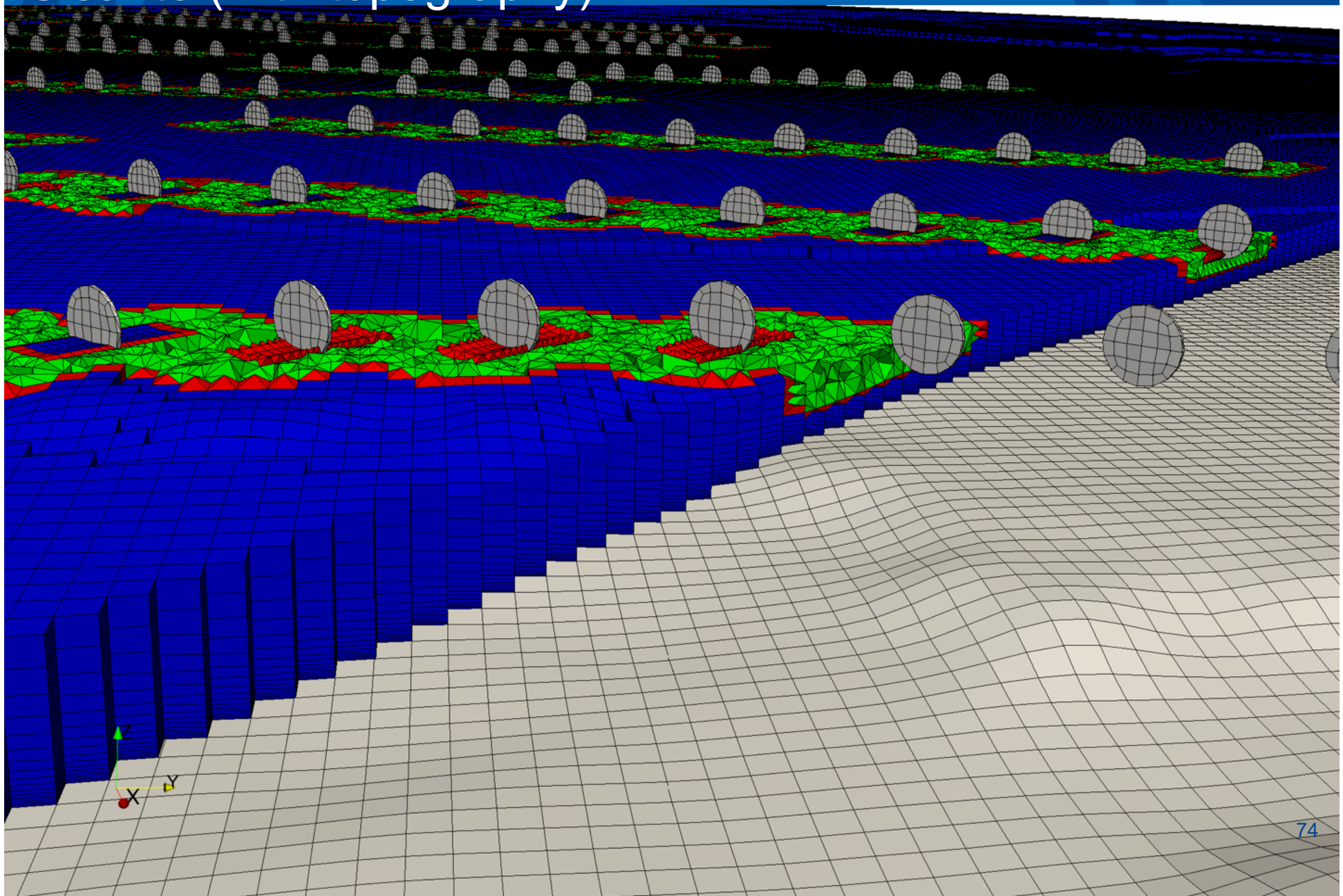
WODS (just Iberdrola)



WODS (complete)



Sisante (with topography)



Thank You!

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