Towards Next Generation Engineering Simulations

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Nuexas

Abel Coll

VELaSSCo

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Layout

- **Our Vision @CIMNE (Numexas & Others)**
  →Simulation Pipeline

- **Do engineering simulations play a role in the HPC context?**
  - **Going large is nice for scalability**
  - **Unfortunately might not be too important from an engineering point of view.**

  →TIME/COST TO SOLUTION rules

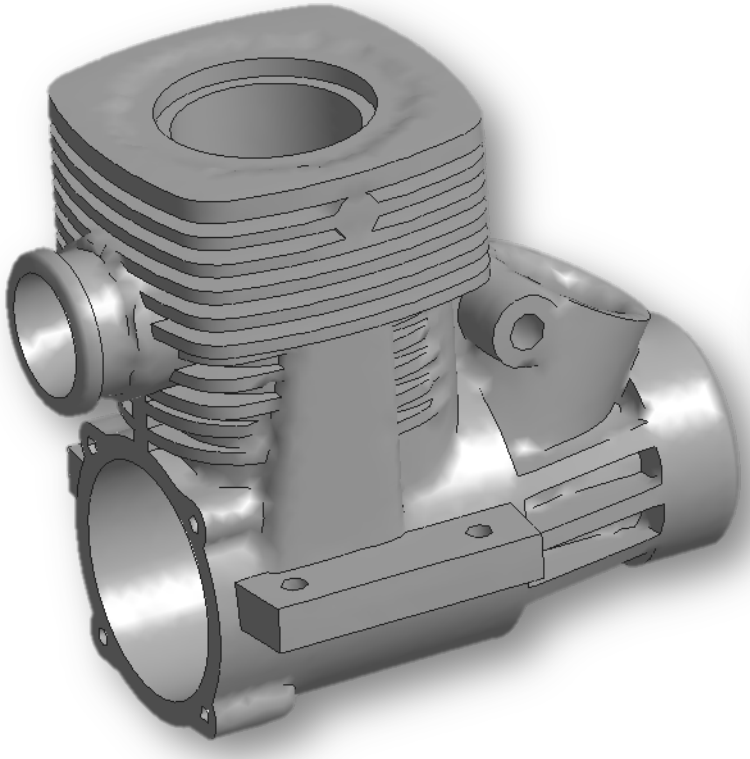
- **Practical Difficulties/petitions to other projects in the area**

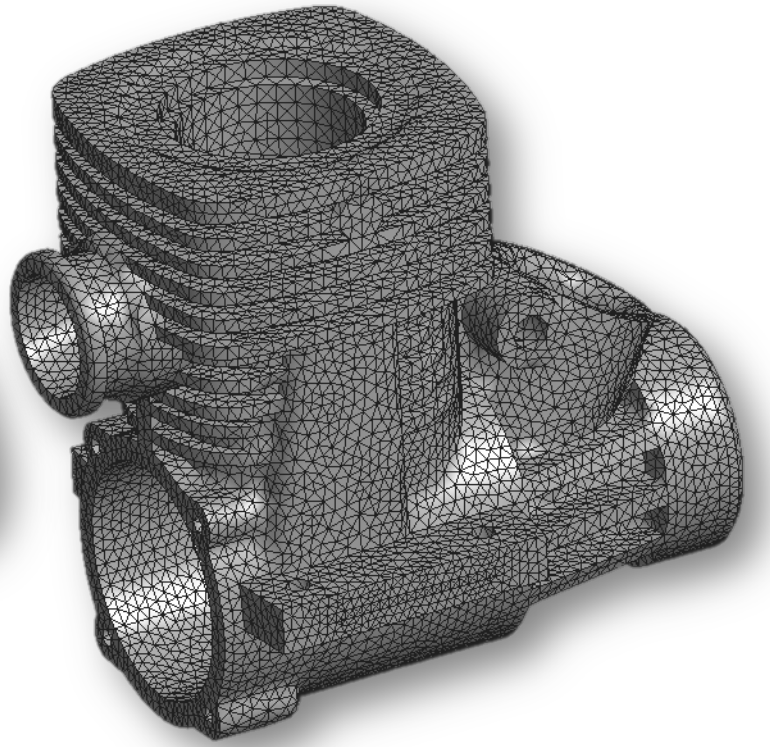
VISION

Industrial Simulation

→ we do not want to solve “cubes” !!

- Reducing calculation time by parallelization
- **Modeling** and Visualization are the bottleneck





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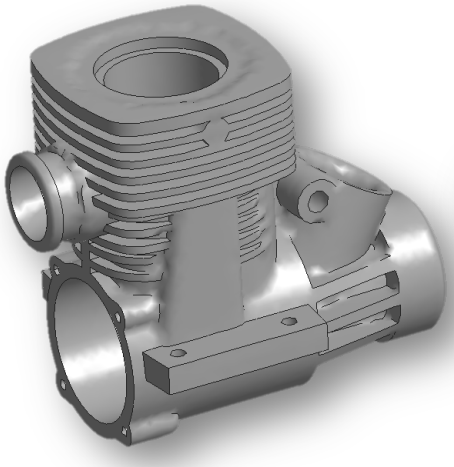
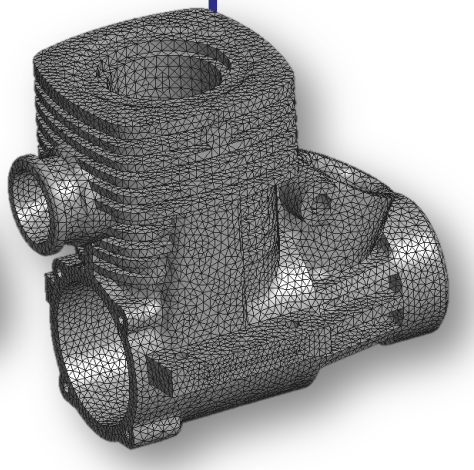
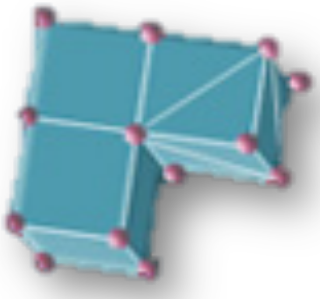
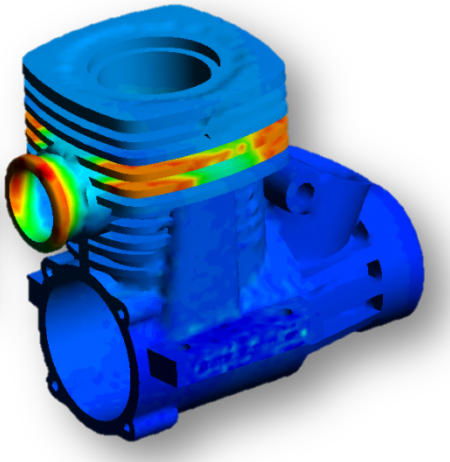
Motivation

Simulation Pipeline









Modeling

- Not Clean Geometry
- Complex Models

Meshing

- Robustness
- Not Scalable

Analysis

- IO
- Scalability
- Efficiency
- Complexity
- Heterogeneous Machines

Visualization

- Connection to the Servers
  - Internet
- Limited local resources
  - Small laptops, tablets, mobiles

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NUMEXAS

Vision (HPC + Big Data + Cloud)

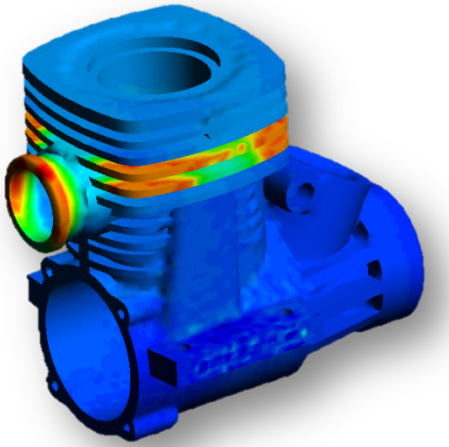
"CLOUD"

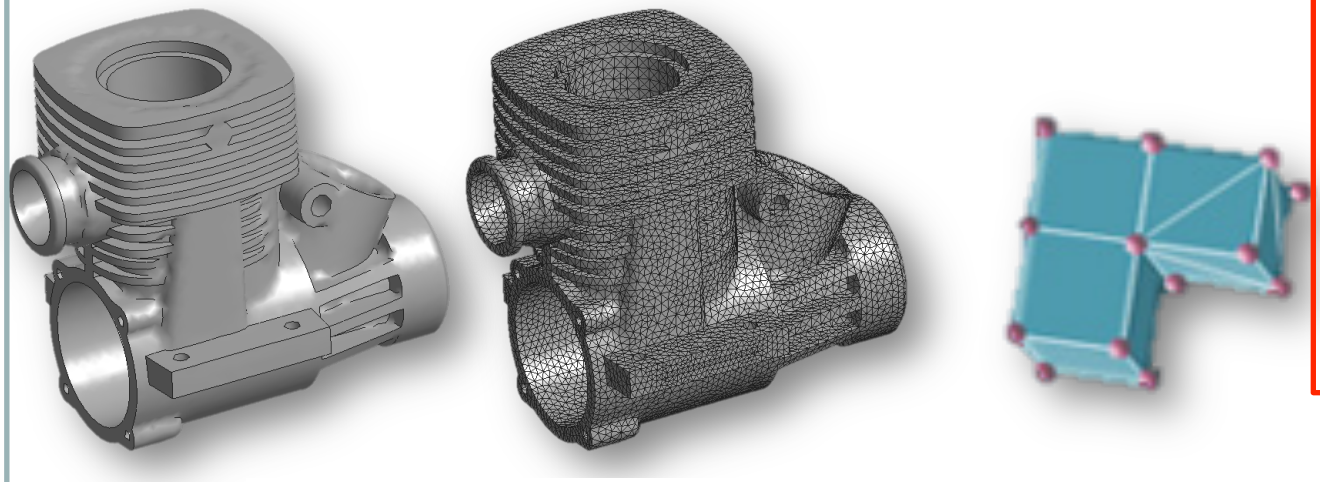
FORTISSIMO

CastInCloud

Read it as "democratize"

The results of the other projects





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"BIG DATA"

Nuxeas

"HPC"

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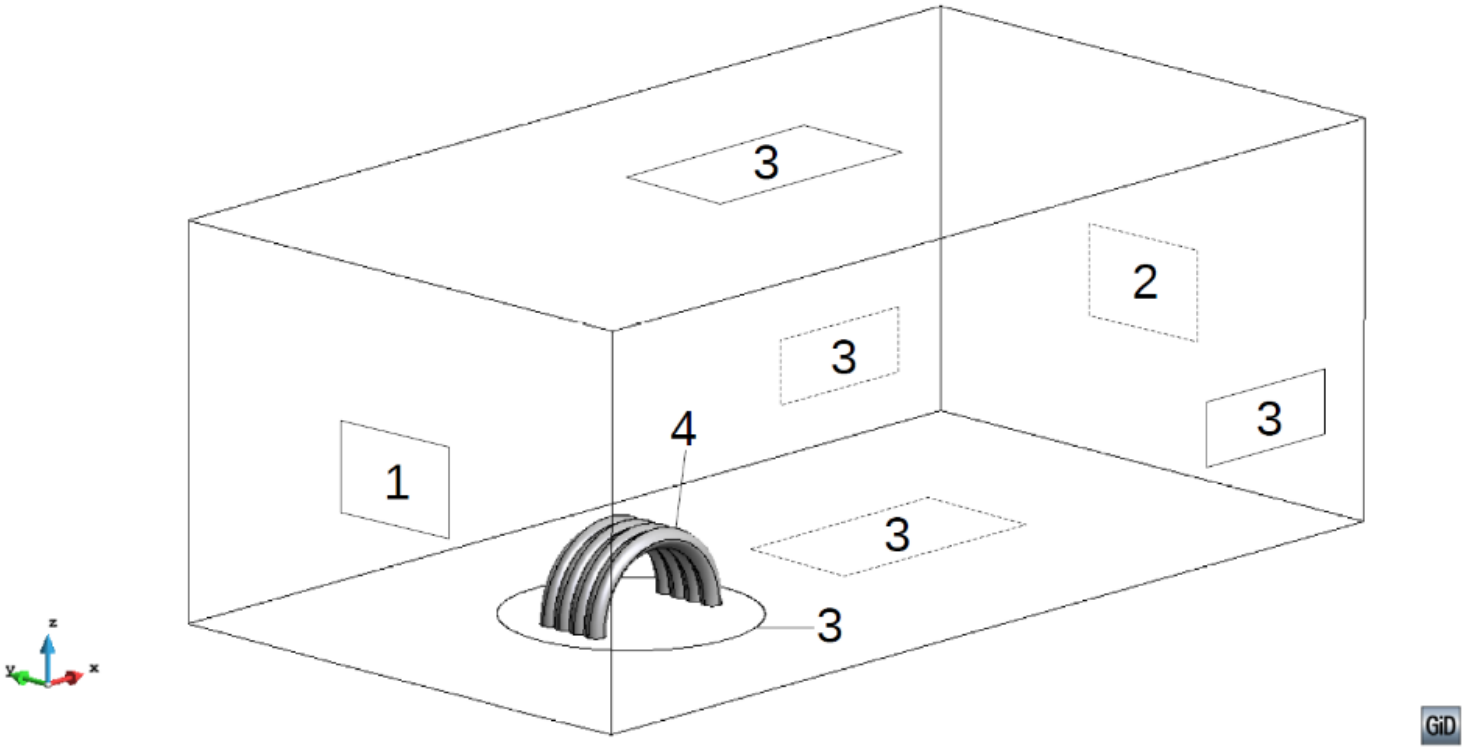
Where are we: today's tech

Works satisfactorily *if you complete the pipeline!*



Fluid Model is validated in controlled configurations. → A lot of validation is going on in collaboration with Dr. Larese and Dr. Wüchner @TUM

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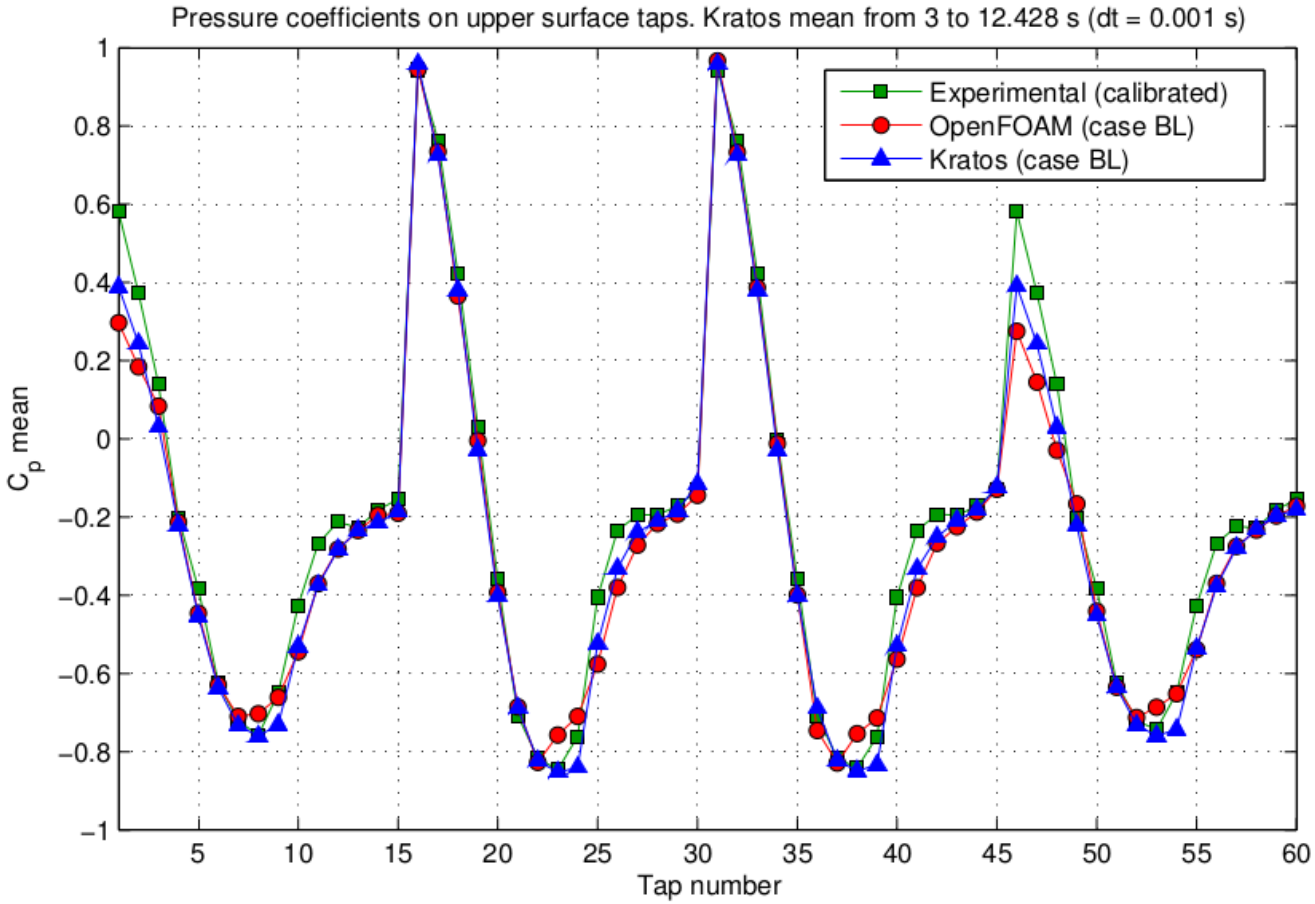

Fluid Model is validated in controlled configurations

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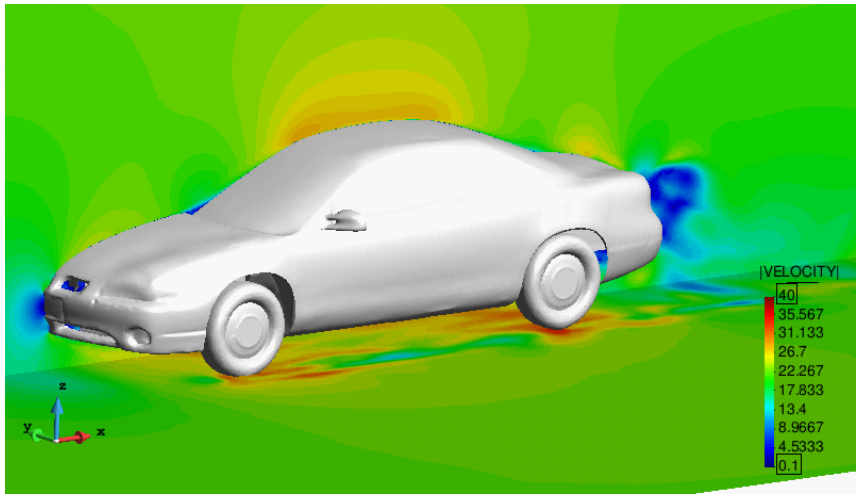
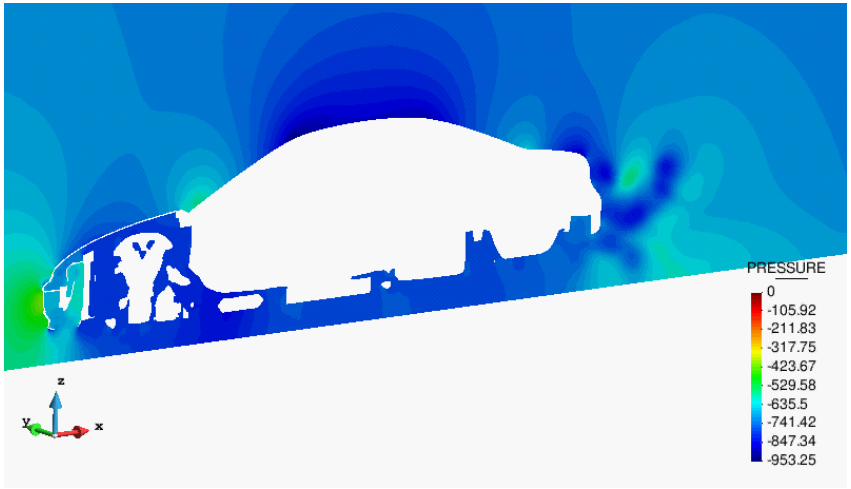
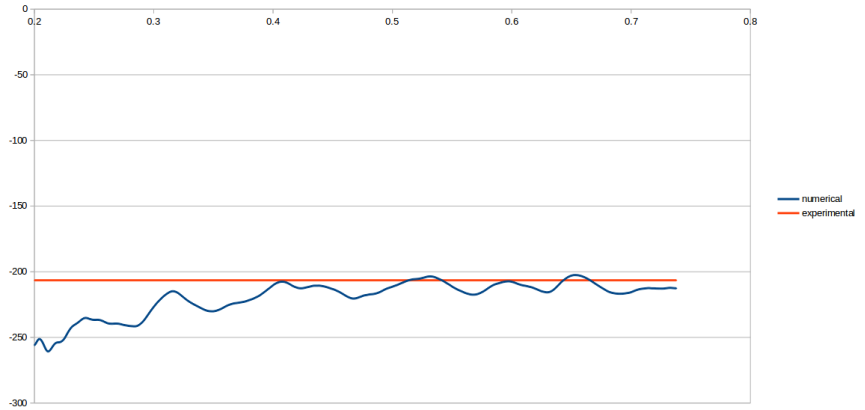
And you can do very complicated things … *if someone gives you a suitable mesh*





MODEL COURTESY OF
Dr. Facundo Del Pin
LS-DYNA



NUMERICAL VS EXPERIMENTAL DRAG

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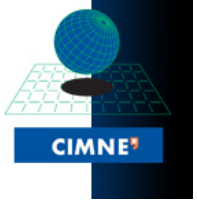
One of the research lines in NUMEXAS was to use "embedded" techniques to Deal with the first 3 points in the pipeline



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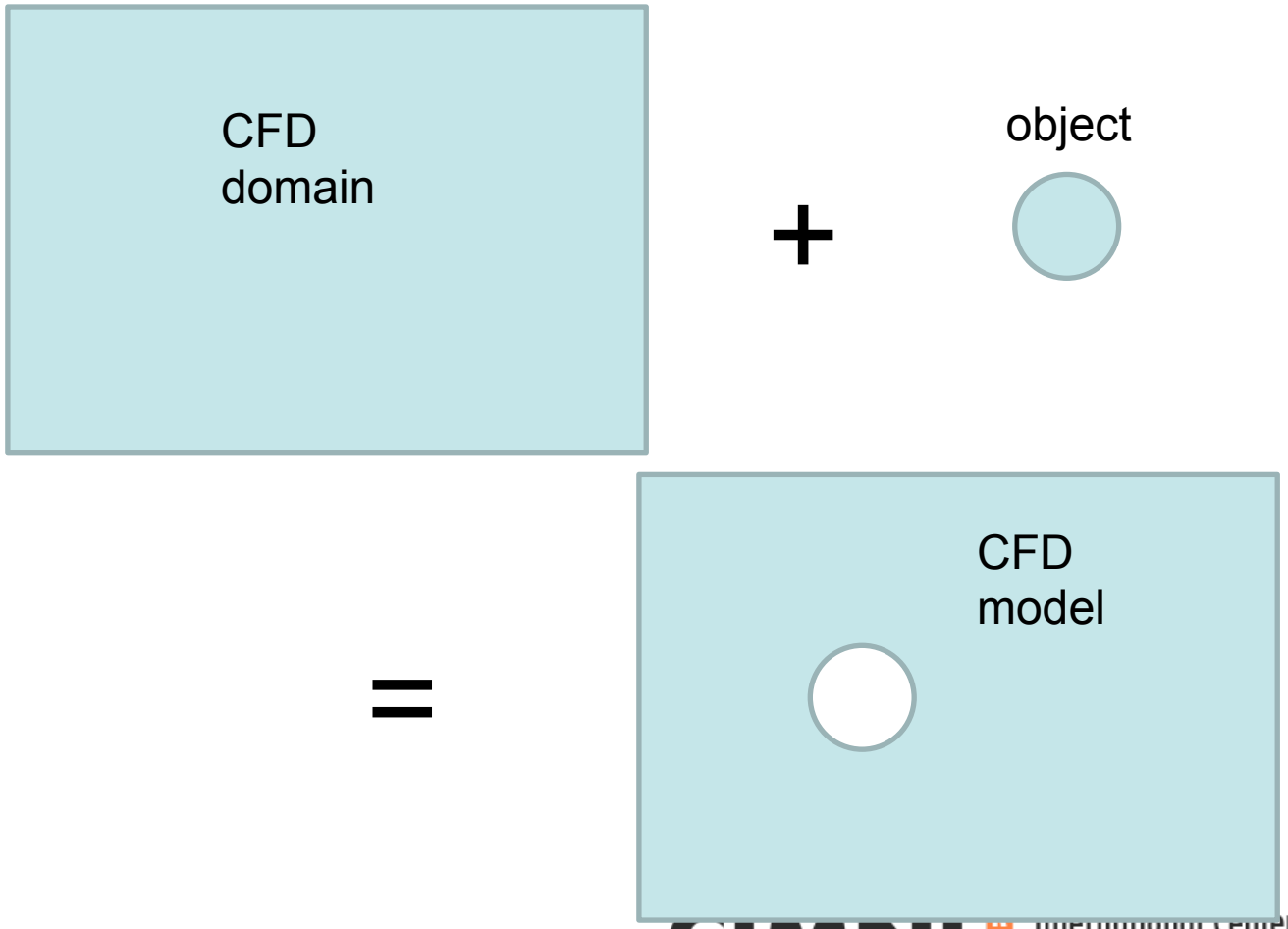
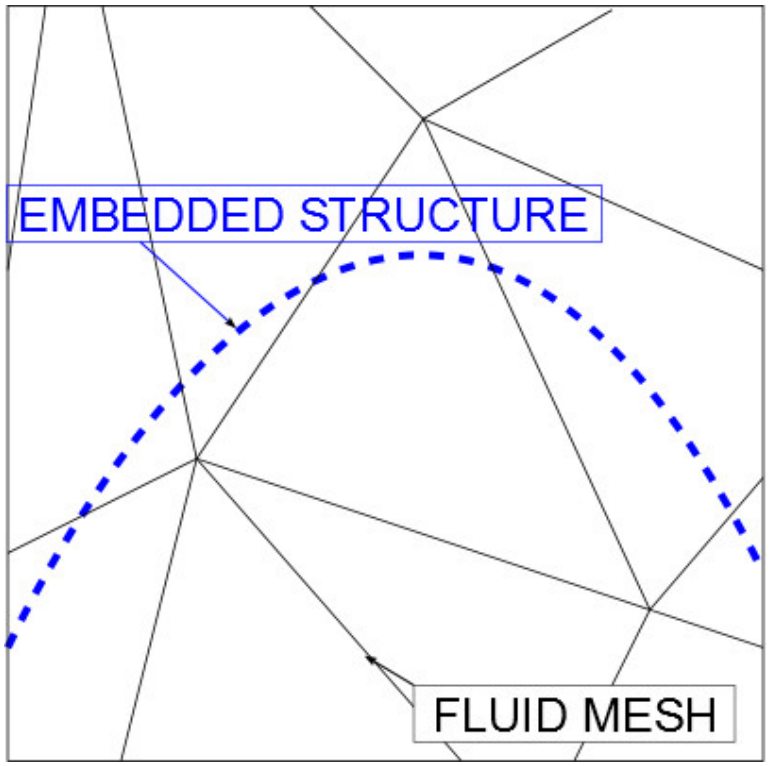
Essential Idea of Embedded Solvers (may know it as Immersed CFD)

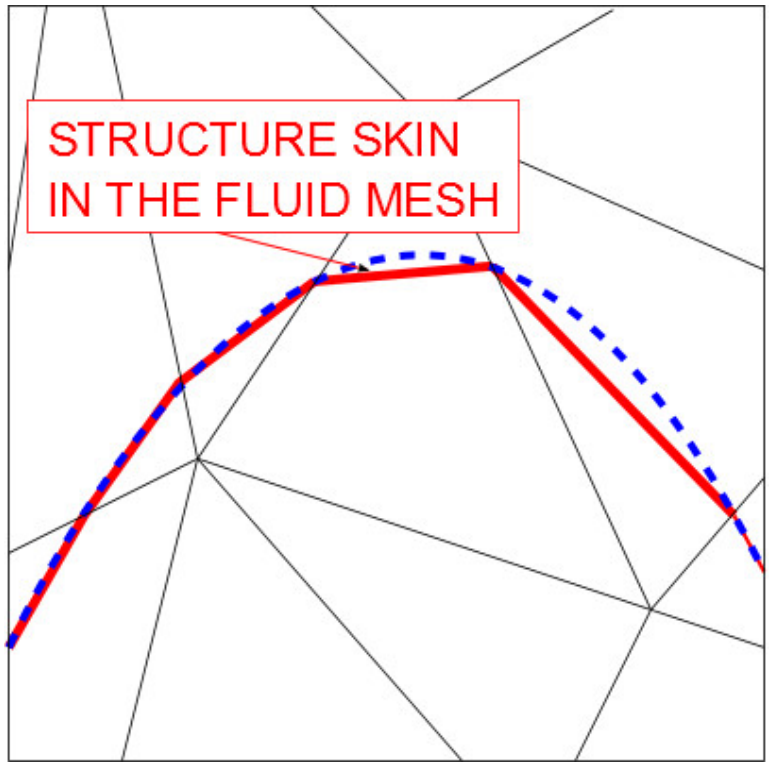
CARVE OUT “a hole” in the CFD mesh



Essential Idea of Embedded Solvers (may know it as Immersed CFD)

CARVE OUT "a hole" in the CFD mesh →
Geometry is approximated as possible → NEEDS FINE MESHES → …and HPC hardware!





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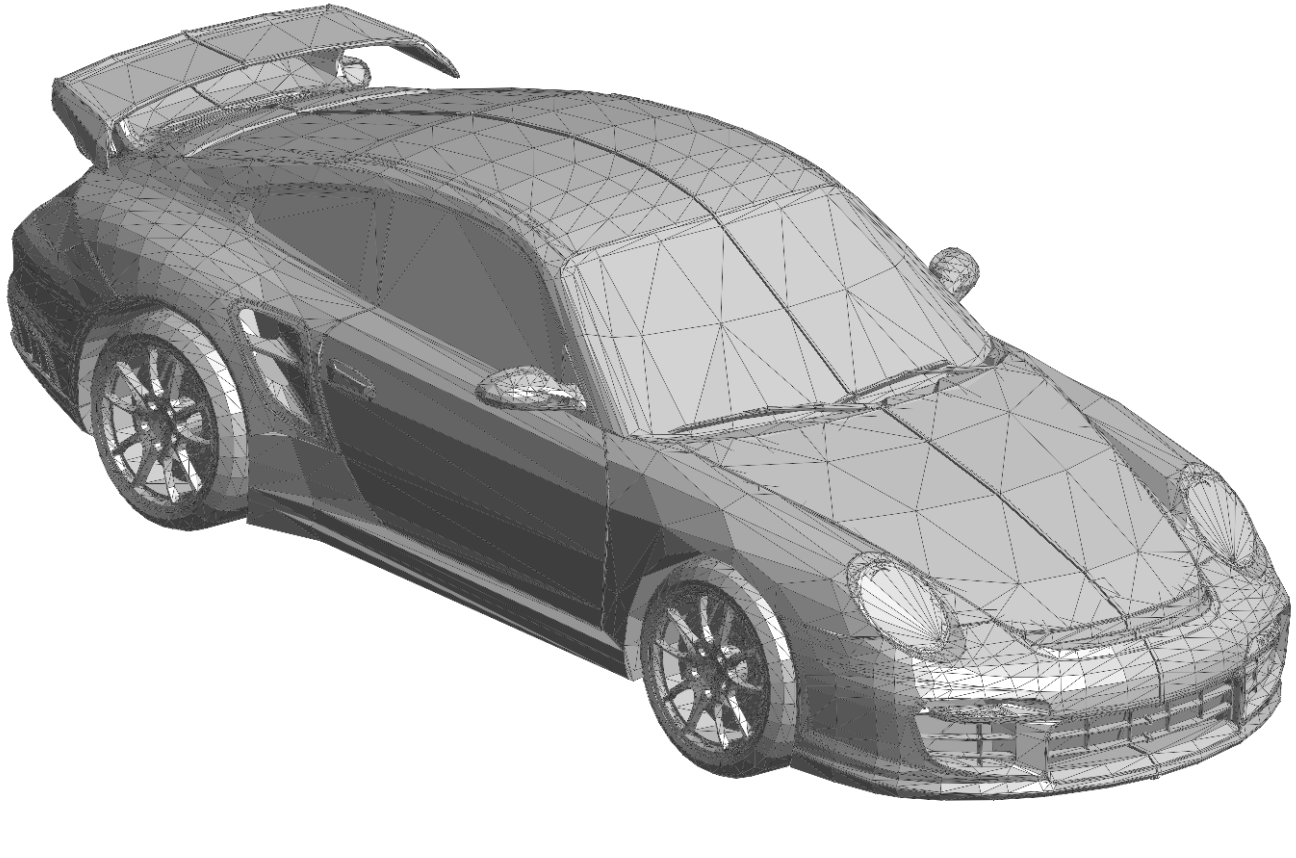
CFD for bodies without a well-defined internal volume



Model as imported from .dae model

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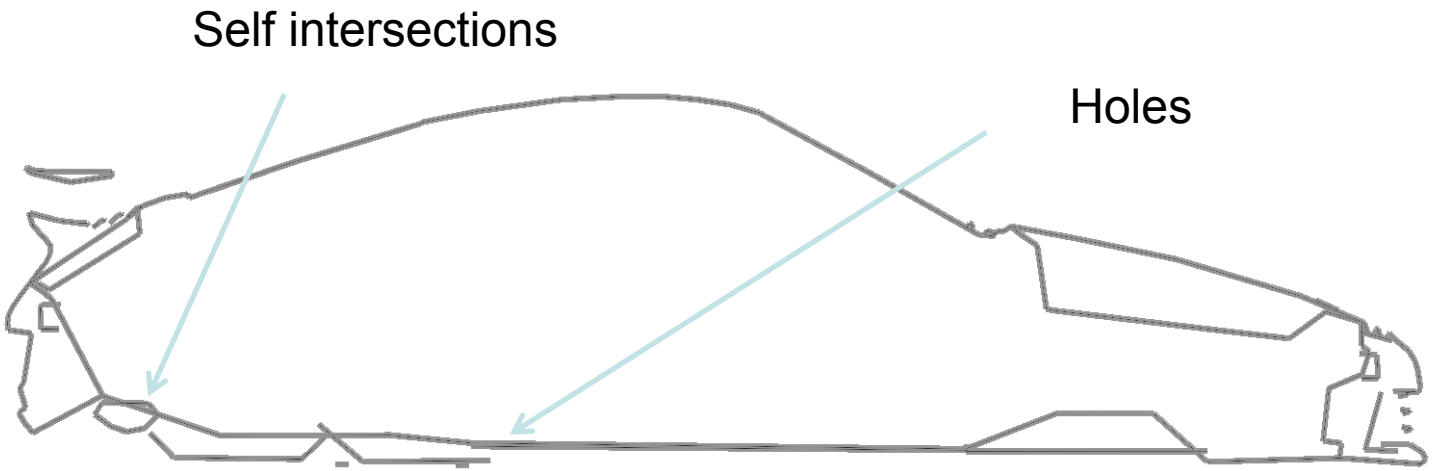
CFD for bodies without a well-defined internal volume



Cut along the center plane – openings and overlaps are apparent

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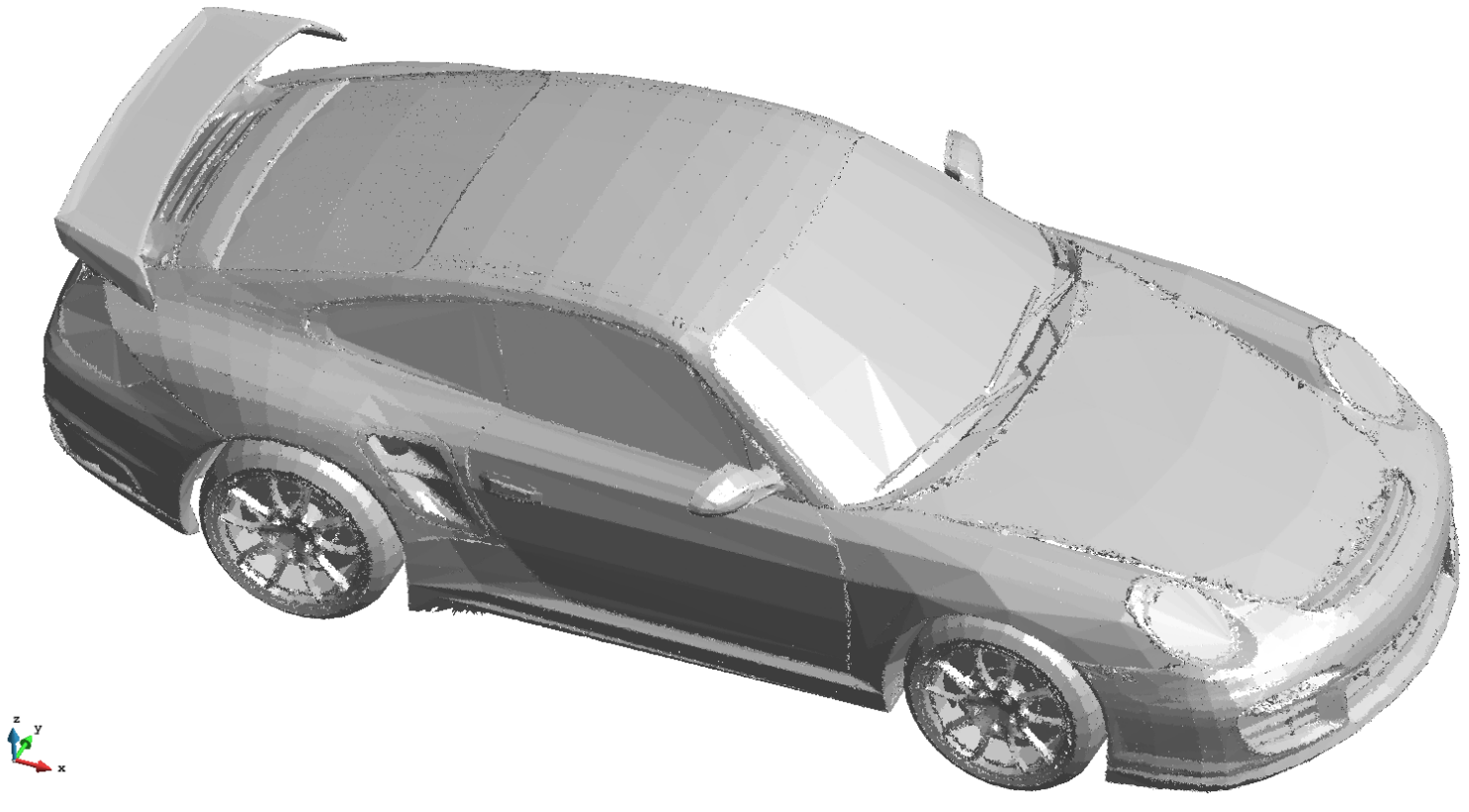
CFD for bodies without a well-defined internal volume



View of the **RECONTRUCTED** geometry (what is actualy taken into account by the flow solver) – **FINE CFD MESH** (By Adaptive Mesh Refinement)

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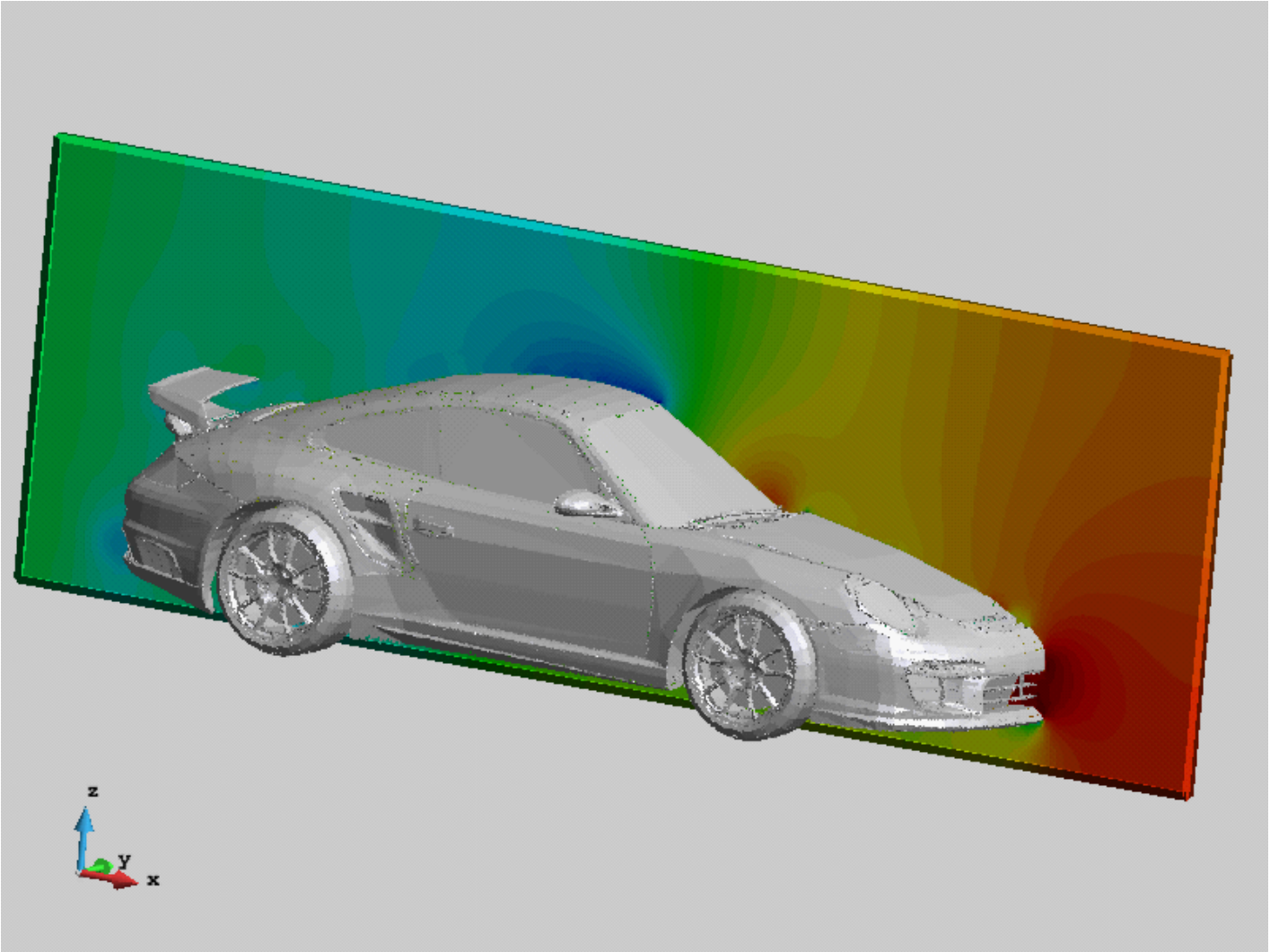
CFD for bodies without a well-defined internal volume



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Do engineering simulations play a role in the HPC context?

Of course!

…however …

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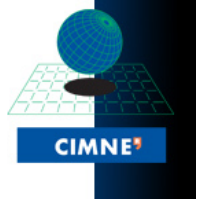

…In HPC,we all tend to do a trick: GO LARGE to be very scalable

The idea is simple … a lot of local work hides the communication cost.

This is the reason for which we all present very large simulations

City of Barcelona

Nuexas

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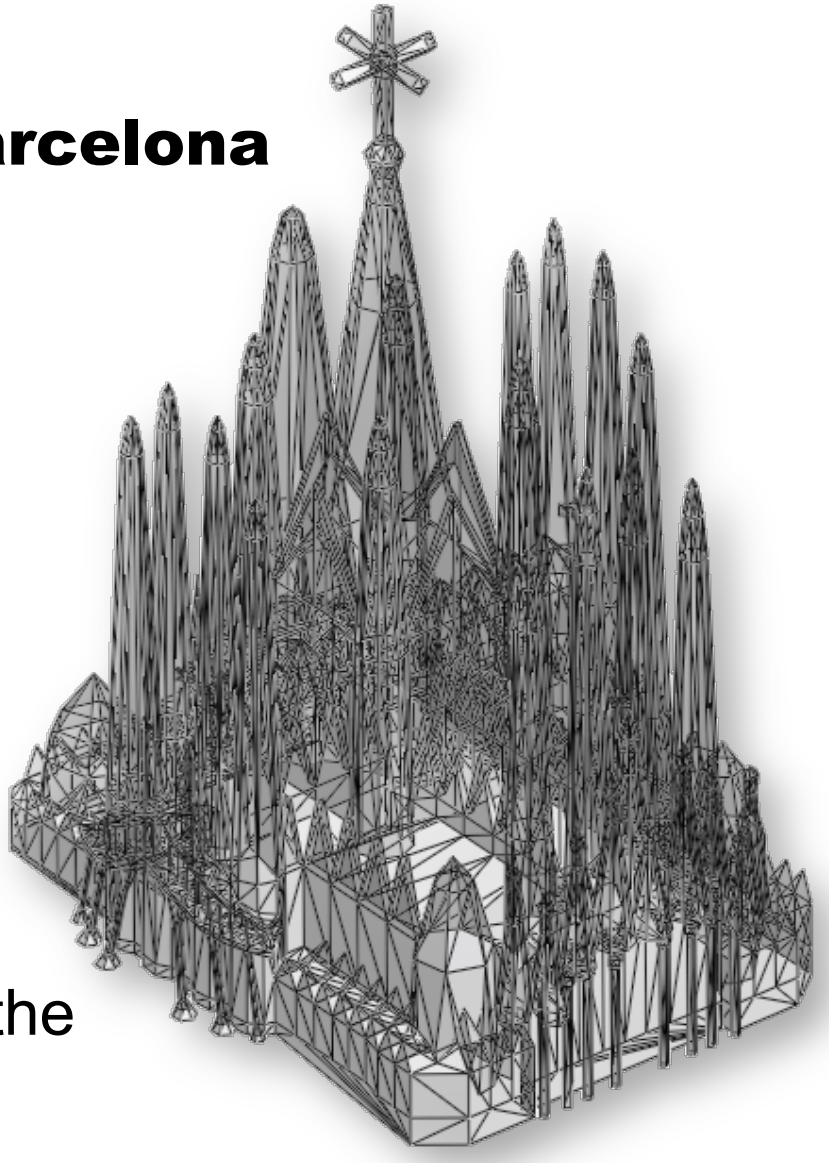
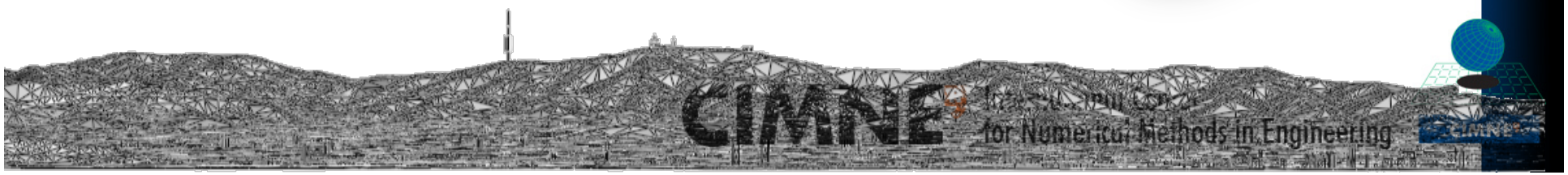


We are in Barcelona

Barcelona Media provide us the model of Barcelona



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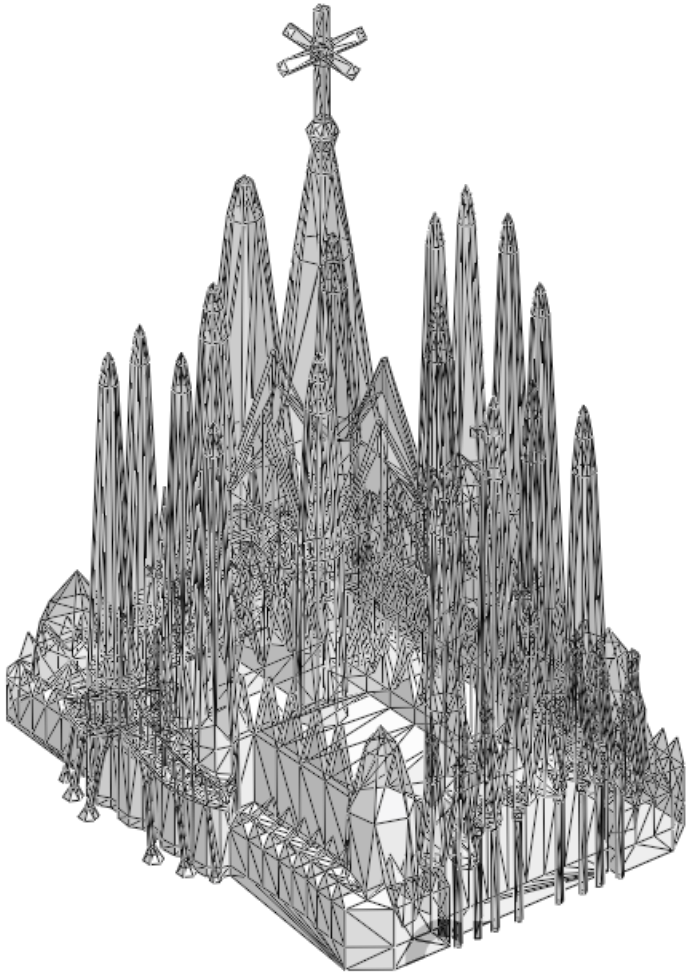
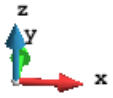
Going Large

5k Surfaces





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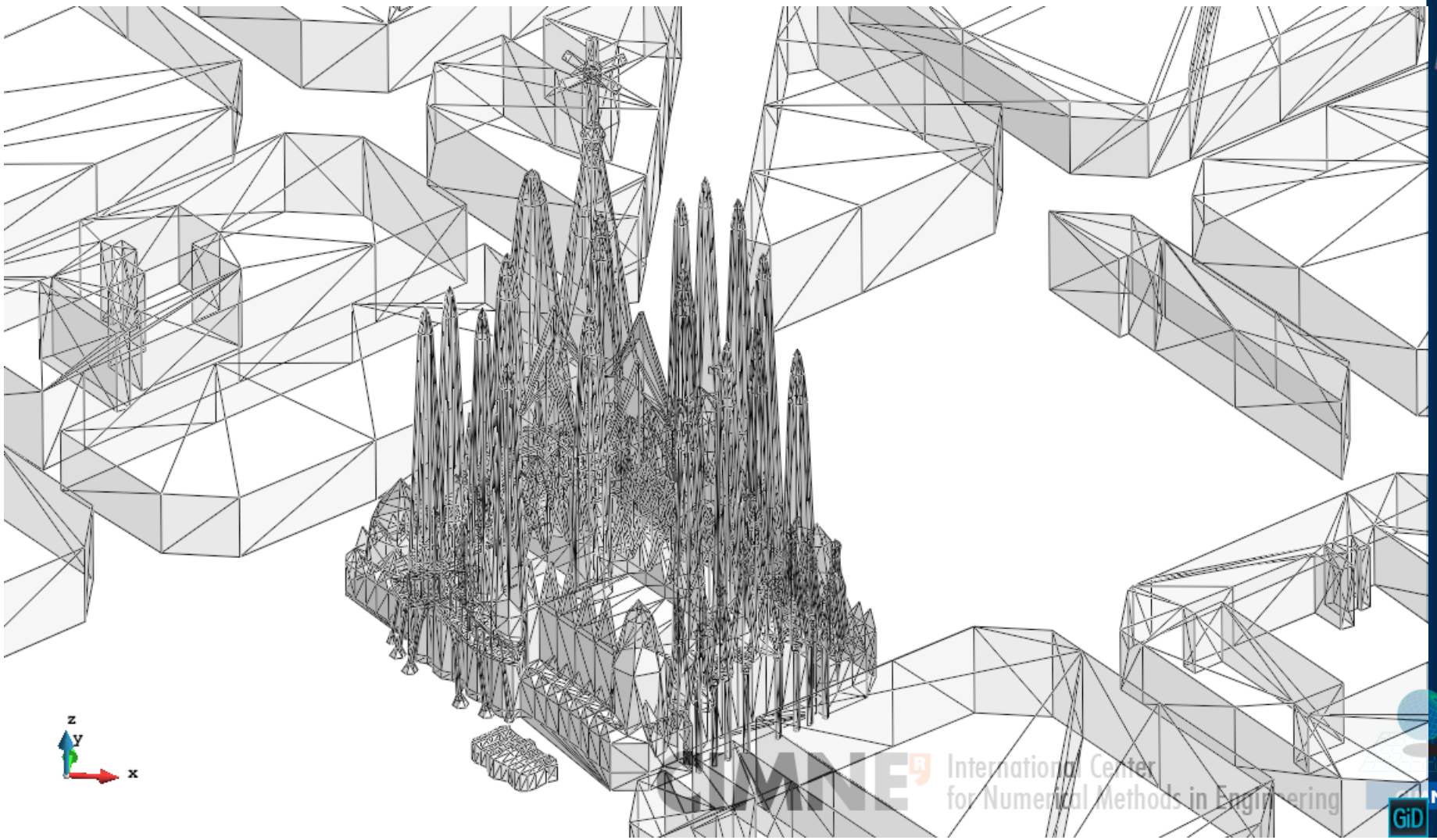
Nu exas

GiD

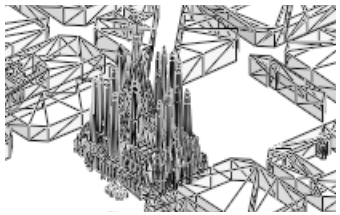
Going Large

7k Surfaces



Going Large

7k Surfaces



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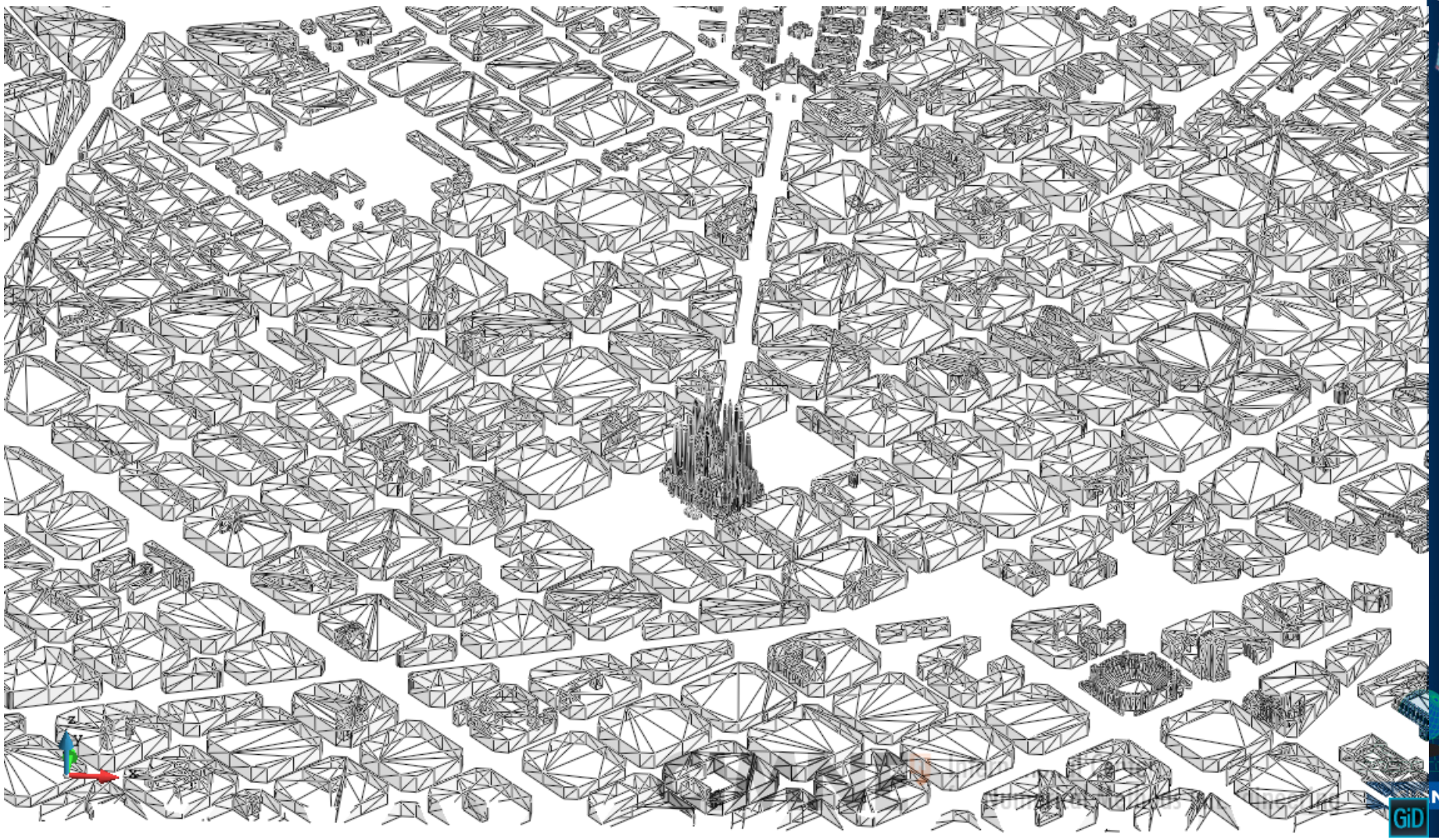
KRATOS MULTI-PHYSICS

Nu exas

Going Large

26k Surfaces



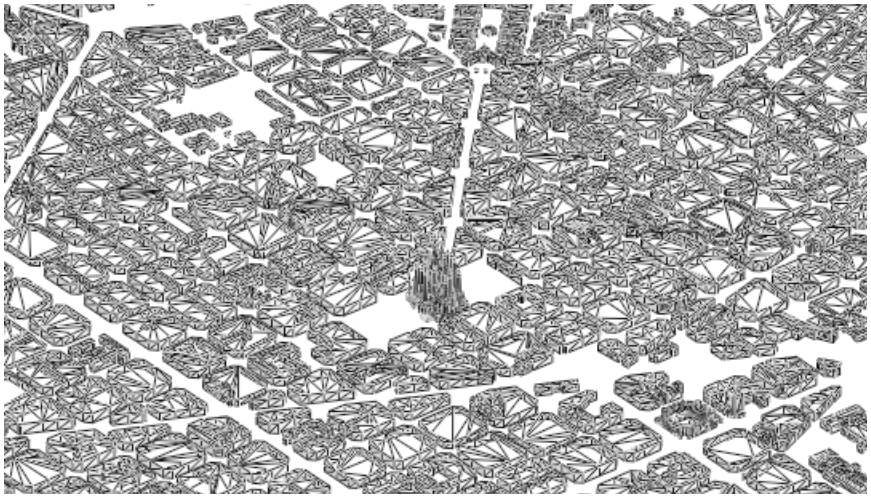
KRATOS MULTI-PHYSICS

Nu exas

GiD

Going Large

26k Surfaces



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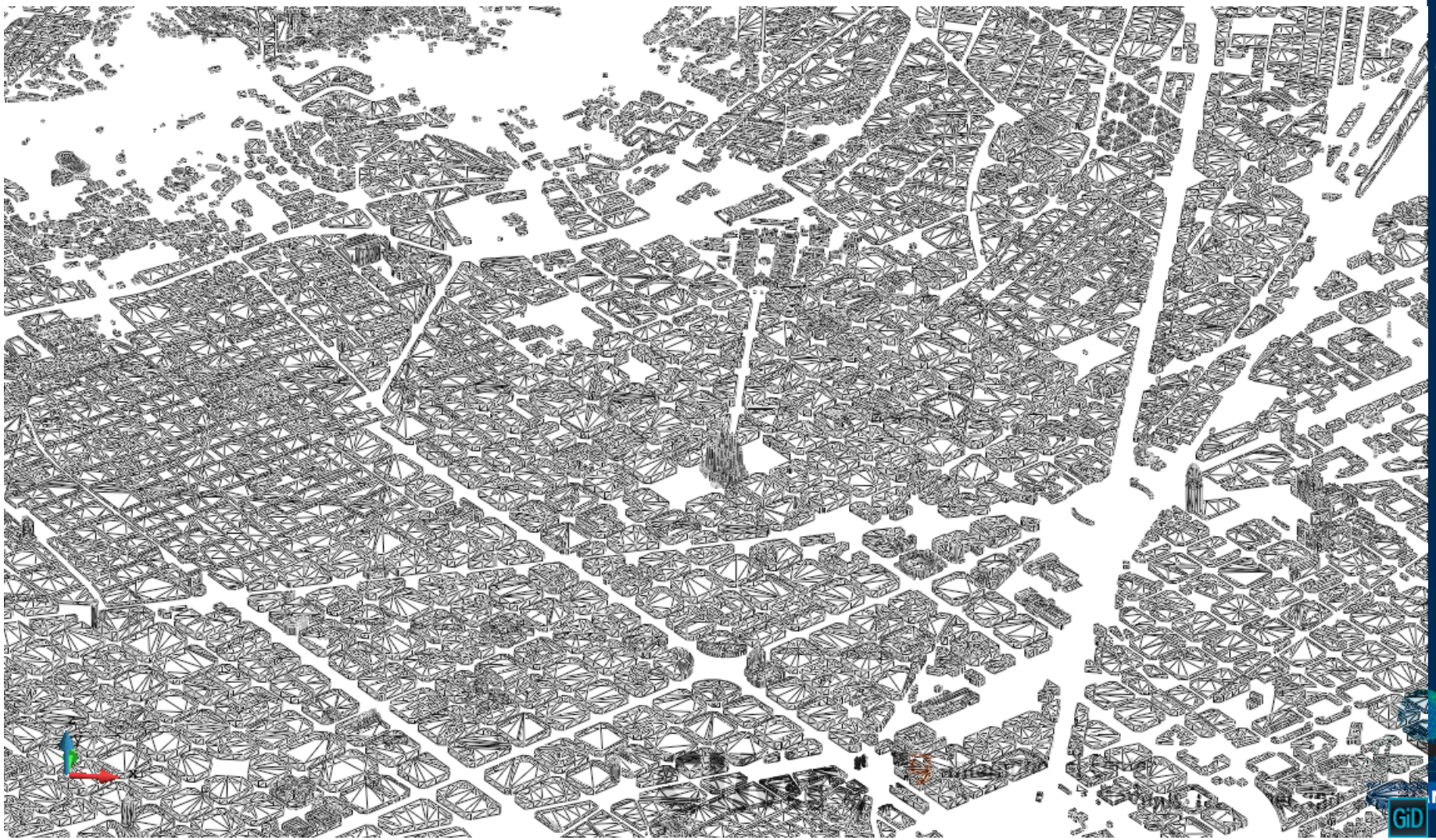
KRATOS MULTI-PHYSICS

Nu exas

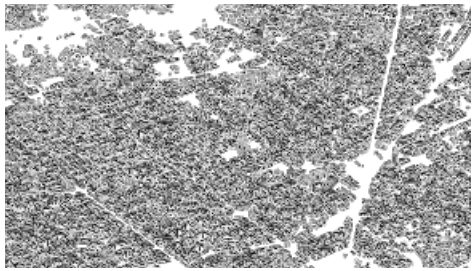
Going Large

130k Surfaces



Going Large

130k Surfaces



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KRATOS MULTI-PHYSICS

Nuexas

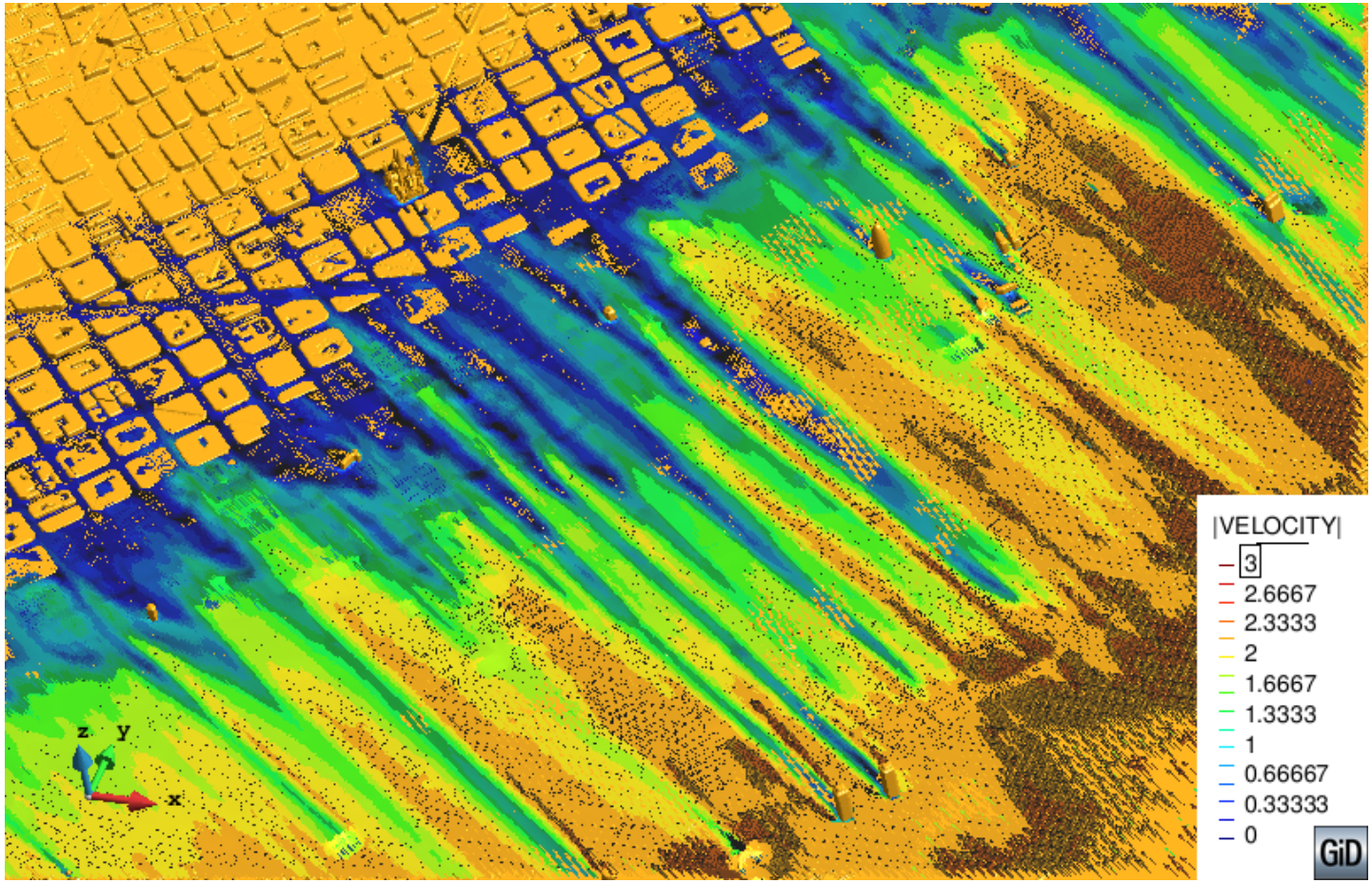
Going Large

797k Surfaces

Going Large

846k Surfaces

Barcelona→detail of “Sagrada Familia”



400M elements correspond to a resolution of 4m.

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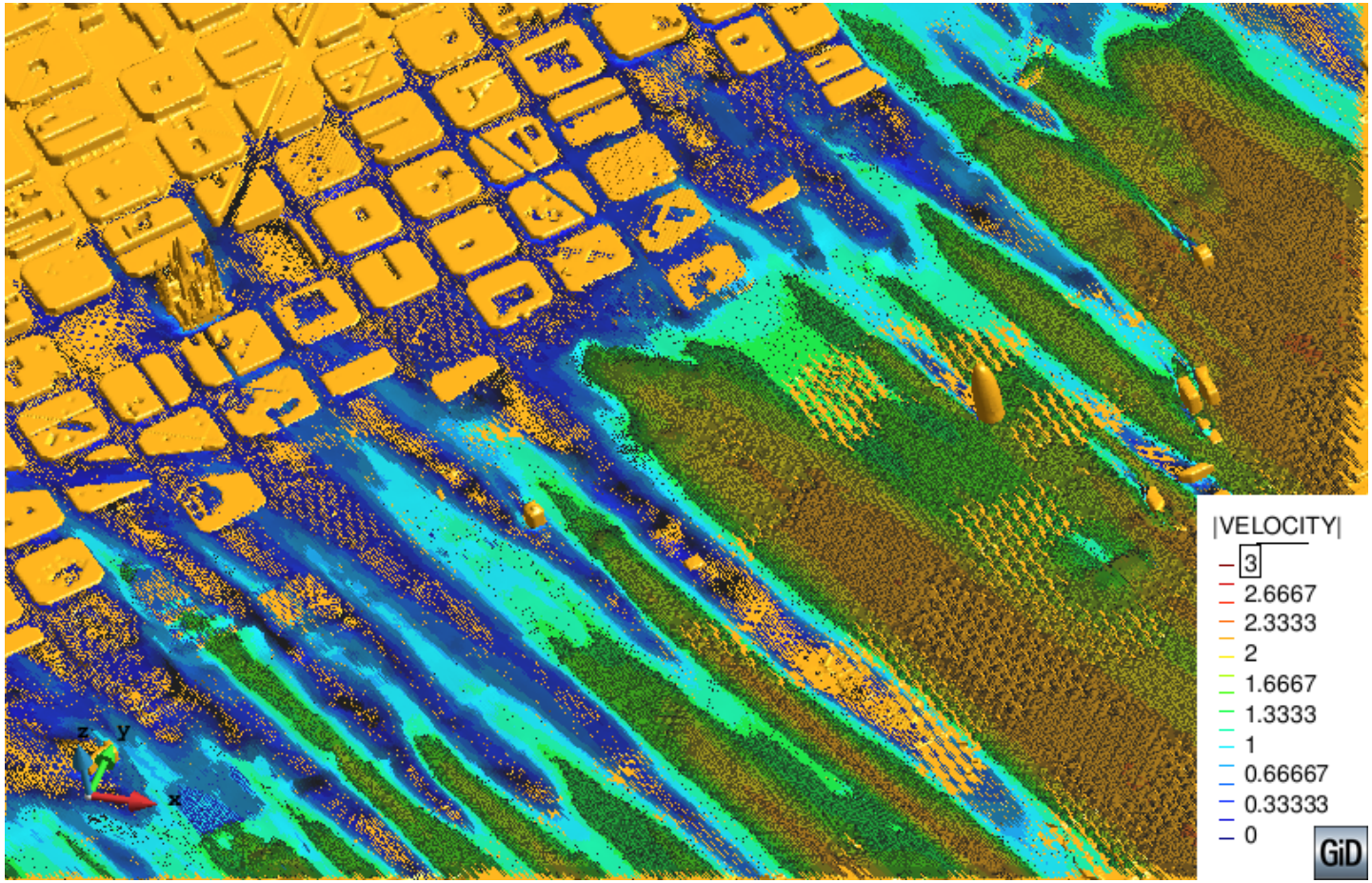
KRATOS MULTI-PHYSICS

Nuexas

Barcelona→detail of “Sagrada Familia”



400M elements correspond to a resolution of 4m.

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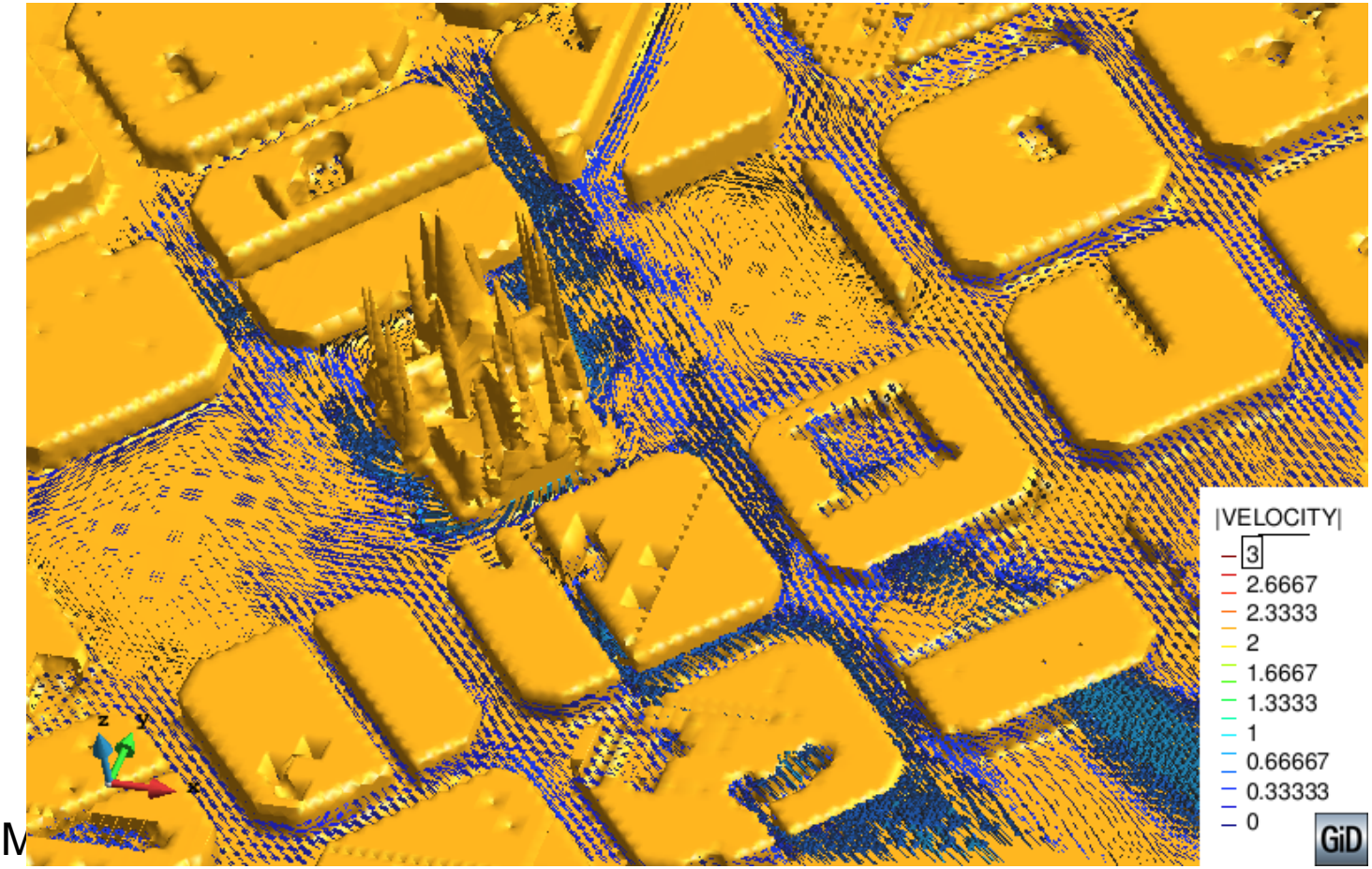
Nuexas

Barcelona→detail of “Sagrada Familia”



M

400M elements correspond to a resolution of 4m.

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The Engineering Community is not interested in going large *per se*

Industrial goals (according to our SME Industrial partners) :

- Reduce TIME TO SOLUTION
  - Pre-processing time
  - Solution time
  - Post-processing time
  - “idle time” (waiting in the queue, transferring data, etc)

Typical Scenarios may be:

- Fixed problem sizes (typically only slightly larger than for “serial” calculations)
- We can see a **growing interest** towards usage of HPC in “**optimization**” → many small-scale parallel runs **(THIS IS ALSO AN IMPORTANT SCENARIO IN THE EXASCALE ERA!!)**

Codes are required to deliver consistent performance on next generation hardware → **DEAL GRACEFULLY WITH INCREASED LEVEL OF PARALLELISM**

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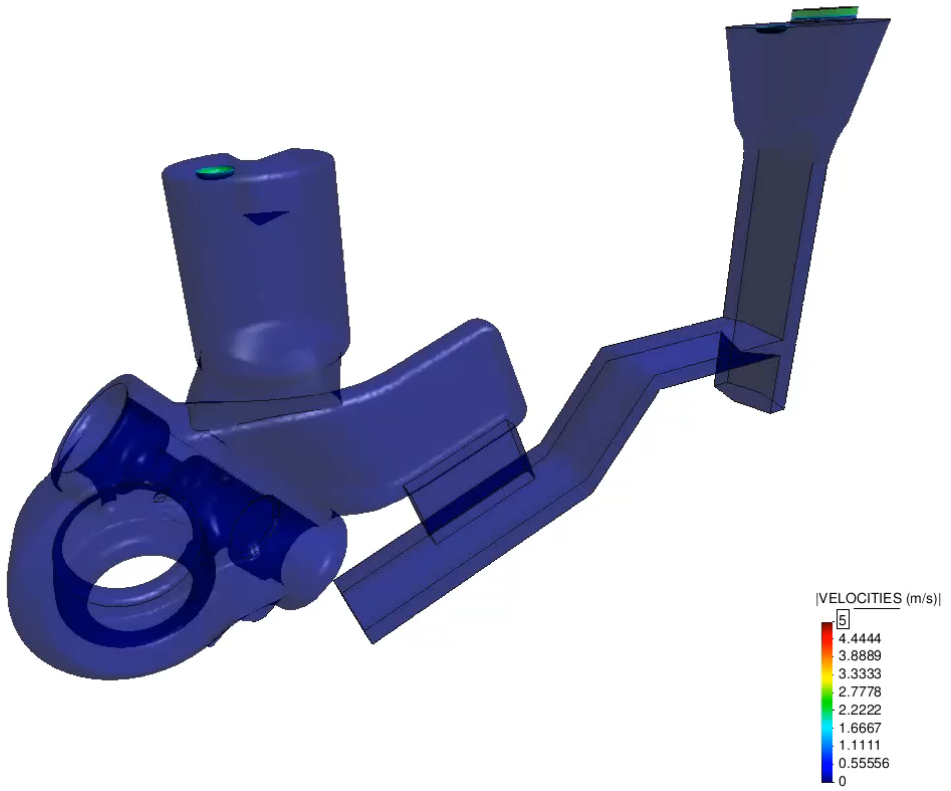
A RECENT CASE STUDY → casting simulation
(geometries by courtesy of Quantech & Altair)

Aluminium Casting Process

Geometries prepared with the Code “**Click2Cast**”. Developed at Quantech and CIMNE (body fitted here. Industry had the technology to generate the mesh)

(Uses the Kratos Flow solver)



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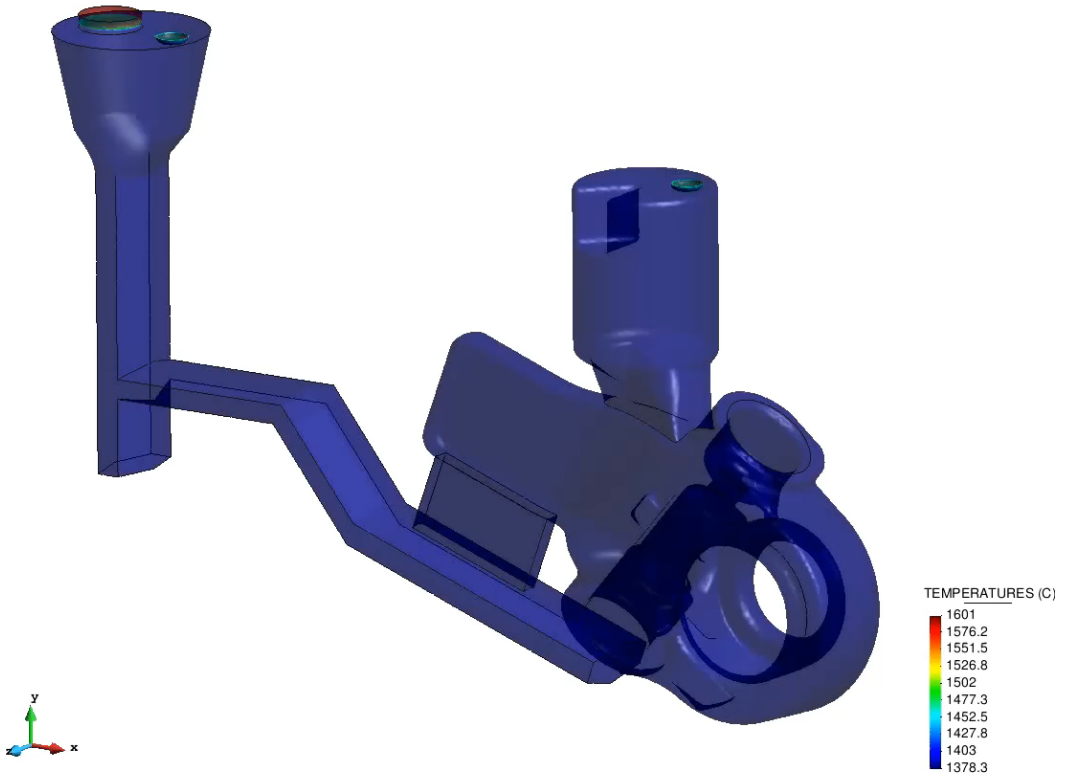
A RECENT CASE STUDY → casting simulation

(geometries by courtesy of Quantech & Altair)

Around 10M elements (larger than a standard serial case)



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A RECENT CASE STUDY → casting simulation
(geometries by courtesy of Quantech & Altair)

CASE SIZE: 10M elements

- **runtime**: approx 44min (800 non-linear time steps, using 192 cores on a Cray XC30) → DOWN FROM 2+ days for OpenMP versión

- **Time Uploading**: approx 10min
- **Time in the queue**: around 9h (met an occupancy peak ☹)

FORTISSIMO

- **Time Downloading**: around 2h
- **Time postprocessing**: around 3h

SOLUTION→ VELaSSCo

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The Idea of VELASSCO

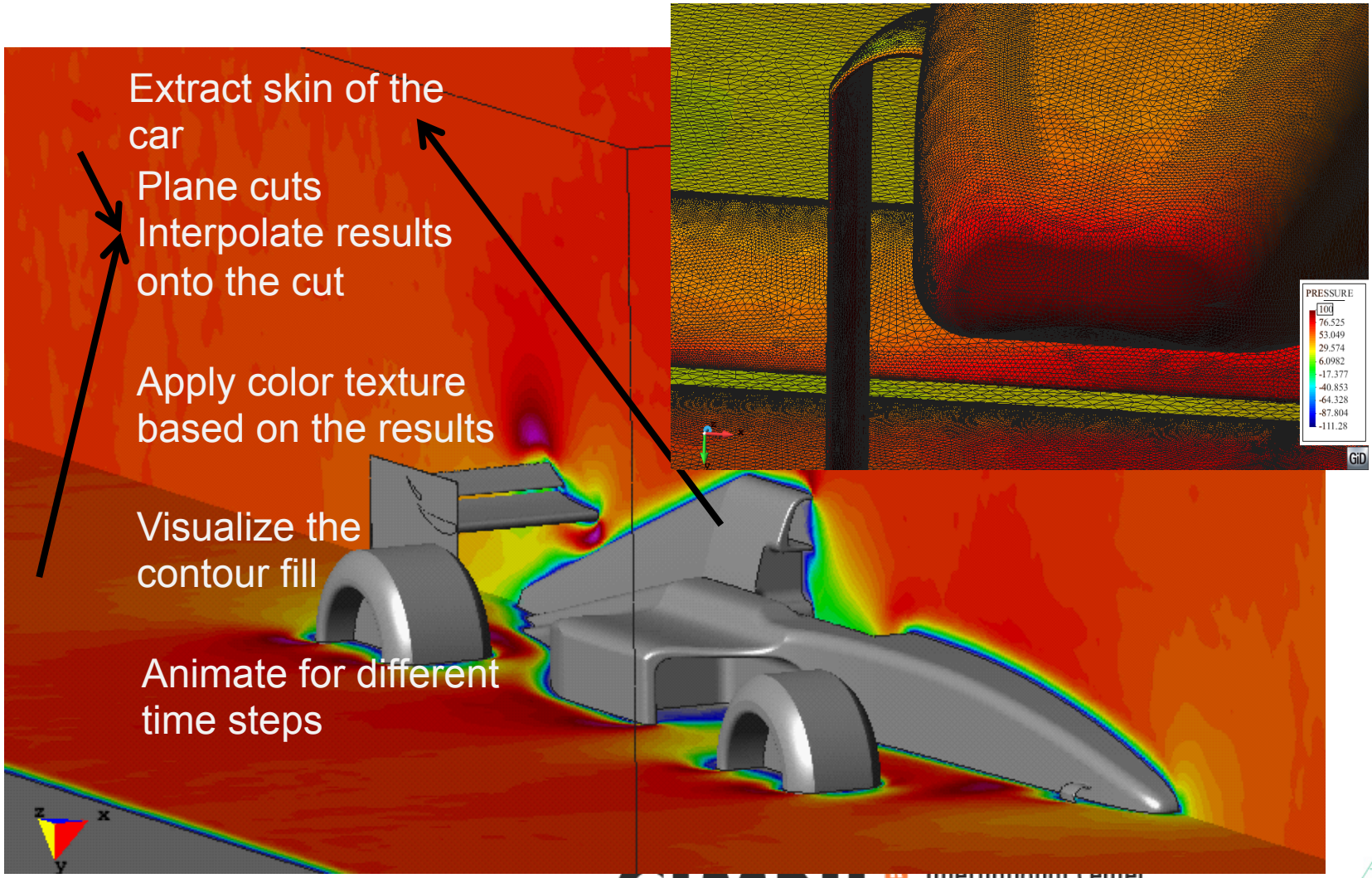
- Data are distributed in HPC computation nodes
- Data generated in the simulation:
  - Mesh
  - Results on mesh

  for each time step! (several thousands)

  (several GB per time step, TB for the whole simulation)

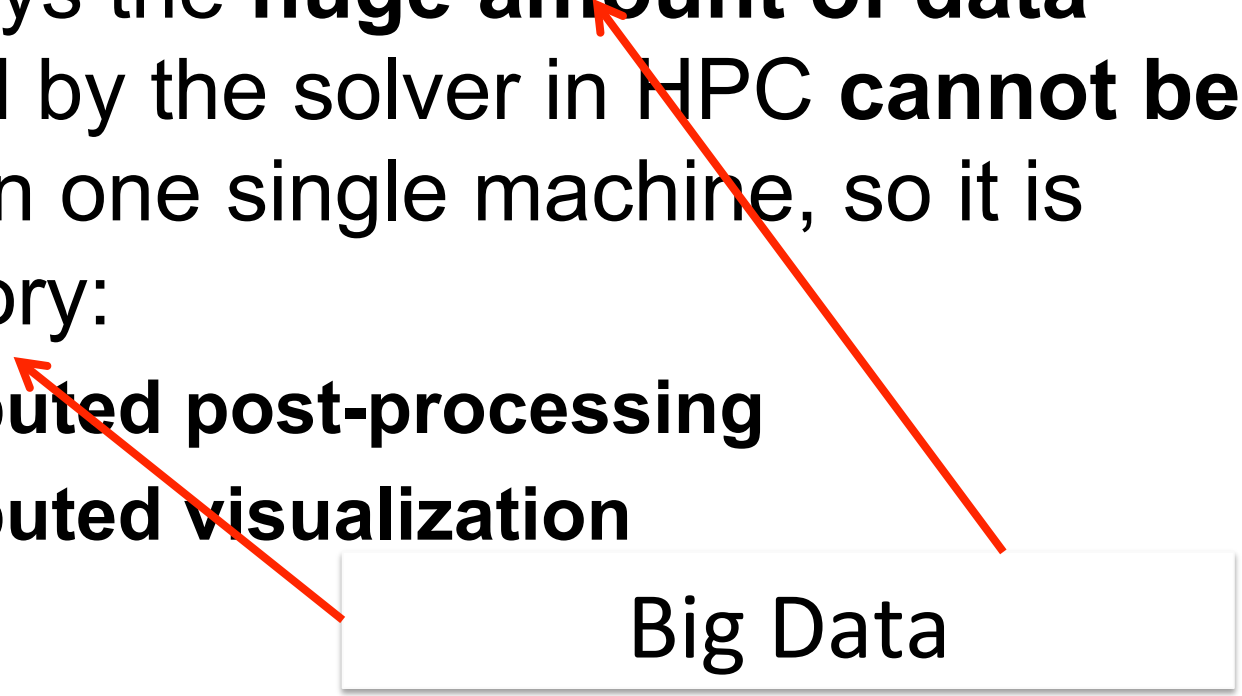
Postprocessing

- Postprocessing operations (data analytics) and visualization of results



Current bottleneck

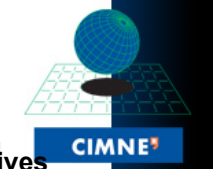
- Nowadays the **huge amount of data** provided by the solver in HPC **cannot be stored** in one single machine, so it is mandatory:
  - **Distributed post-processing**
  - **Distributed visualization**



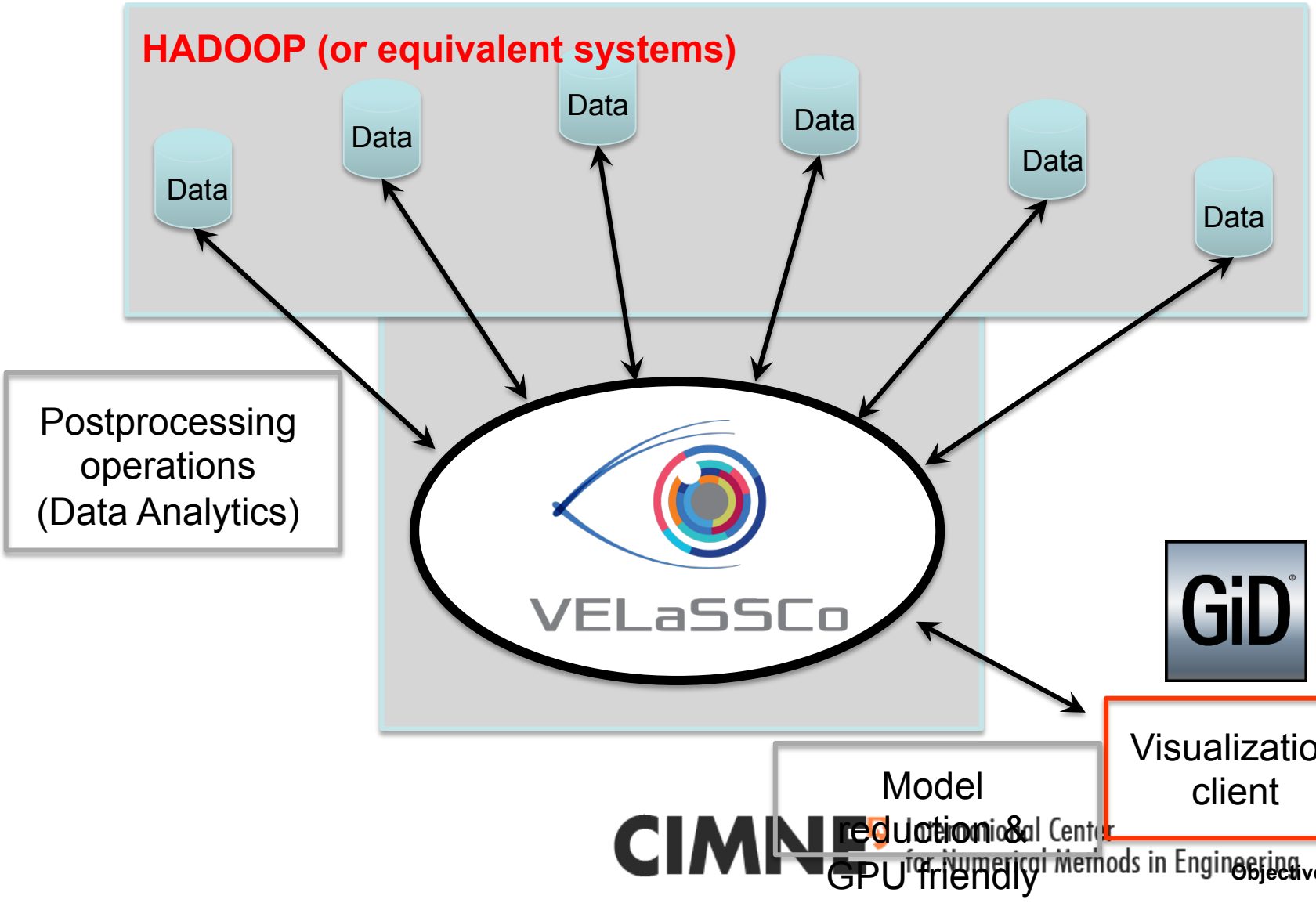
Objective of VELaSSCo

- The main **objective of VELaSSCo** project is to build the VELaSSCo Platform, a system that performs distributed **post-processing operations and visualization of very large simulations**.

- To address this objective, VELaSSCo brings together **Simulation** and **Big Data.**



VELaSSCo Platform



Some comments

MPI versión was TWICE FASTER than the OpenMP (per core)

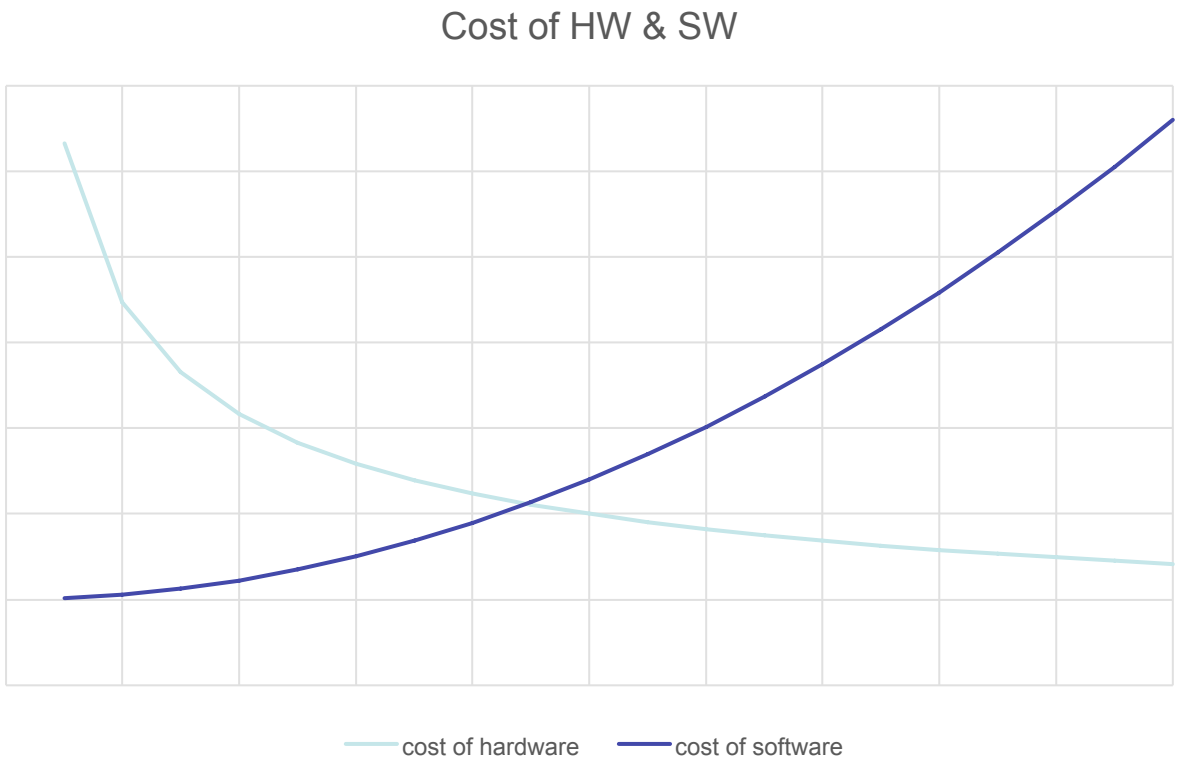
→ **We believe this is related to dynamic memory management**

→ **A PETITION : please generate some good OpenMP allocator for C++.** (I would personally love to have a discussion offline with experts on the subject)

Note that this is also very important for MPI+X. may it could be that some form of MPI nesting will be better?

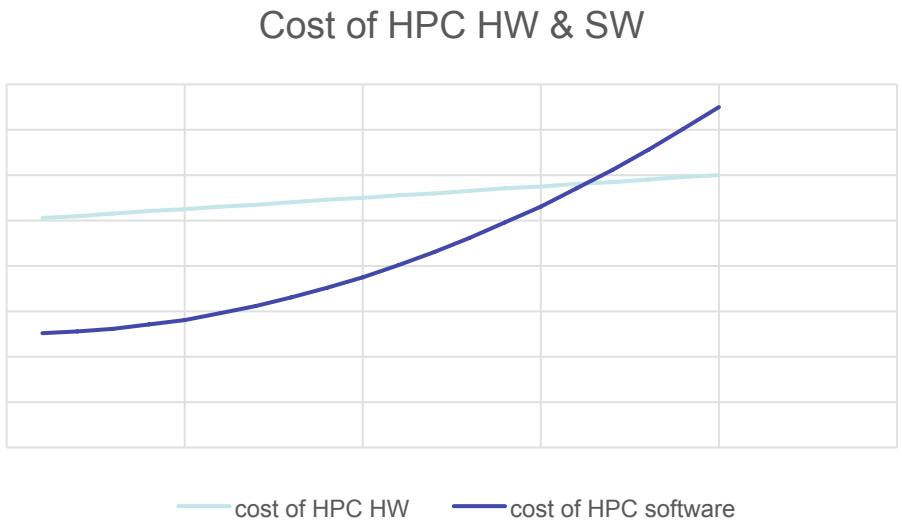
Final Thoughts

It is easy to find in the internet graphs like the following



Admittedly referring to consumer hardware (NOT HPC)

Of course for HPC cost is not really going down, since the limits are being constantly pushed



However the complexity of harvesting performance is also increasing! That is COST OF SOFTWARE also increases.

→ HPC **software** also needs funding instruments.

Thank you for listening

And … we are open for collaborations

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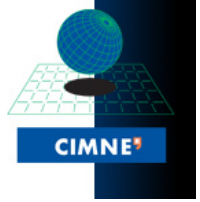

Acknowledgments:

Projects

- **NUMEXAS**:

  NUMERICAL **M**ETHODS AND TOOLS FOR KEY **EX**ASCALE COMPUTING CHALLENGES IN ENGINEERING AND **A**PPLIED **S**CIENCES

  http://www.numexas.eu/

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