NUMEXAS Embedded solvers for Industrial CFD Applications

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Layout

- Why Embedded Solvers? Motivation
- Simulation Pipeline
- Objects with well defined internal volume
- Objects without a well defined internal volume
- Future Challenges

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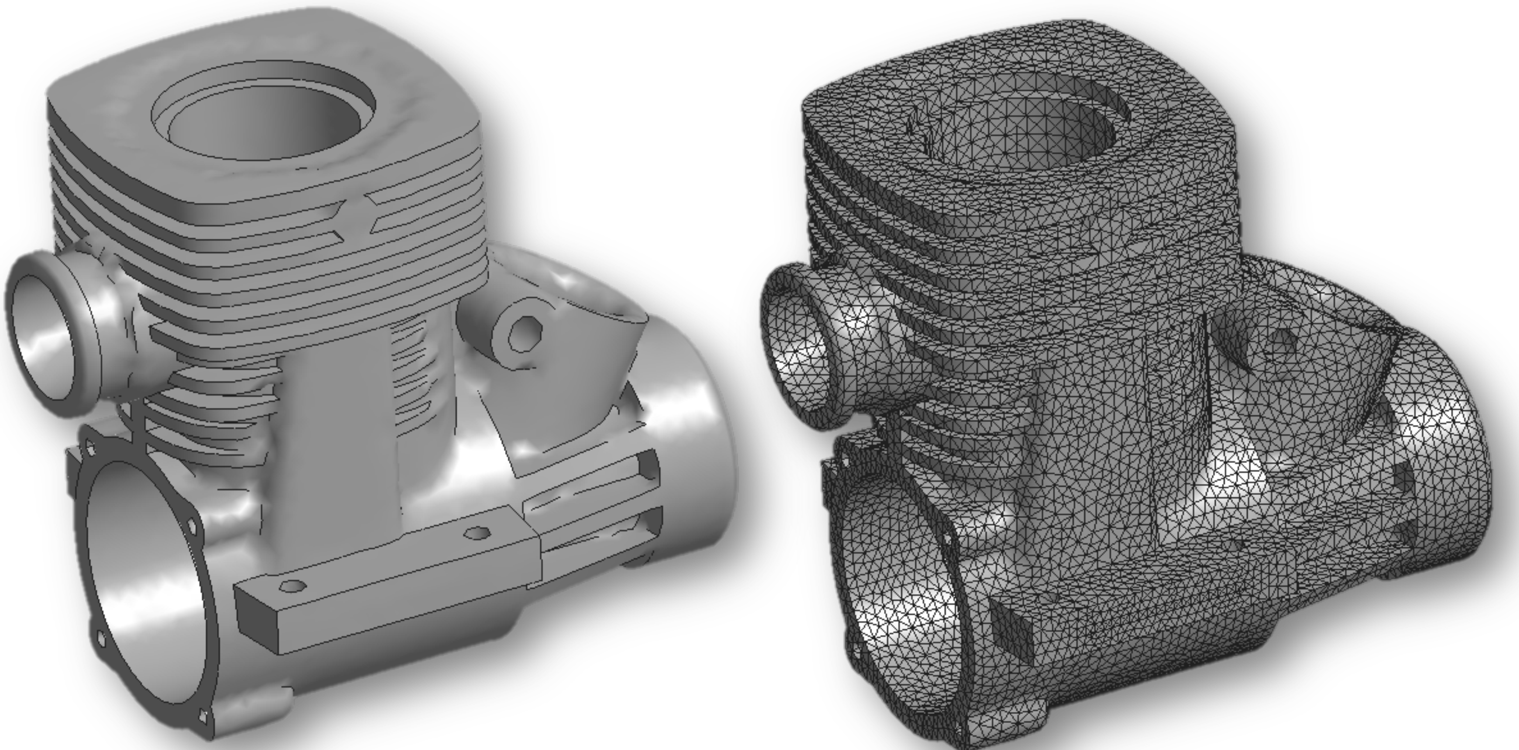
Motivation

Industial Simulation

→ we do not want to solve "cubes" !!

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



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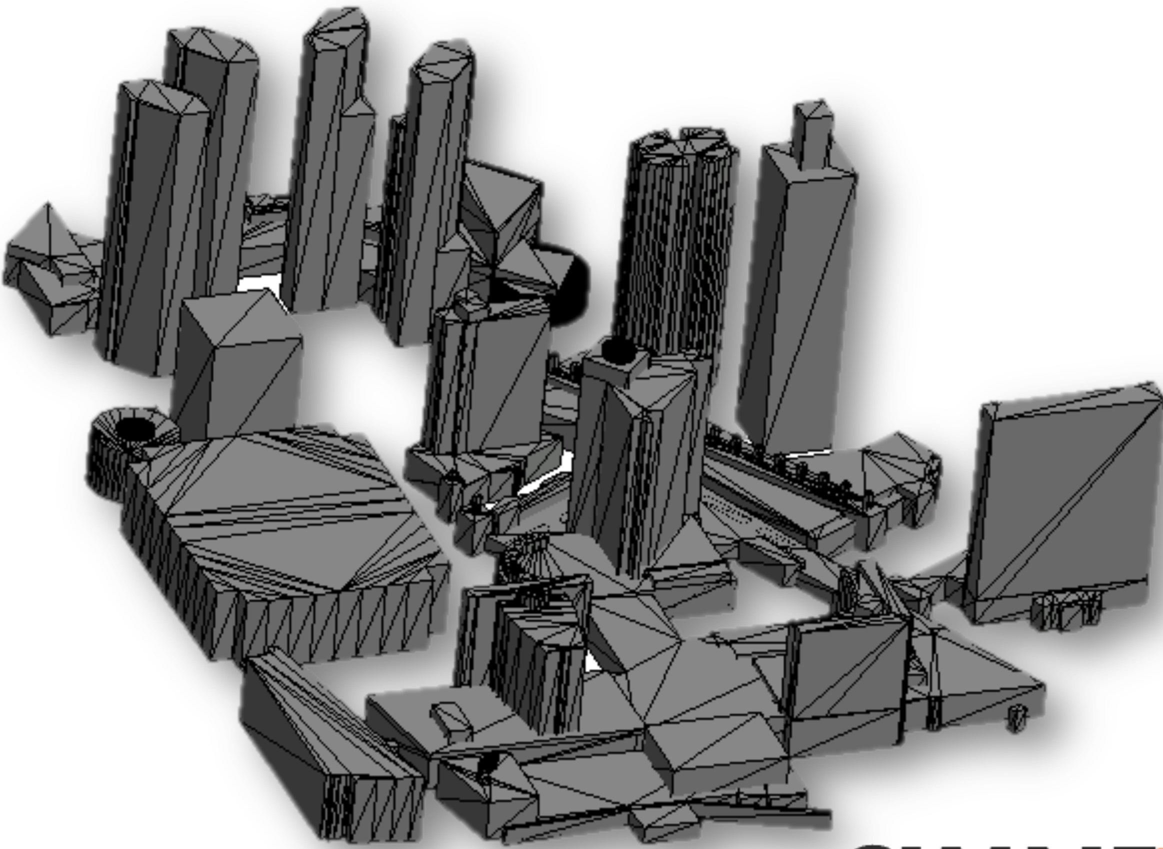
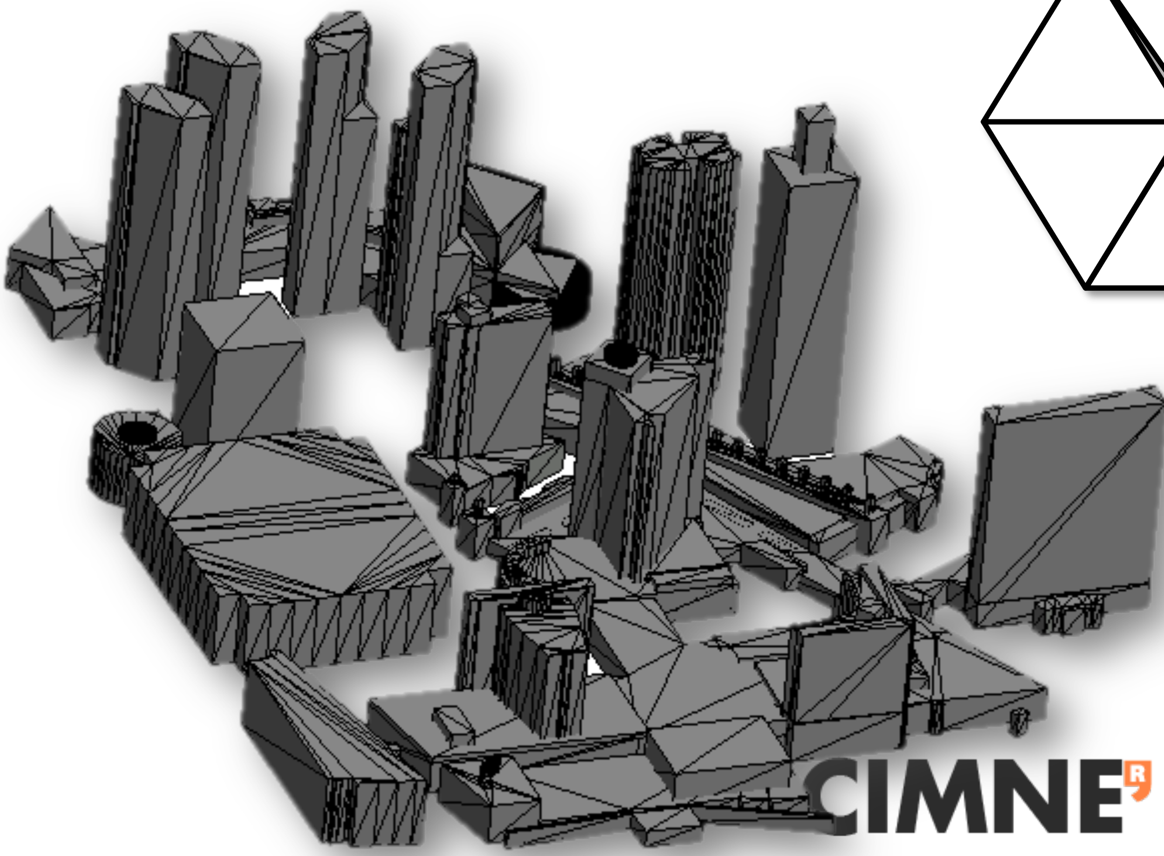
Motivation
Industrial Models

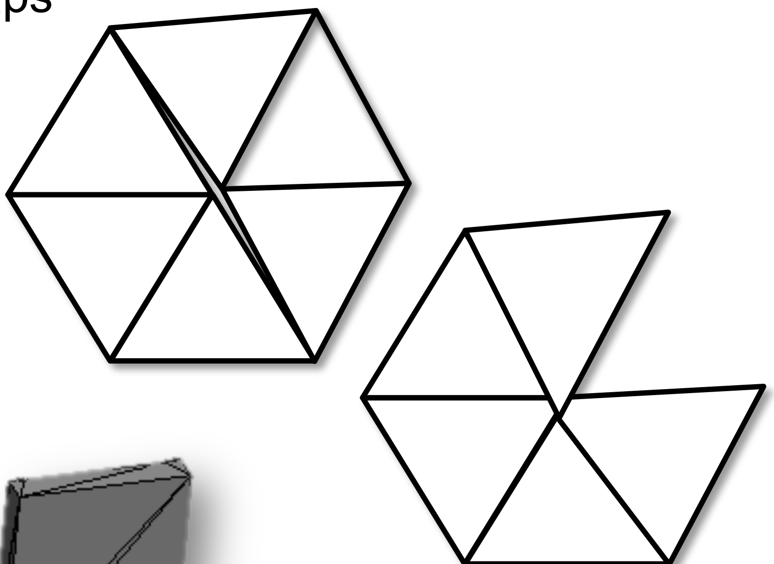
- STL-like non conforming meshes are all over the place.
- Also the standard for 3D printing!!



Motivation
Industrial Models

- STL is a common format
- STL files usually have gaps and overlaps





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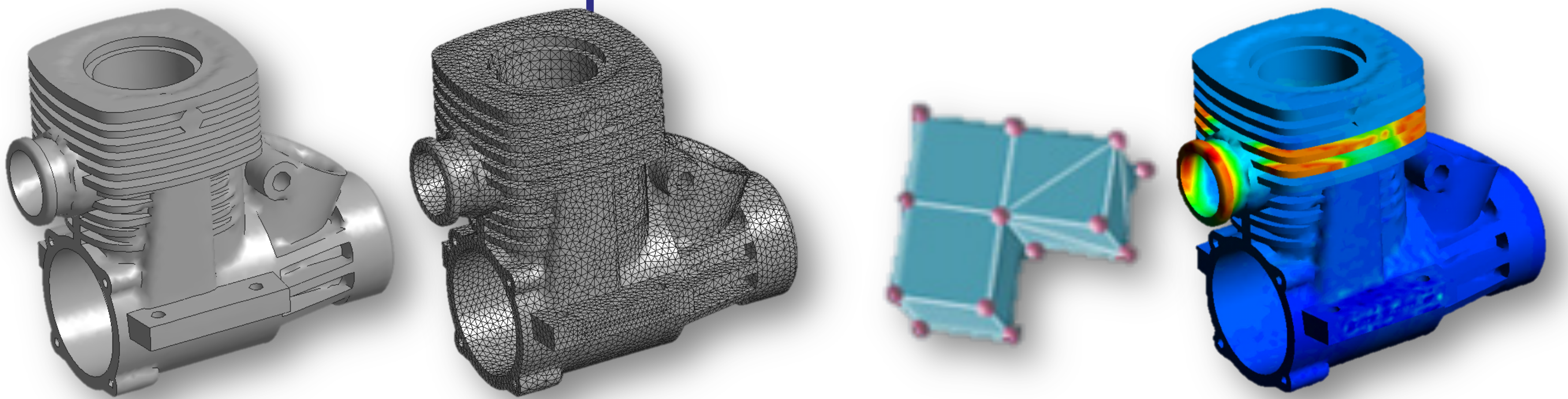
Motivation
Simulation Pipeline



Modeling

- Not Clean Geometry
- Complex Models

Meshing

- Robustness
- Not Scalable

Analysis

- Scalability
- Efficiency
- Complexity
  - FSI
- Heterogeneous Machines

Visualization

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

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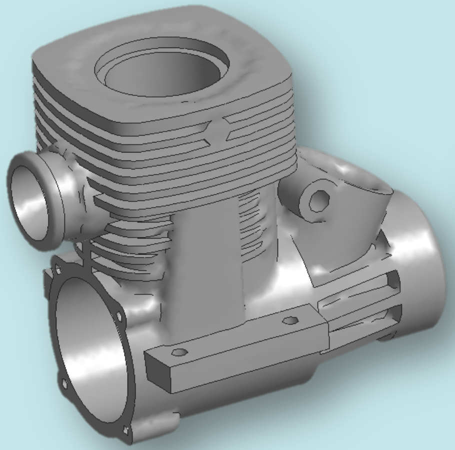
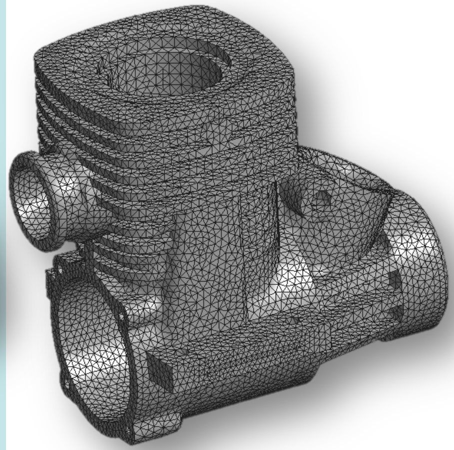
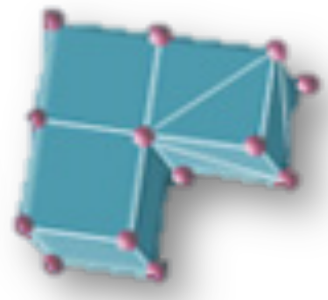
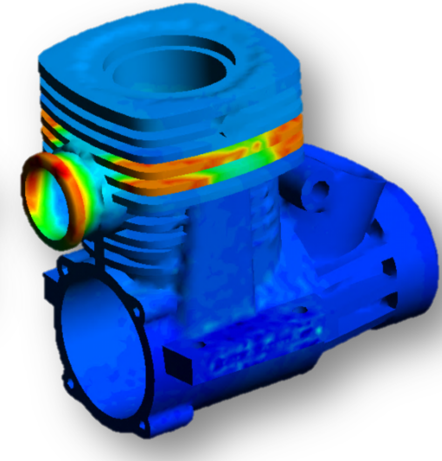
Challenges

Simulation Pipeline









Modeling

- Avoid Cleaning
- Allow deformations of the domain

Today's presentation about:

Embedded Approaches

(using STL-like discretizations)

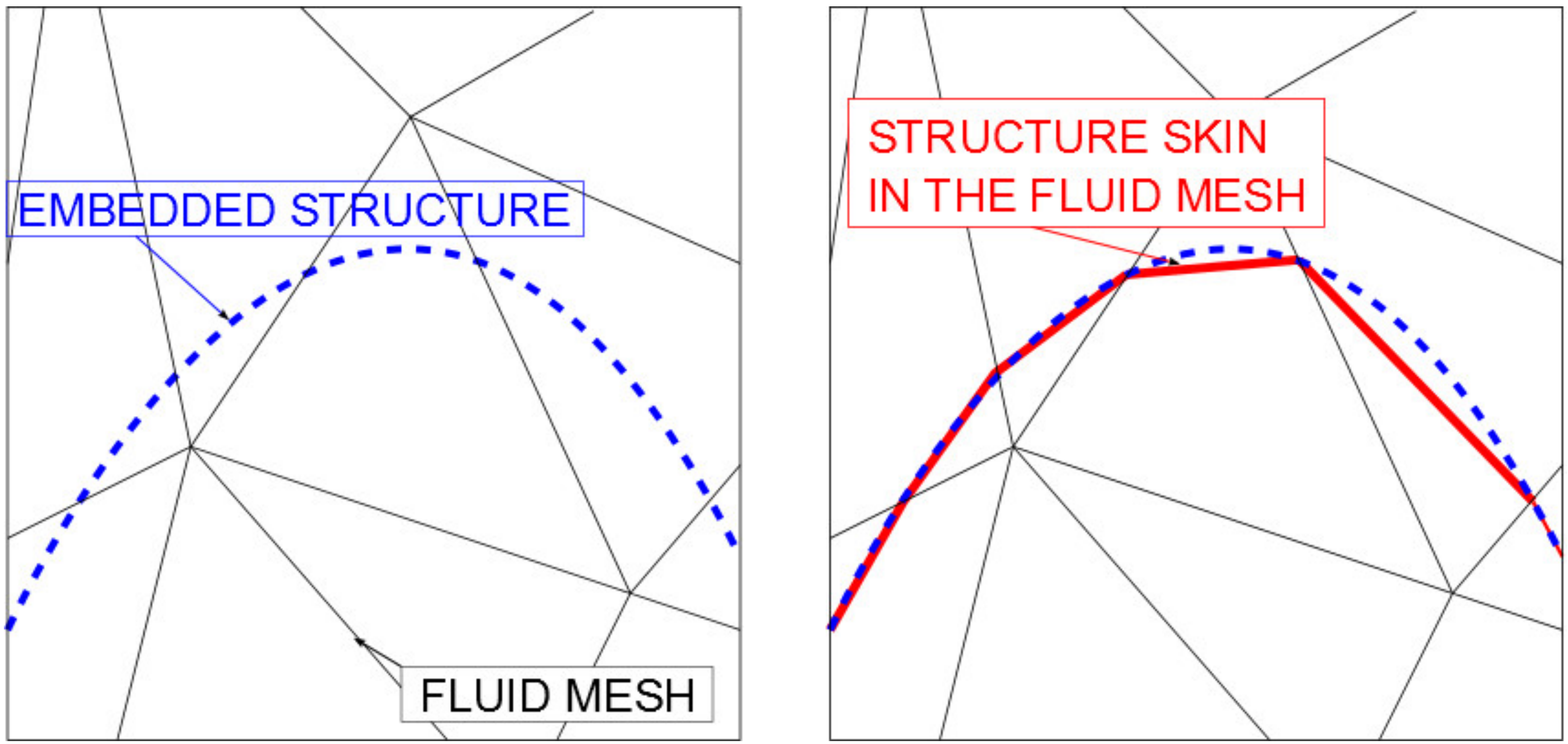
- **Simplify model preparation**
- **Allow topology changes, moving domains**

DOWNSIDE→ less accurate. Use if needed!!

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

CARVE OUT "a hole" in the CFD mesh →

Geometry is approximated as possible → TOUCHES ALL OF THE PIPELINE!



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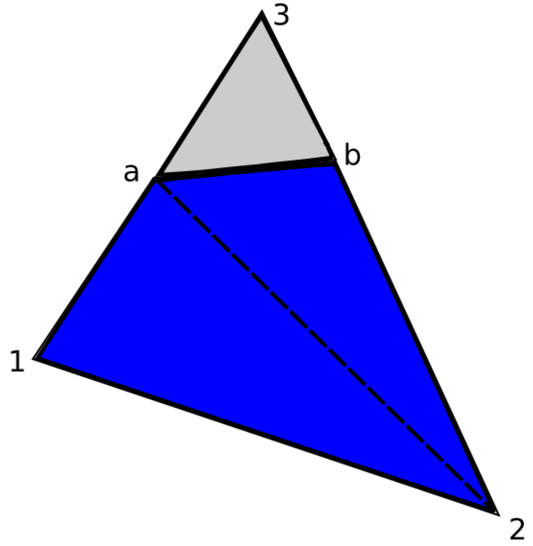
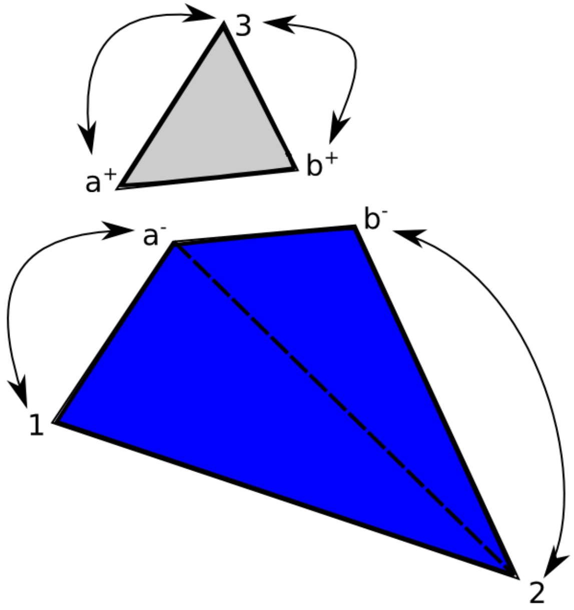
Essential Idea of Embedded Solvers (may know it as Immersed CFD)

Cut elements are subdivided, and conditions are imposed on the "virtual nodes" → details of the CFD implementation are NOT the objective of Todays talk





Motivation
Simulation Pipeline

Everything in the current presentation is implemented within the

KRATOS

Framework

www.cimne.com/kratos

Kratos
What is?

A Program for Engineering Calculation

Engineers

Framework for parallel Multi-physics programs development

Developers

OPEN SOURCE (BSD Licence)

Everyone

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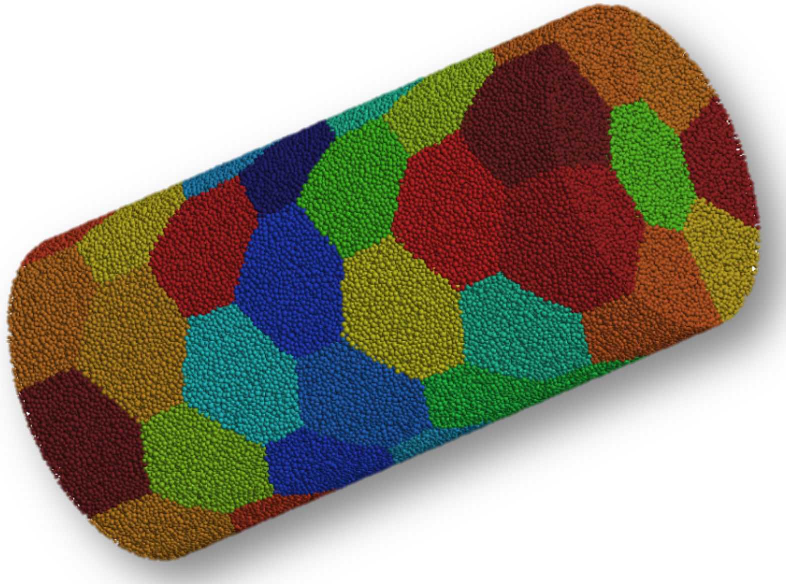
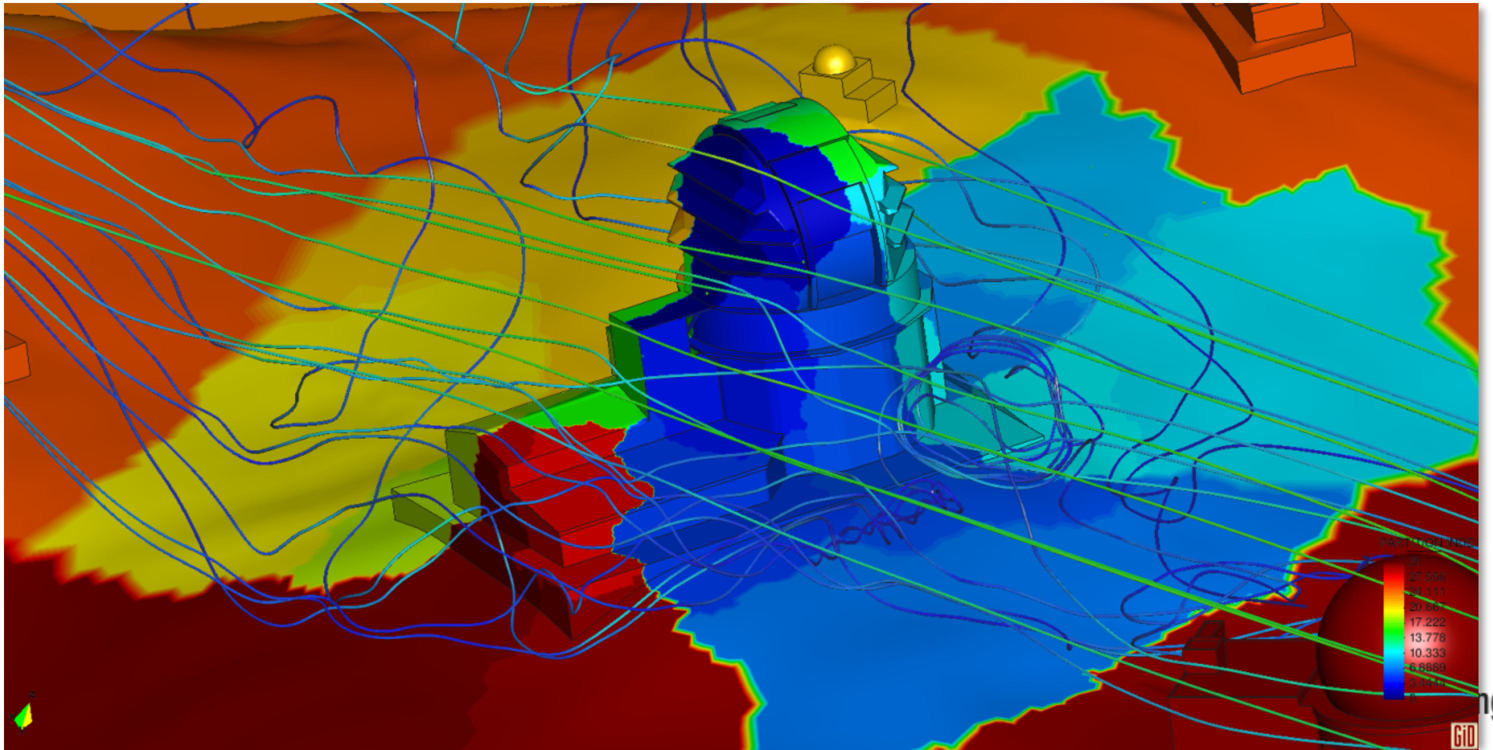
Kratos

HPC

- SMP (OpenMP based)
- MPI
- GPU support (OpenCL based)





CFD for bodies with a well-defined internal volume

In many cases it is required **to compute the flow of a fluid "around" objects.**

The **best case** scenario is when the "**outer skin**" of the object is **provided** → it is possible to distinguish "inside" from "outside", and hence to deactivate the part not needed.

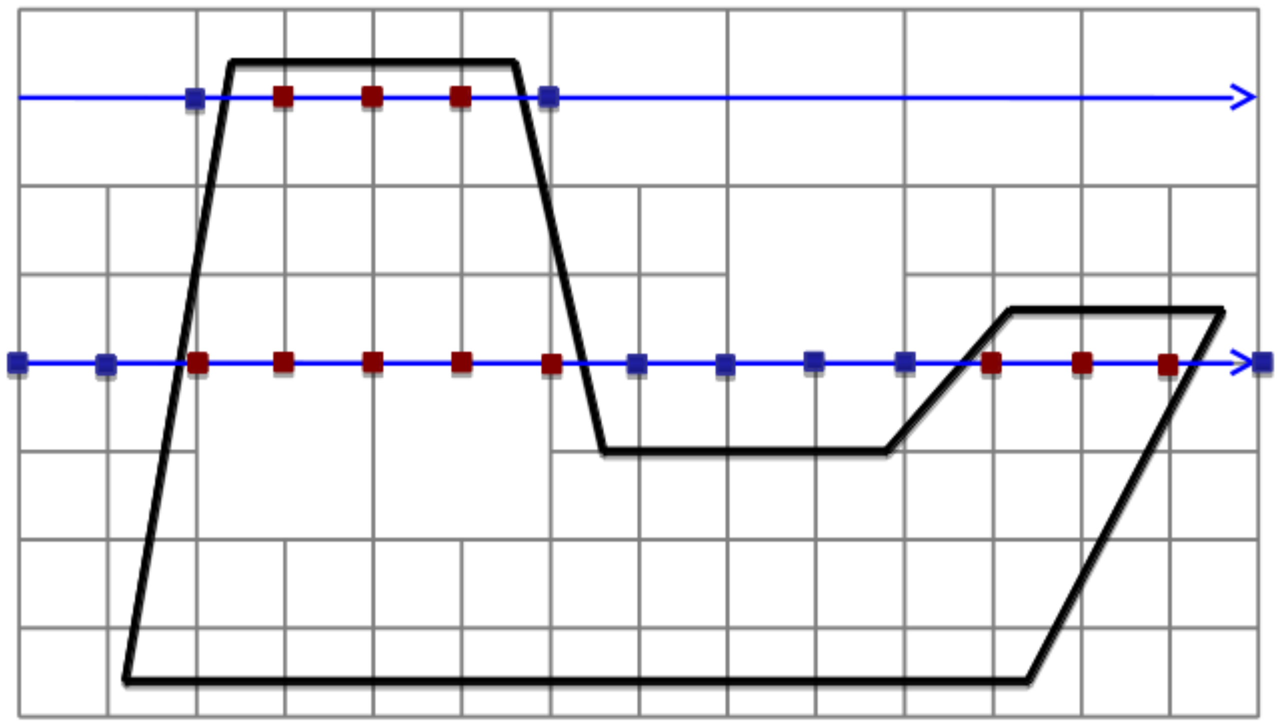
A robust technique to do this is RAYTRACING

In the hypothesis of a well defined skin:

- **Raytracing** can be done in parallel since the inside/outside decision is **embarassingly parallel**
- Given an arbitrary point in space one may univocally decide concerning its status
- Can be done robustly even for stl meshes

3D printing relies on this conditions

Essential Idea of Raytracing



- “far away” is *outside*
- If i cast a ray from an outside point, inside/outside status changes every time a surface is crossed

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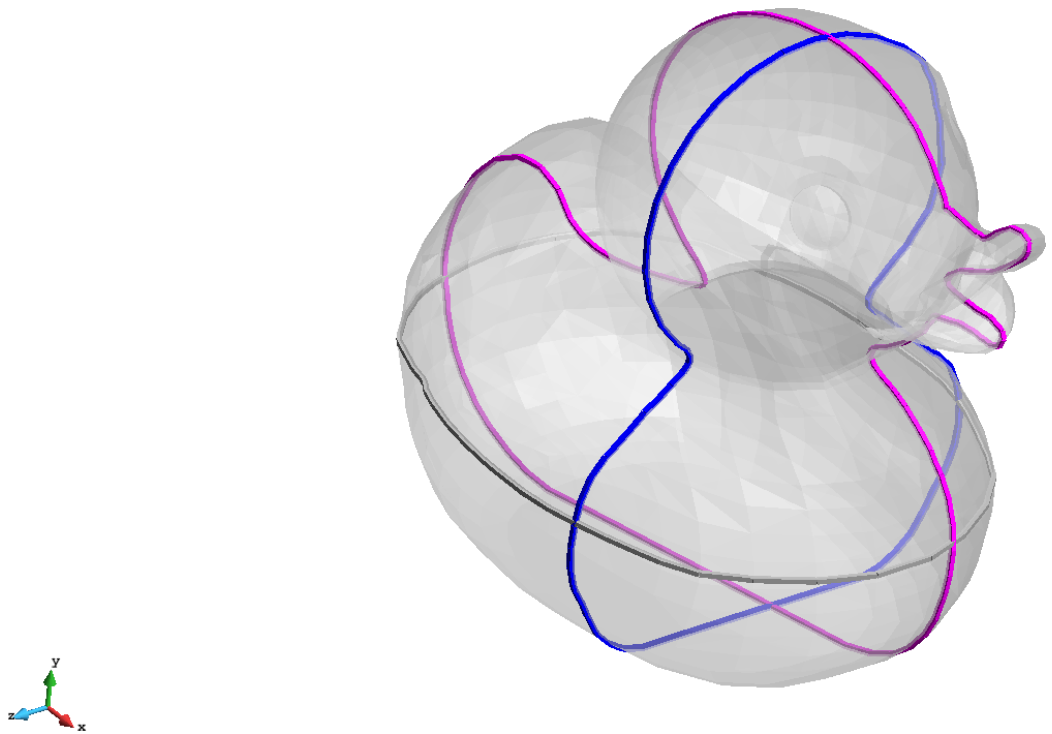
A simple example: a “duck”

Simple, nicely closed, surface



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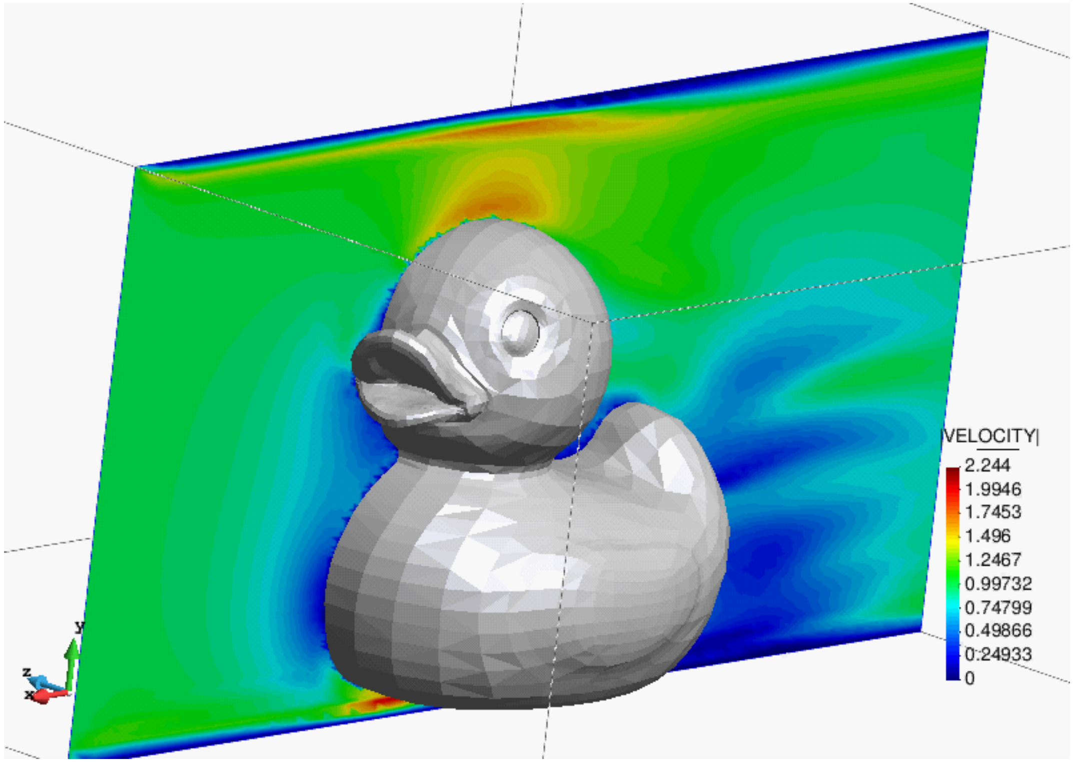
Flow around our "duck"



Important advances of having an internal volume:

- A **continuous "levelset" distance** function can be defined
- A **metric tensor** can be computed based on the levelset function, allowing anisotropic refinement
- One **portion** of the domain can be **deactivated** – less computational effort
- Easier formulations for CFD

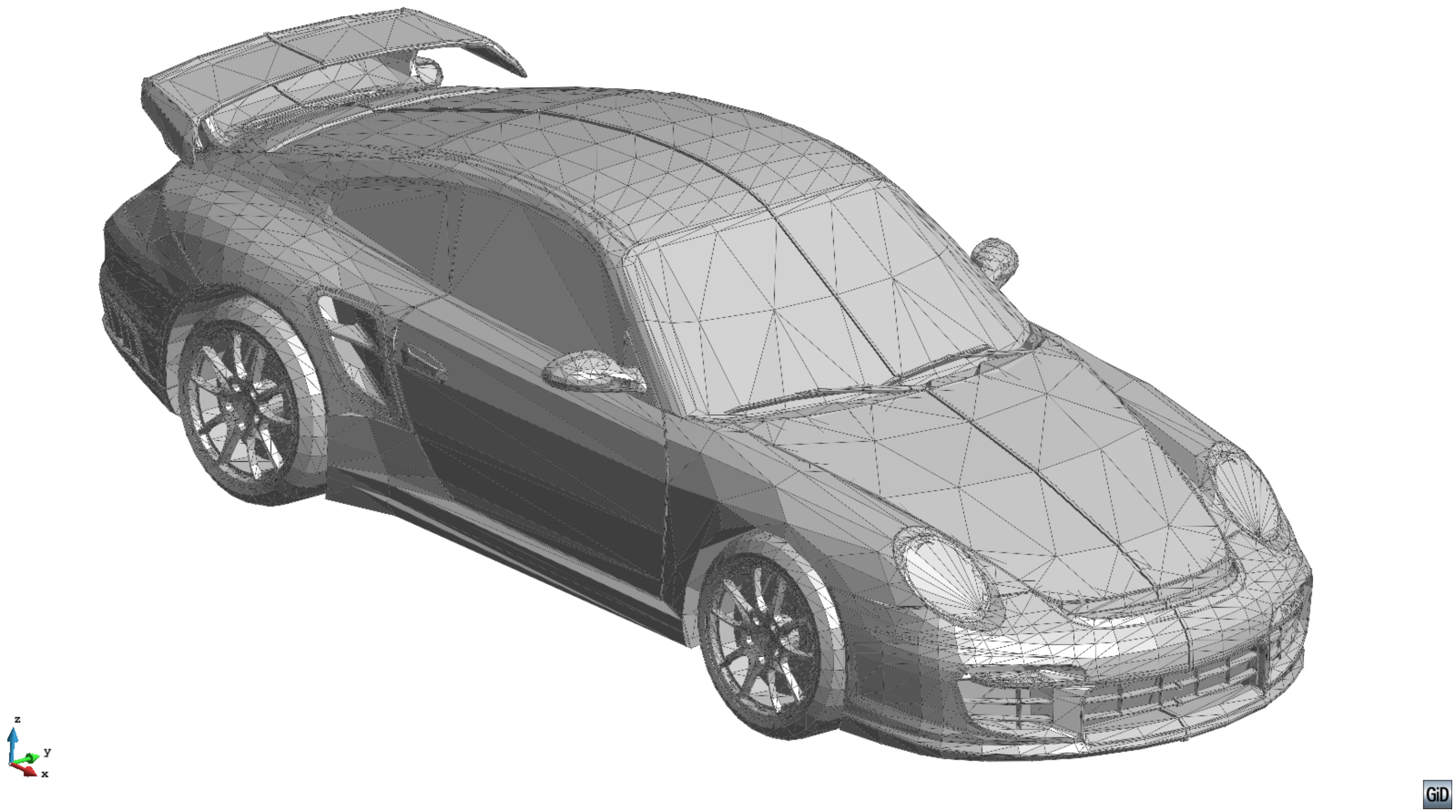
CFD for bodies without a well-defined internal volume

Unfortunately the **practice is different**:

needs of graphical modelling do not match the needs of computing
→ inside/outside often not important for visual results

Let's consider a model of a car as downloaded from the internet (original CAD not available to us)

CFD for bodies without a well-defined internal volume



Model as imported from .dae model

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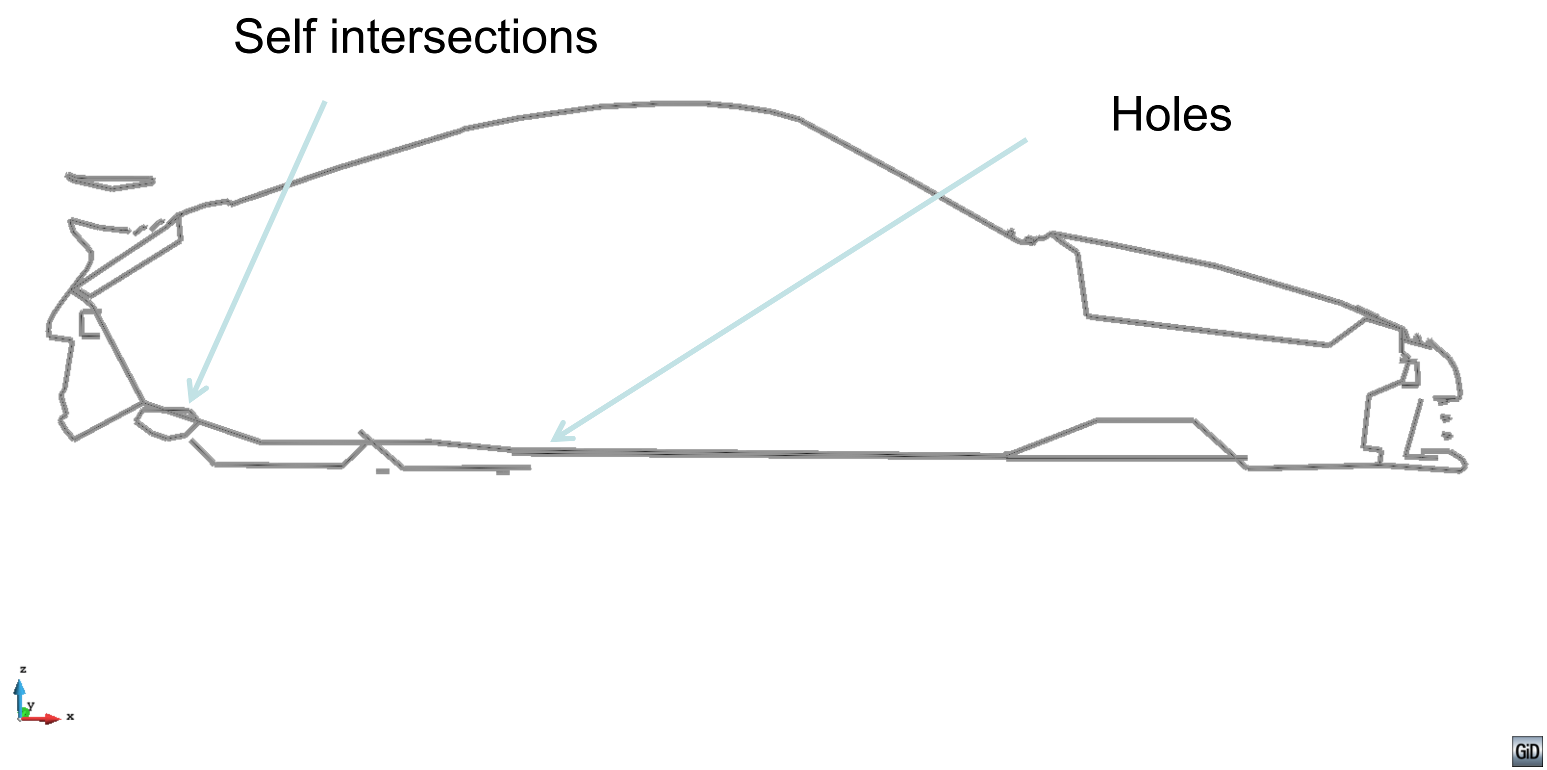
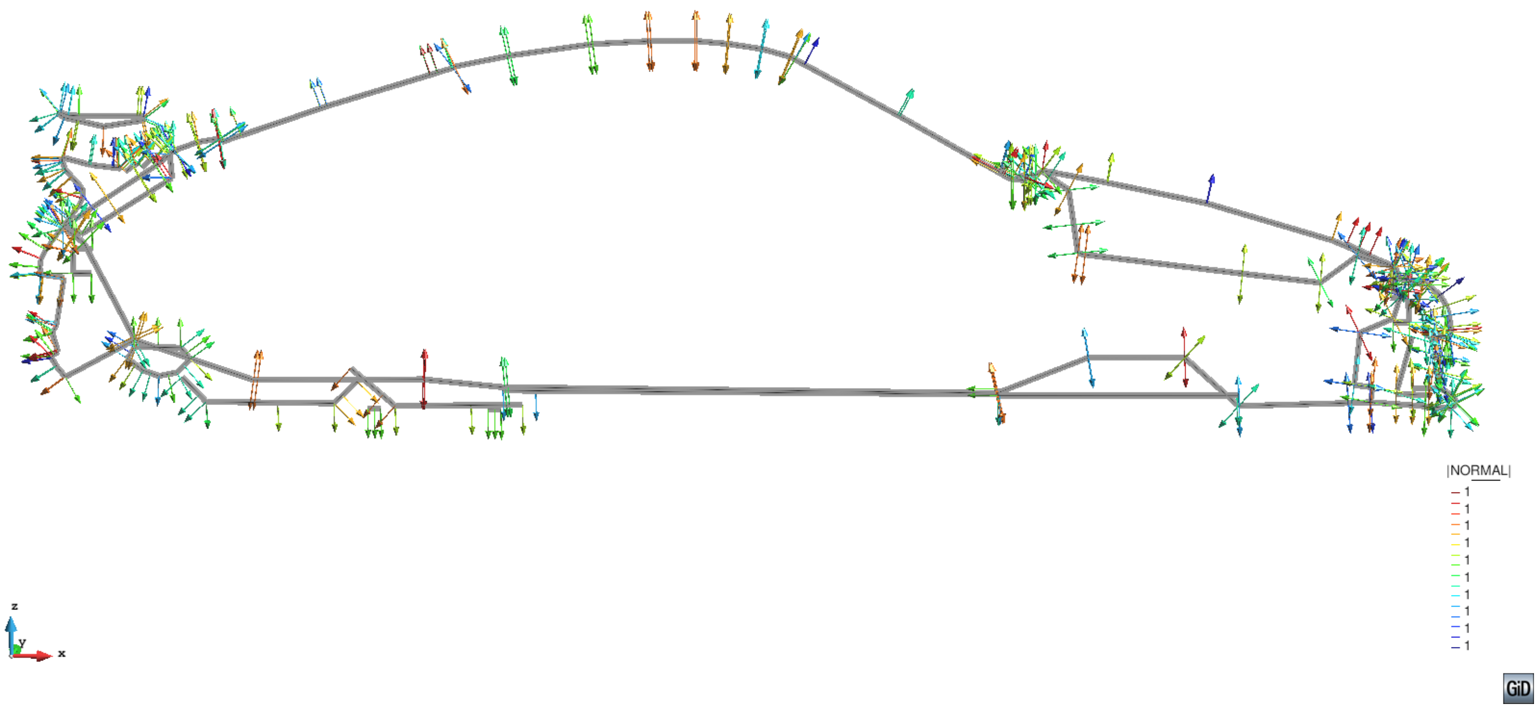
CFD for bodies without a well-defined internal volume



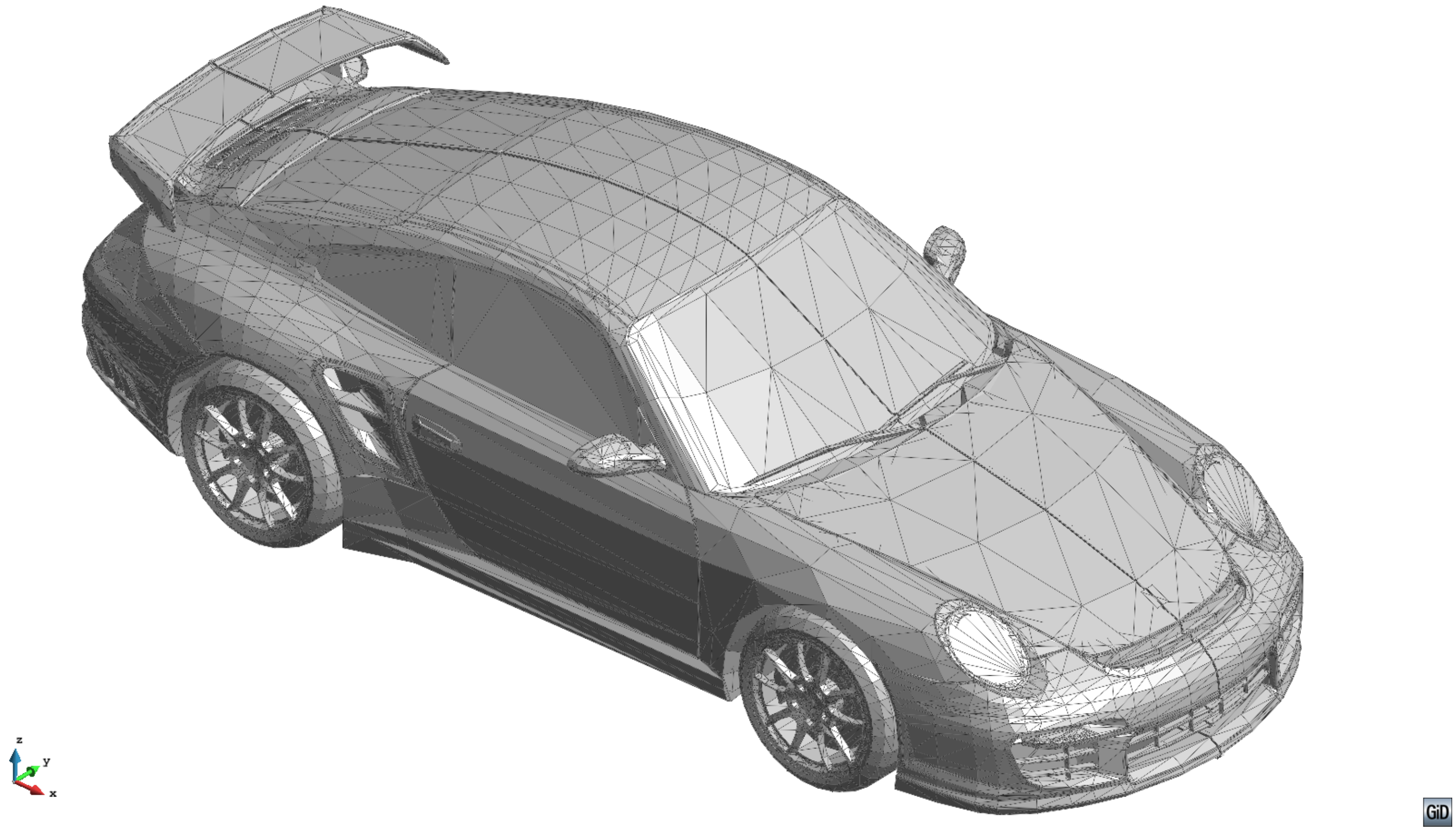
Cut along the center plane – openings and overlaps are apparent

CFD for bodies without a well-defined internal volume



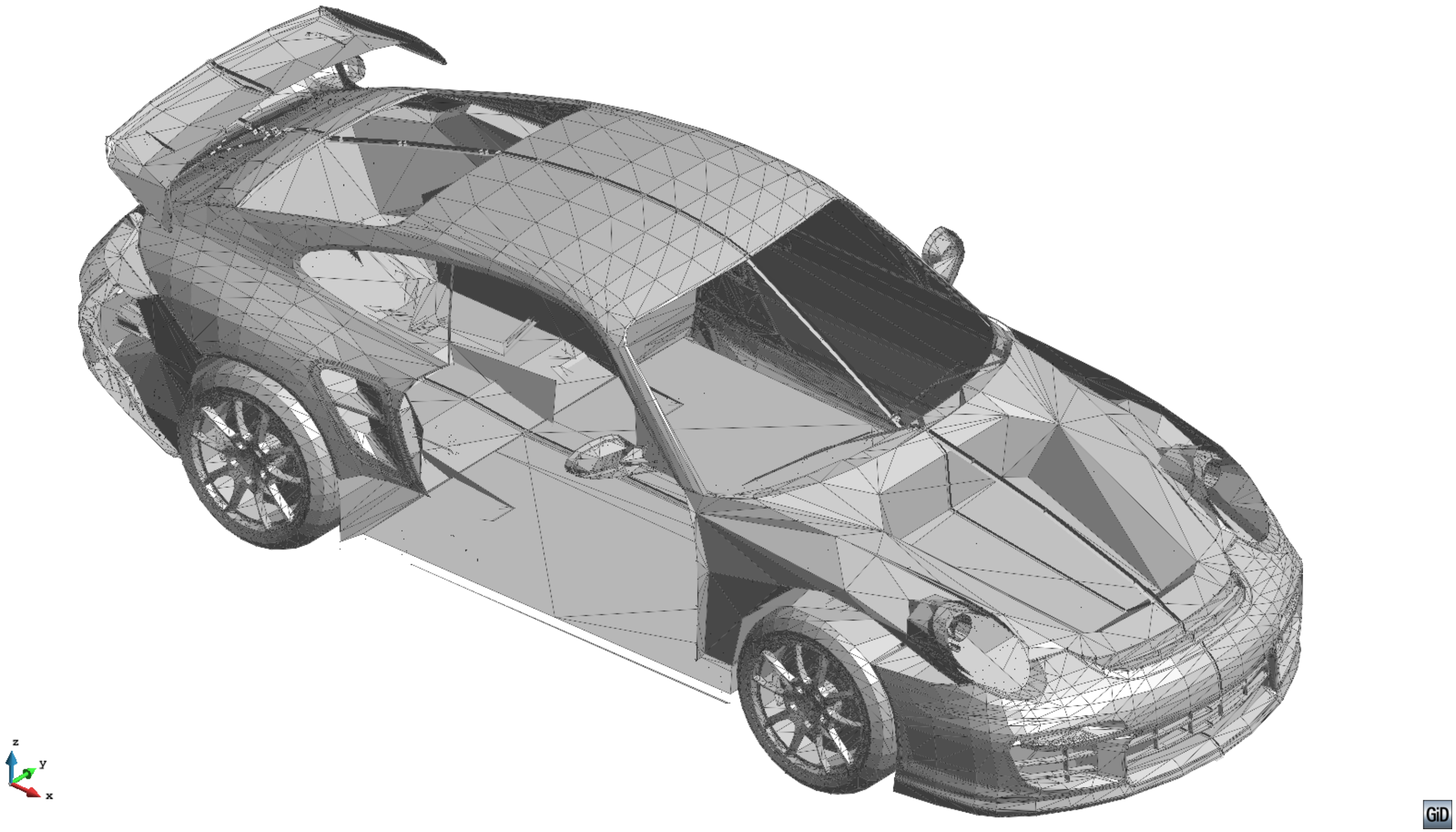
Cut along the center plane – NORMALS – double sided surfaces!!

CFD for bodies without a well-defined internal volume



"Positive" Orientation (towards the observer)

CFD for bodies without a well-defined internal volume



"Negative" Orientation (normal looks away from the observer)

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CFD for bodies without a well-defined internal volume

Features of the model

- Gaps & overlaps
- T-joints
- Double-sided and single-sided surfaces

Essentially ***as bad as it gets***

What to do?

Our answer is to impose "slip" boundary conditions (extension to wall law modelling is obvious) on cut elements, allowing flow on the two sides

→ SURFACE TRIANGLES AS "OBSTACLES"

CFD for bodies without a well-defined internal volume

IDEA:

COMPUTE CFD ON BOTH SIDES OF EACH OBSTACLE

That is, compute CFD everywhere

A simple 2D example explains it visually:

[2D discontinuous pressure]

CFD for bodies without a well-defined internal volume

The essential idea is that for each Tetra in the mesh we identify the single cut plane that "best approximates" all the surfaces that cut through the element → such cut plane is univocally determined in terms of an **Element-Discontinuous distance function**.

Highlights:

- ***Best approximation always defined (even for multiple cuts)***
- ***Cutting plane is defined even if a "signed distance" would not be possible***
- ***Single-sided objects can be taken into account***

All the details of the method can be found in:

CONTRIBUTION TO THE FLUID-STRUCTURE INTERACTION ANALYSIS OF ULTRA-LIGHTWEIGHT STRUCTURES USING AN EMBEDDED APPROACH
D. Baumgärtner, J. Wolf, R. Rossi, R. Wüchner, P. Dadvand
Monography N 152
http://www.cimne.com/tiendaCIMNE/tmp/111142843049/M152.pdf

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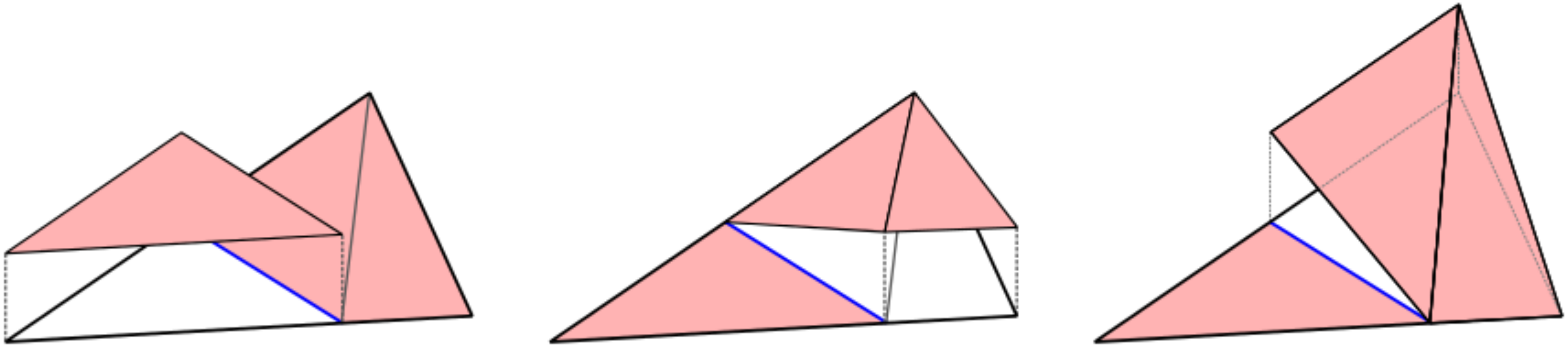
CFD for bodies without a well-defined internal volume

Different Options in how to do this.

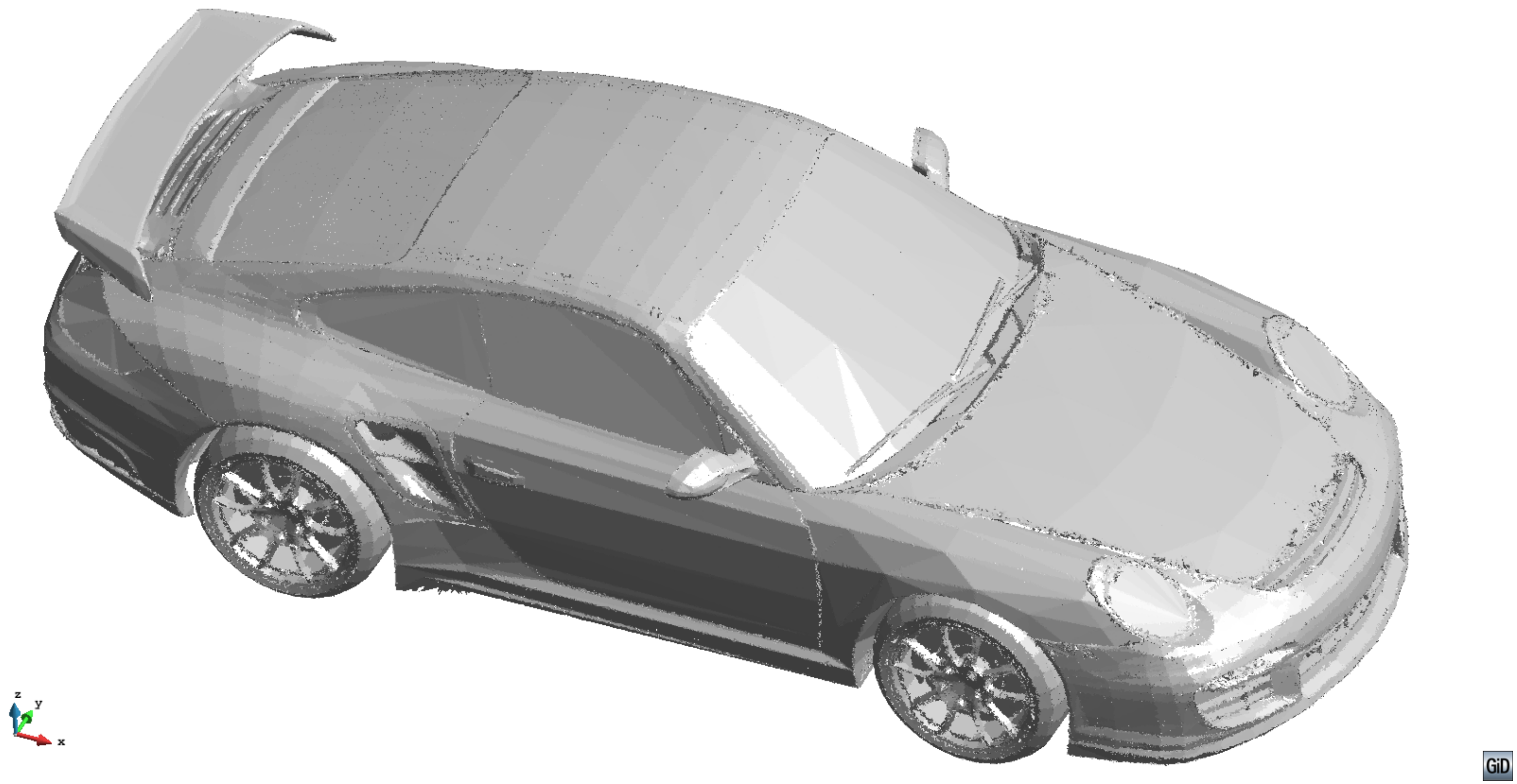
In current examples we ***modify the FE space*** *by replacing the shape functions by others that* ***EMBED THE DISCONTINUITY***

→ constraint is applied ON THE KINEMATICS

R.F. Ausas et al./Comput. Methods Appl. Mech. Engrg. 199 (2010) 1019–1031



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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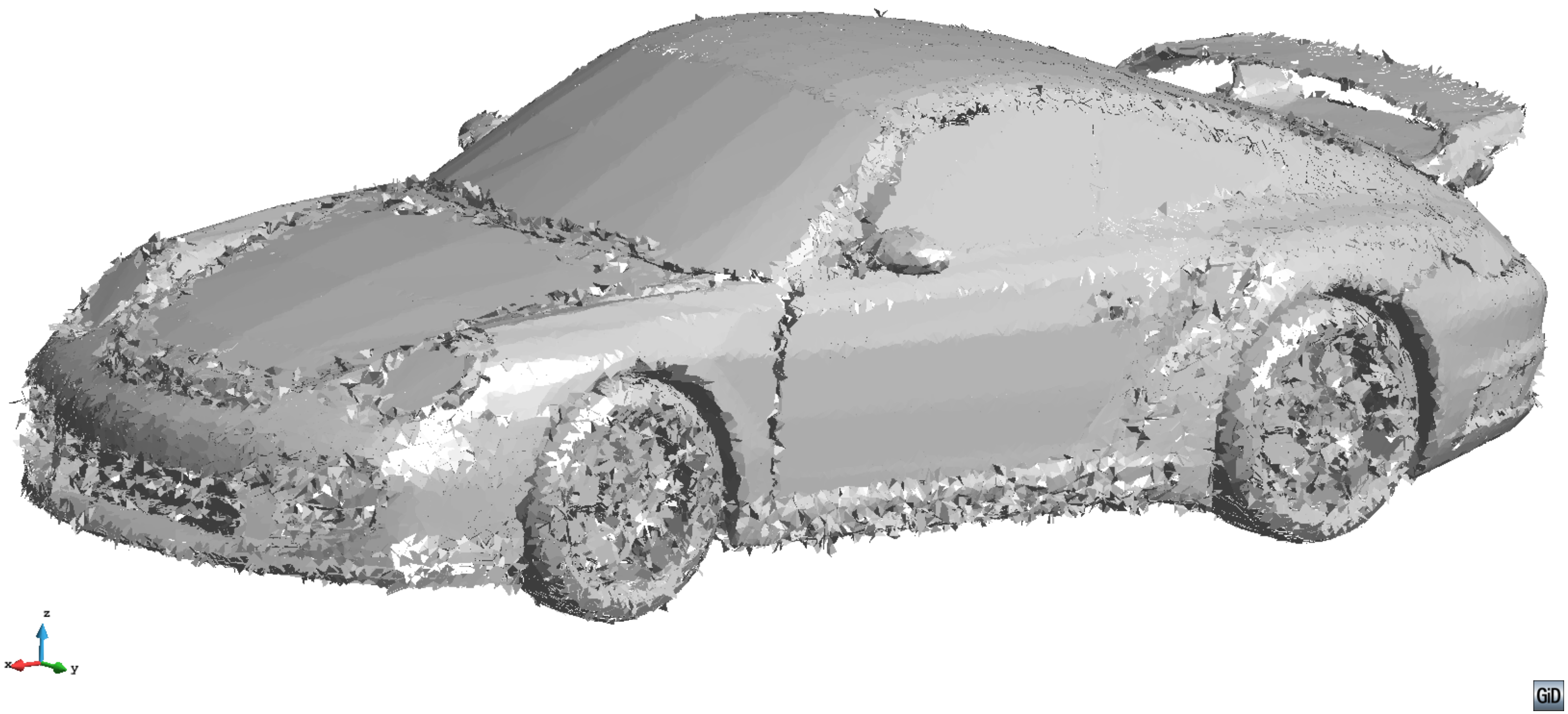
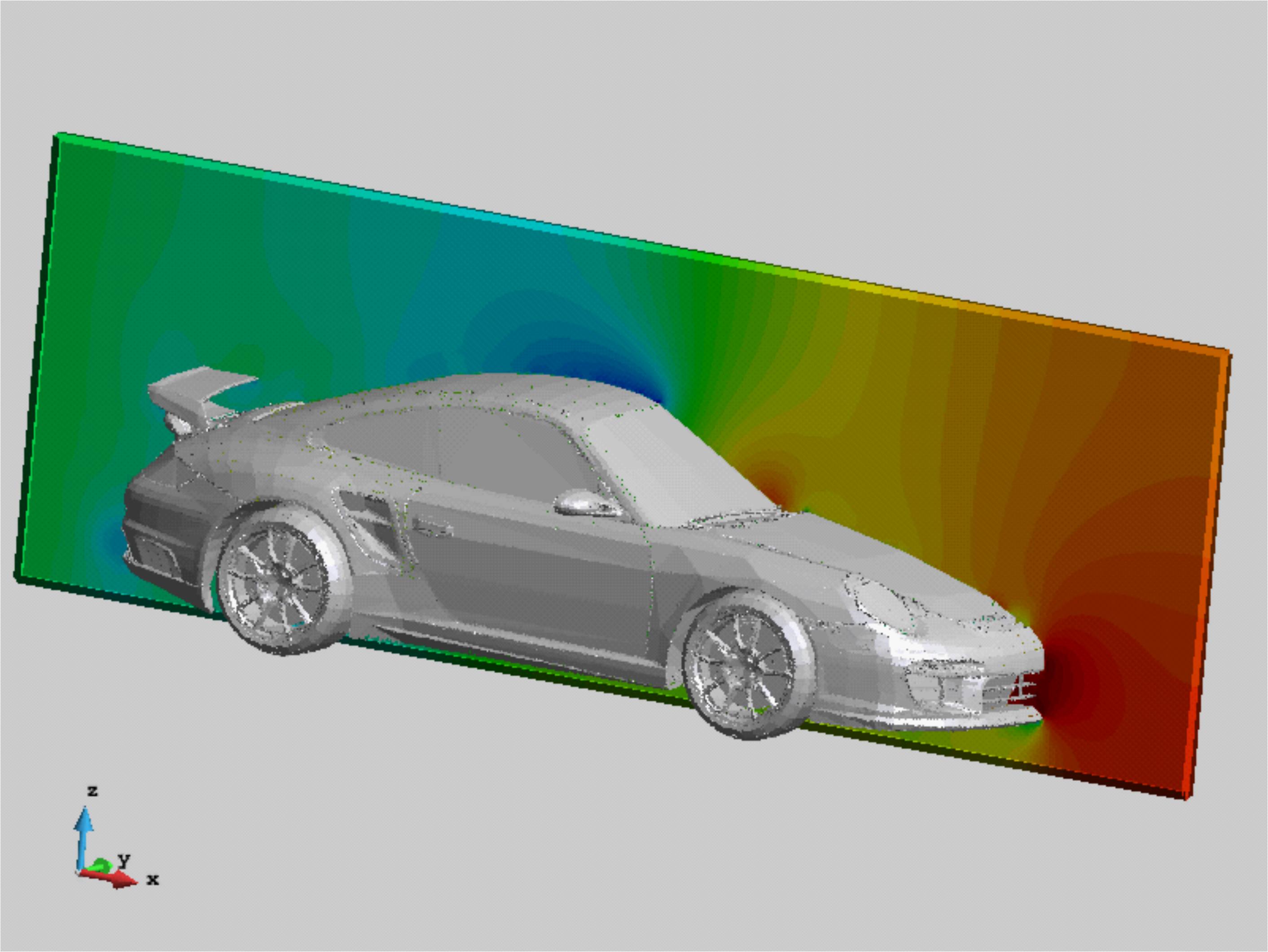
CFD for bodies without a well-defined internal volume



View of the RECONTRUCTED geometry (what is actualy taken into account by the flow solver) – COARSE CFD MESH → details are lost!!

CFD for bodies without a well-defined internal volume



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CFD for bodies without a well-defined internal volume

17M elements

Around 6h to perform a simulation of 20s on a HLRN Cray XC40

Everything is parallel so much larger models should be used to take advantage of large machines!!

But note note also that 1-2 of the future Xeon PHIs (16Gb fast RAM) will be already able to handle relevant problems → IF BANDWIDTH AS PROMISED ATTRACTIVE ALTERNATIVE!!

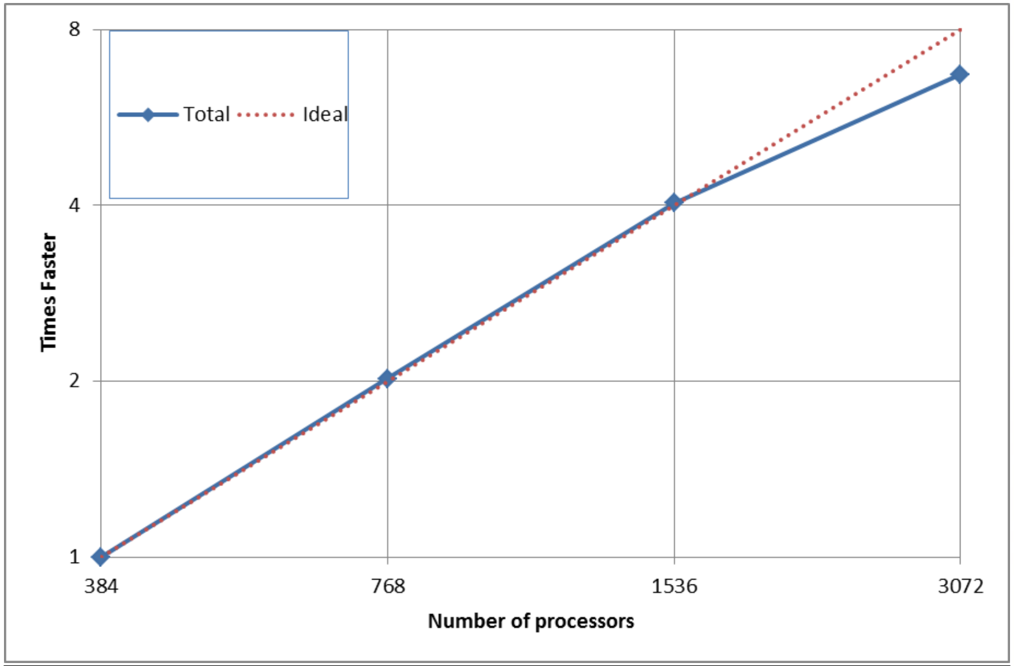

Figure 6: *Strong scalability for the wind tunnel test up to 3K cores (SLIGHTLY LARGER EXAMPLE)*

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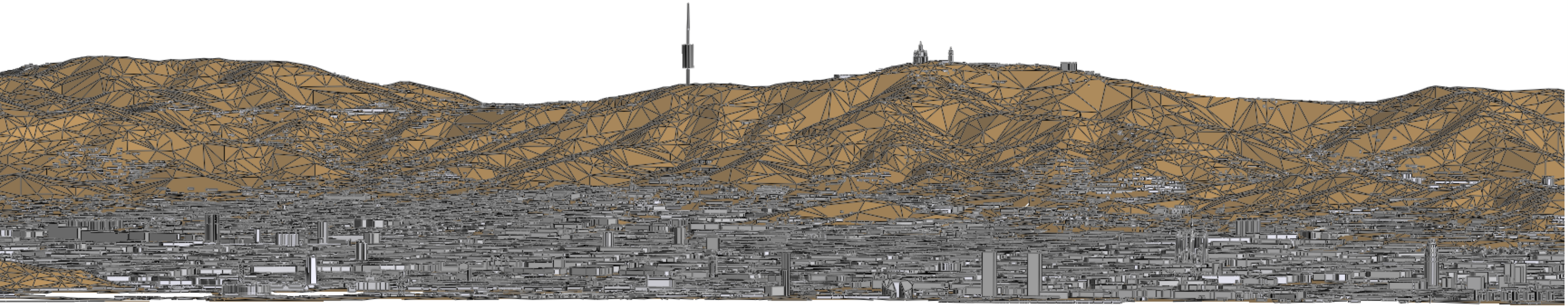
TOWARDS EXASCALE



Triangulated model of the city of Barcelona

→ extremely dirty geometry

TOWARDS EXASCALE

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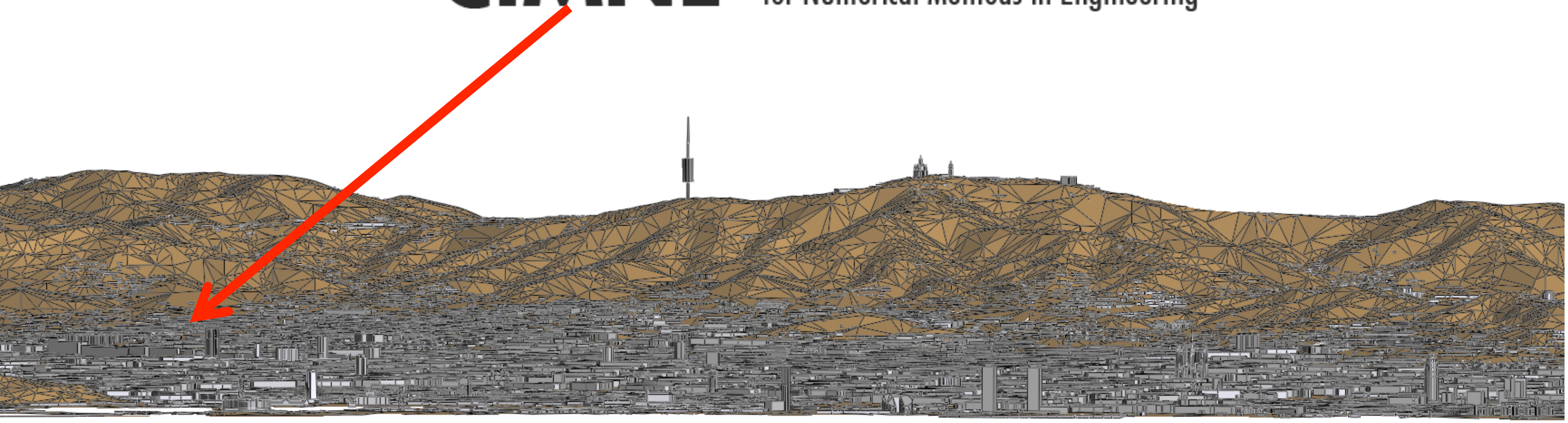

EXTREMELY LARGE MESH NEEDED!!

→ volume will contain 2000M elements

→ Will not fit on "few" processors →Good testcase for the "towards exascale challenge"

→ Now working on BCs

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Scalability

Scalability at the beginning of NUMEXAS

- Results presented problems
- Two main blocks in the solution: “Build” and “Solve”
- Build was scaling perfectly
- Solve (Trilinos based) was not scaling → **Decision taken to work on this**

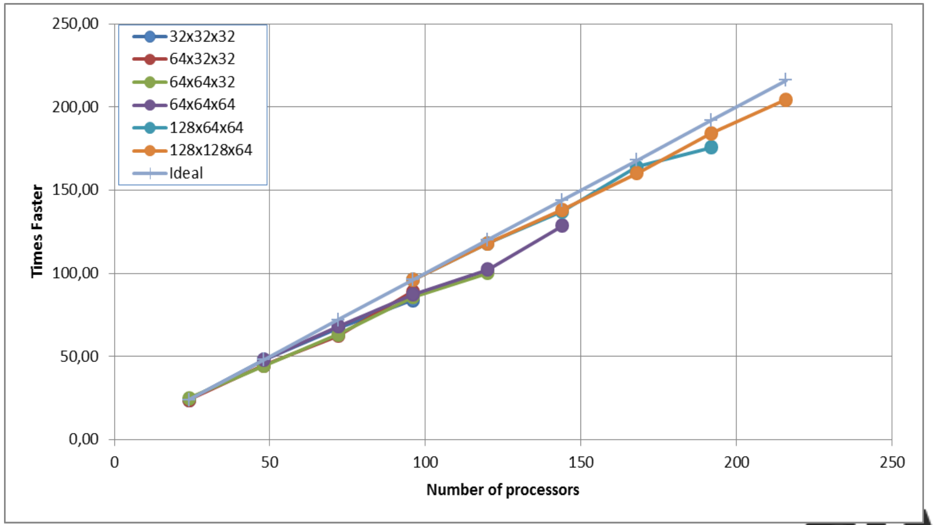

Figure 3: Scalability of the build part for the laminar cube

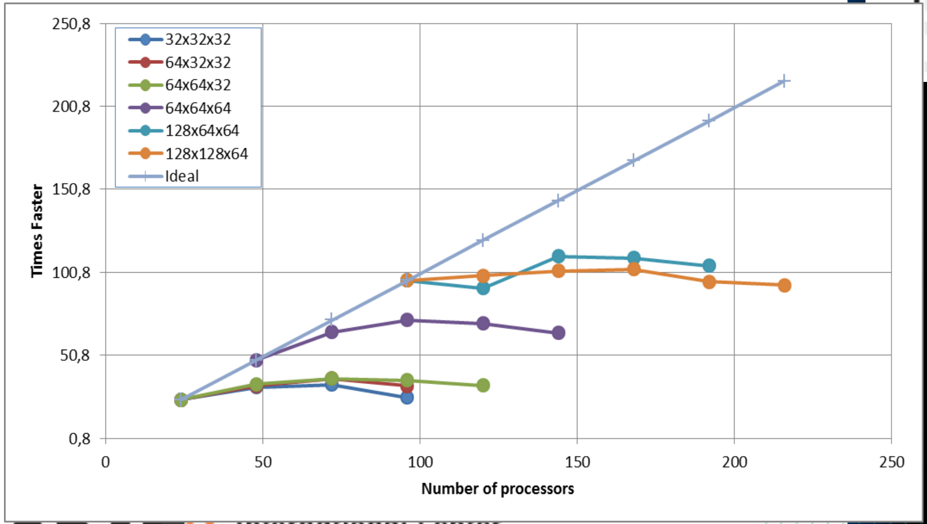

Figure 4: Scalability of the solve part for the laminar cube

AMGCL Solver
Formulation

Let's consider a system in the form:

$$Ax = b.$$

The idea is to express the solution "x" as

$$x = y + Z\lambda.$$

Where Z will be a sparse matrix defind so that non zero rows STRICTLY SPAN ONE SINGLE MPI PROCESS.

The idea is that we are adding a new variable, so we need to introduce one further restriction in the solution of the system. This restriction is:

$$Z^T \left(A \left(y + Z\lambda\right)\right) = Z^T b.$$

Overall the modified system is equivalent to

$$\begin{pmatrix} A & AZ \\ Z^T A & Z^T AZ \end{pmatrix} \begin{pmatrix} y \\ \lambda \end{pmatrix} = \begin{pmatrix} b \\ Z^T b \end{pmatrix}$$

With $E = Z^T AZ$

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AMGCL Solver
Formulation

The idea is to condense statically the lambdas as

$$\lambda = -E^{-1}AZy + E^{-1}Z^{T}b.$$

After substituting in the first equation we get

$$\left(I - AZE^{-1}Z^{T}\right)Ay = \left(I - AZE^{-1}Z^{T}\right)b$$

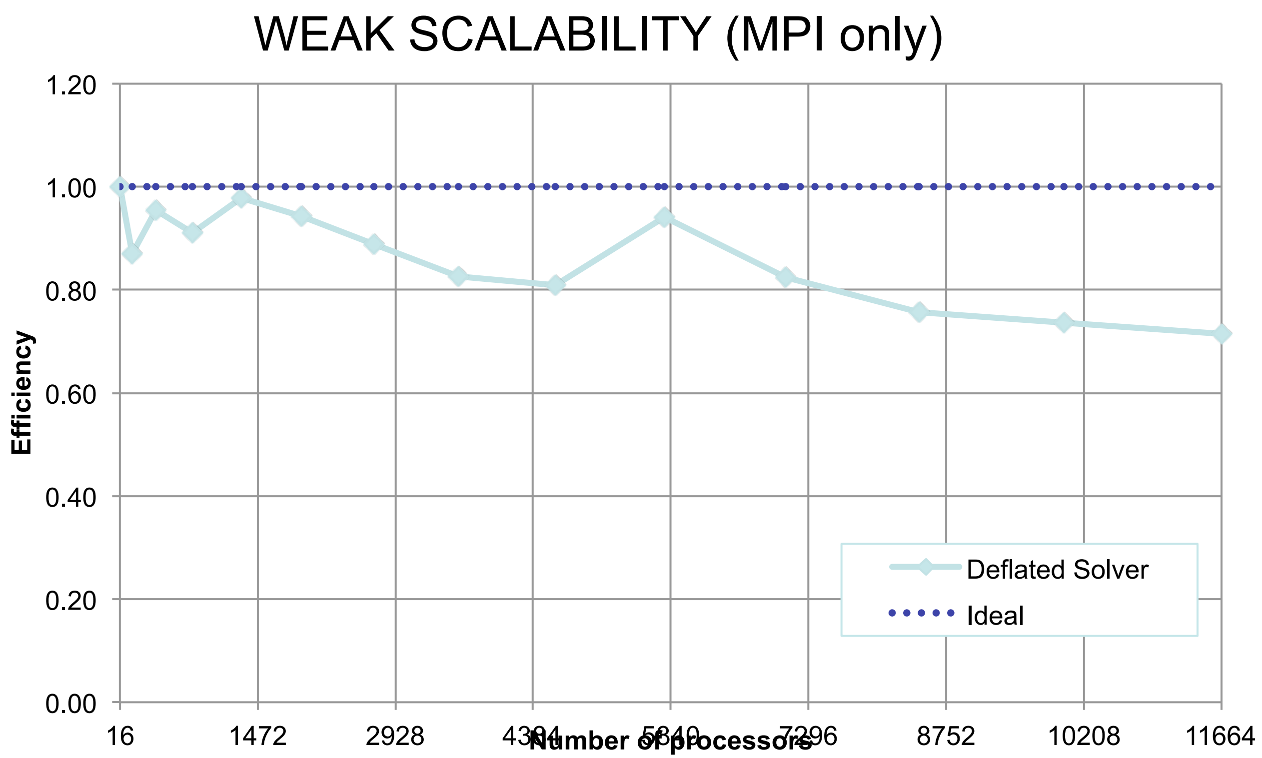
Which can be expressed as a projection as

$$P\left(Ay\right) = P\left(b\right).$$

Defining a system we can effectively solve for “y”. Given “y” one can compute “lambda” as a post process and finally obtain the final result.

AMGCL Solver

Deflation at the MPI level + AMG at the local level



Numexas is collaborating to the MPI version of "AMGCL" (together with Dr. Demidov, the library author)

- 2 level library (multilevel is possible)
- MPI+X (X = OpenMP/OpenCL/CUDA depending on the backend)
- **Algorithmically scalable solver**

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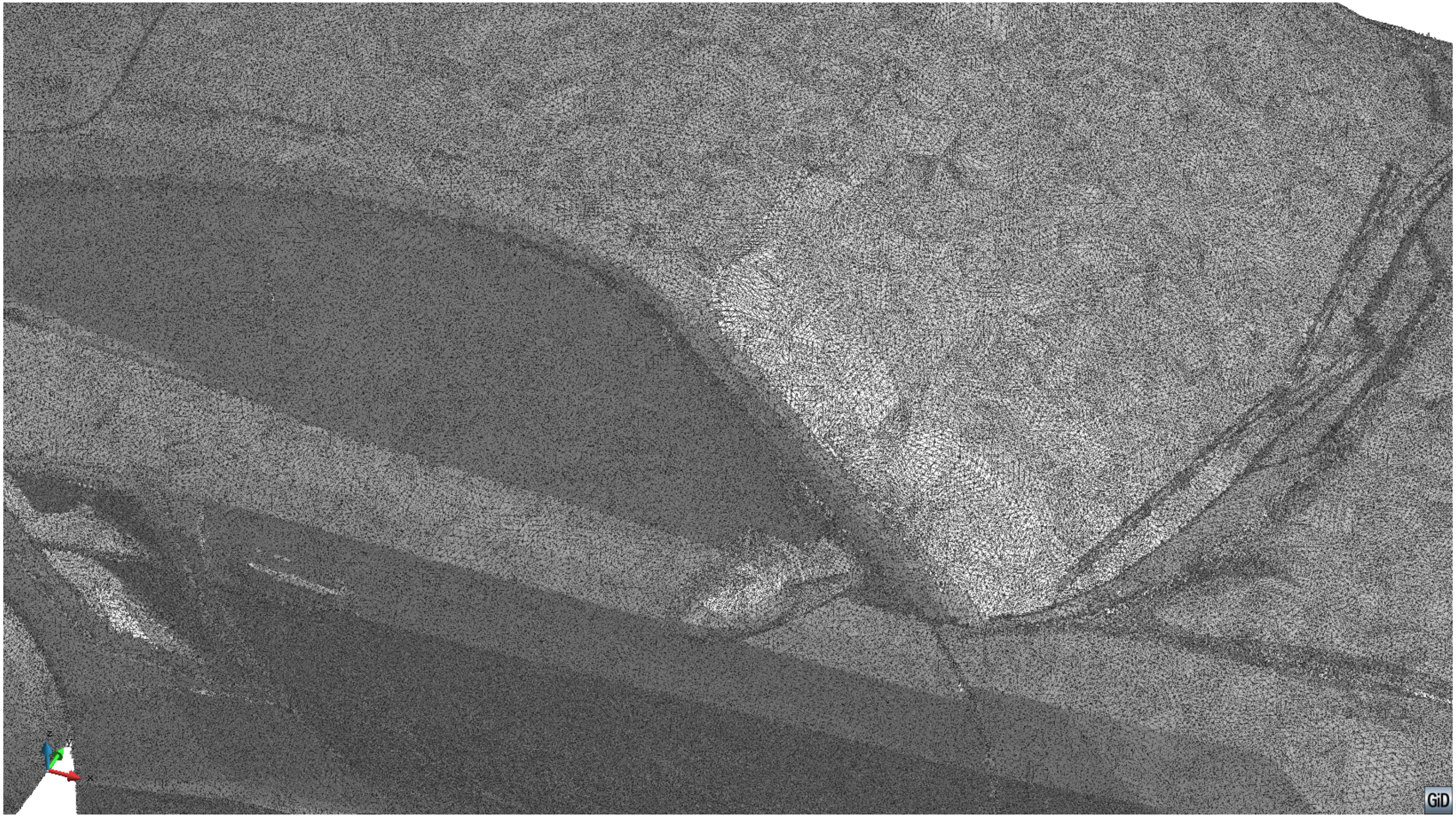
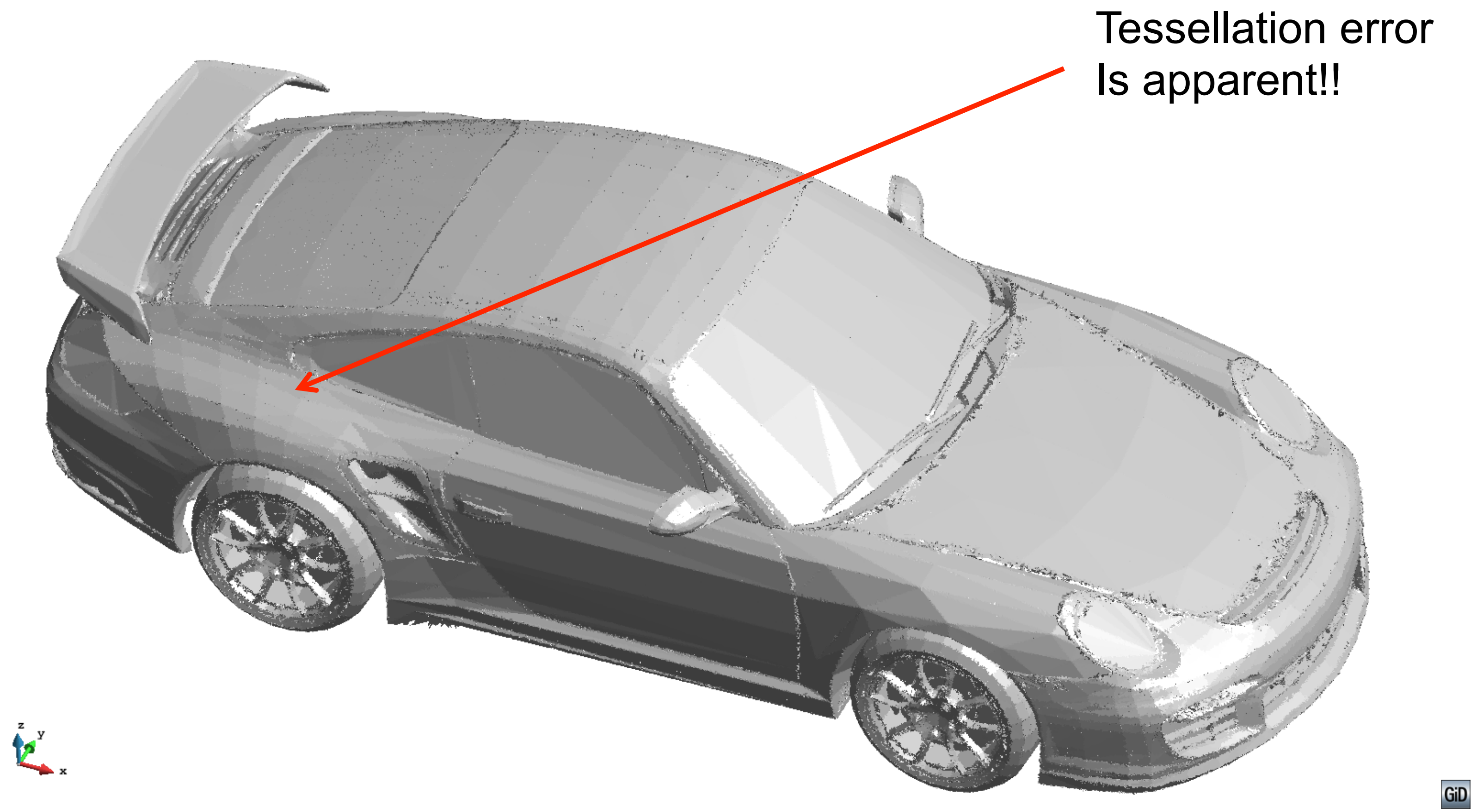
OPEN CHALLENGES

CFD mesh much finer than the original 3D model triangulation



OPEN CHALLENGES



Original Surface was triangulated ➔ it already contained discretization errors

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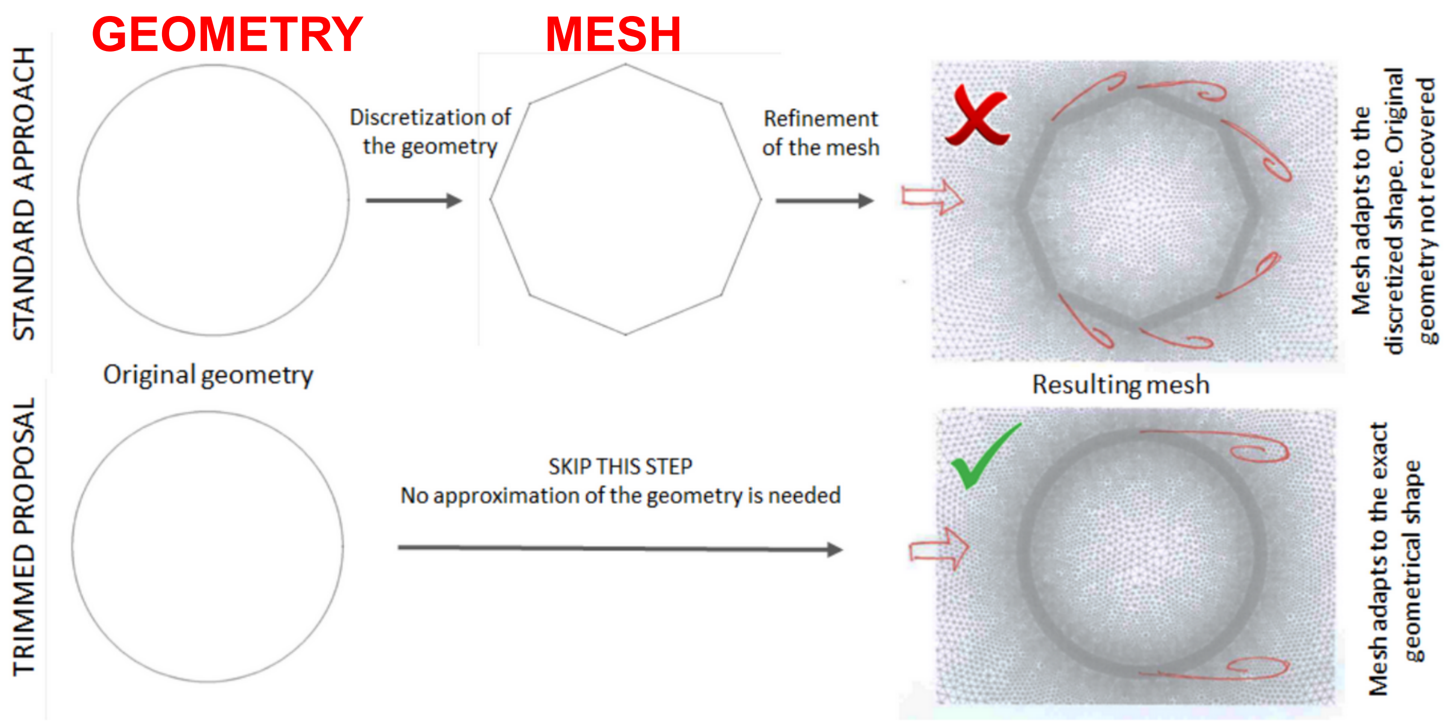
OPEN CHALLENGES

CFD error will be governed by the error in the initial triangulation!!
→ **Ongoing effort to work directly with TRIMMED MULTIPATCH NURBS (following ideas of Isogeometric B-rep analysis [Breitenberger 2015])**



First results soon to be published in the M.Sc. thesis of Mr. Matthias Mayr

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OPEN CHALLENGES

SIMULATION OF MOVING BODIES

→ **Ongoing work on importing multibody animations**

Acknowledgments:
Projects

- **NUMEXAS**:

NUMERICAL METHODS AND TOOLS FOR KEY EXASCALE COMPUTING CHALLENGES IN ENGINEERING AND APPLIED SCIENCES

http://www.numexas.eu/

COOPERATION

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KRATOS MULTI-PHYSICS

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