



Exascale Computing Challenges in Engineering

Numexas and Velasco

POOYAN DADVAND

MIGUEL PASENAU

EUGENIO OÑATE

CO-DESIGN

Guilin 2013

Layout

- **Who are we**
- **Motivation**
- **Kratos**
- **GiD**
- **Industrial Exascale Chalanges**

Who are we?

International Center for Numerical Methods in Engineering

Created in 1987 in
collaboration with
UNESCO



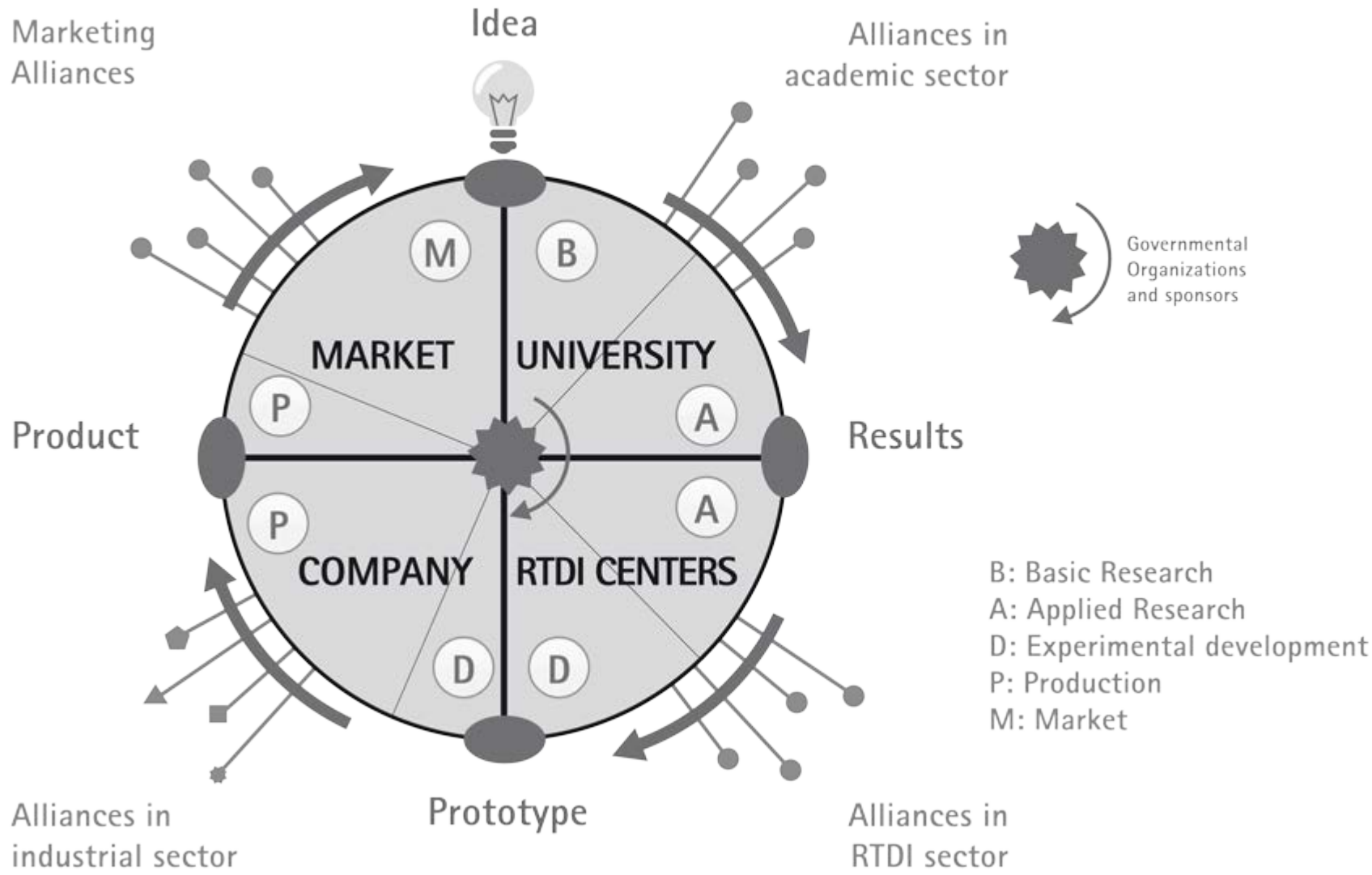
Consortium:



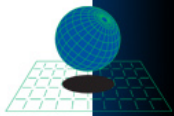
Specialized

Training + Research + Technology Transfer





INTERNATIONAL BRANCHES



CIMNE's Classrooms

The CIMNE Classroom Network currently has thirty members, located mainly in Spain and Latin America.

Espanya: 8

Latinoamérica

Argentina 5

Brasil 2

Chile 1

Colombia 2

Cuba 1

El Salvador 1

Guatemala 1

México 3

Perú 1

Venezuela 3



Personnel

Staff	254
Post Doctoral Researchers	52
Affiliated Scientists (UPC)	24
RTD staff	106
PhD Students	36
Administration and services staff	36

2012		2012		2012	
Argentina	9	Ecuador	1	Peru	1
Australia	1	France	1	Romania	1
Belgium	1	Germany	1	Russia	1
Brazil	1	Greece	1	Slovenia	1
Bulgaria	1	Holland	0	Spain	133
Chile	5	India	1	Tunisia	1
Colombia	11	Iran	4	Turkey	1
Costa Rica	1	Italy	10	United States	1
Cuba	1	Luxembourg	1	Uruguay	1
Czech Republic	0	Mexico	3	Venezuela	1
Dominican Republic	1	Morocco	1	TOTAL	226

CIMNE regularly welcomes teachers and students from over 35 different nationalities.

Activities from 1987

Courses and seminars: 509



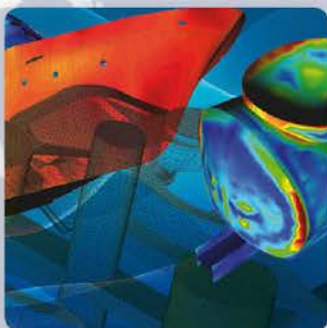
Conferences: 135



Publications: 1395



RTD projects: 1643



Spin-Off Companies: 13

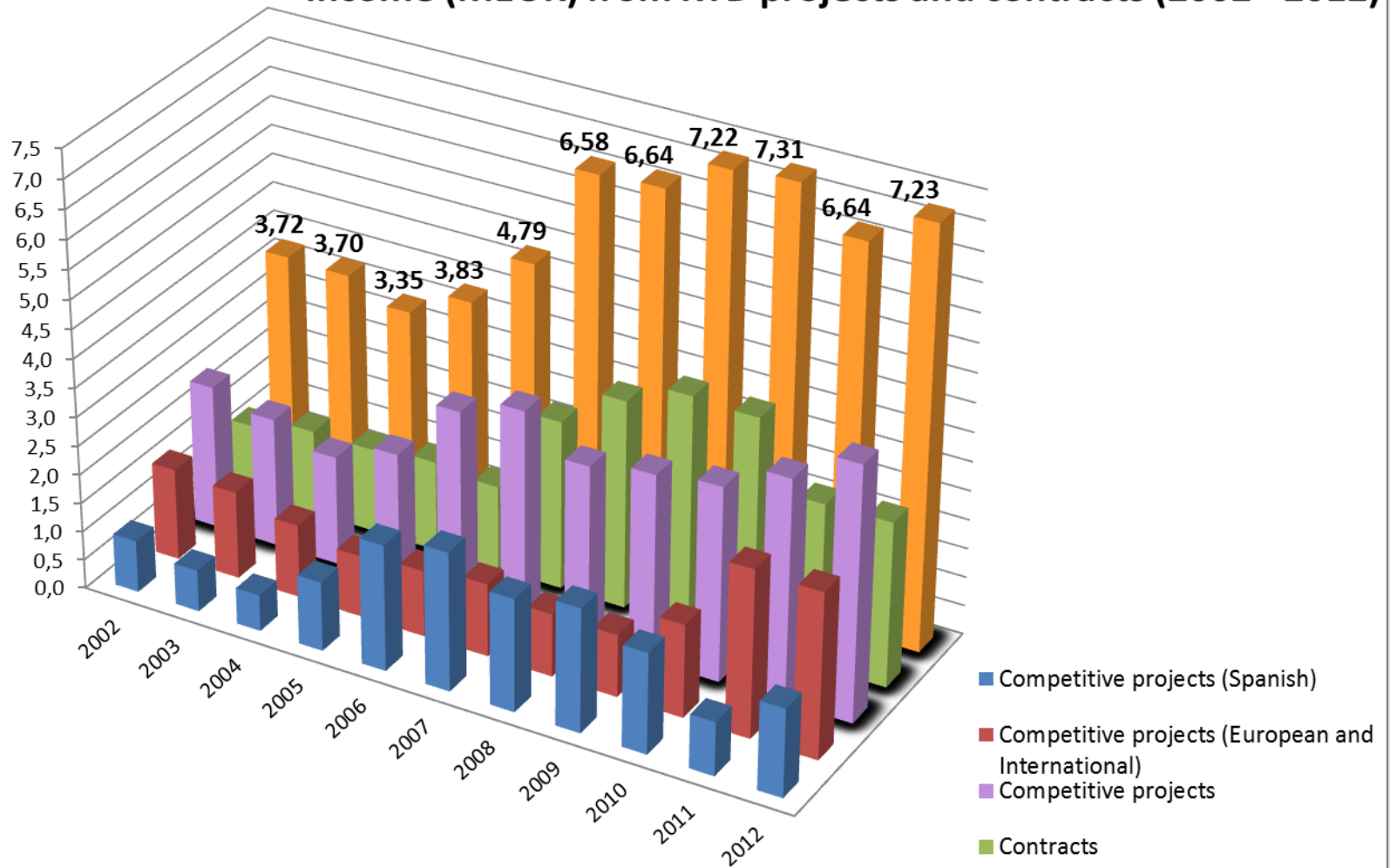


CIMNE Classrooms: 29



Information at 30/09/2013

Income (MEUR) from RTD projects and contracts (2002 - 2012)



Research, development and innovation (RDI) Departments in CIMNE:

- Computational Physics and Large Scale Computing
- Aerospace Engineering
- Civil Engineering
- Building, Energy and Environment (BEE GROUP)
- Marine and Naval Engineering
- Technology Transfer Services (TTS)
- Bio-Medical Engineering
- Socio-Economic Research
- Pre and Post processing
- Information and Communication Technologies

PRE AND POST PROCESSING SOFTWARE

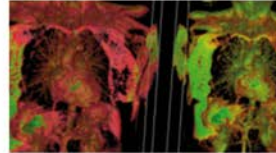
GID



A universal and adaptive pre and postprocessor for computer simulation in engineering and applied science.

Developed and marketed by CIMNE since 1998
www.gidhome.com/

DIPPO



Digital image processing platform.
Developed and marketed by CIMNE since 2011

ENGINEERING SYSTEMS AND HARDWARE

Inflatable structures



Inflatable pavilions, shelters and bridges for applications in engineering and architecture.

Developed in cooperation with Building Ingeniería y Arquitectura SL and Tensairity Structures SL.

Marketed by BuildAir since 2002
www.builair.com

COLLABORATIVE WORK PLATFORMS

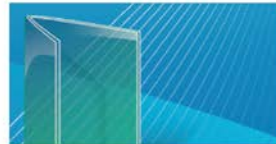
FRAKTALIS



Fully customizable Web application that creates virtual communities where users can communicate, share information and work collaboratively.

Developed and marketed by CIMNE since 2009
www.fraktalis.com/

SIGPRO



Integrated software platform for the management of the research and financial activities and reports in RTD projects.

Developed by CIMNE

EDUCATIONAL SOFTWARE

SoftEducatiu



Educational software for interactive learning about structural design and finite element method

Developed and marketed by CIMNE

Mi colegio en red (MCR)



Integrated communications and services management system for schools via the Internet.
Since 2000

LHINGS



Lhings is a cloud platform designed to provide access and links to all kind of things and let users management, share and interact with those things anywhere and when they like.

Developed and marketed by Lyncos SL in cooperation with CIMNE
www.lhings.com

DECISION SUPPORT SYSTEMS

BEACHING



Information system for management of tourism activities in beach areas.
Developed by CIMNE and marketed by TAOC SA since 2011
www.beaching.com/

SIE



Information system for management of energy consumption in public buildings and municipalities.
Developed by CIMNE
Marketed by Gassó Auditors SL and CIMNE since 2005

FLOOD



Artificial neuronal network package.
Developed by CIMNE

ROBOCOPT



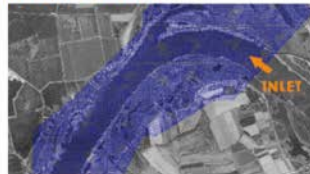
Interpolated platform for robust optimization in engineering.
Developed by CIMNE

ROEM



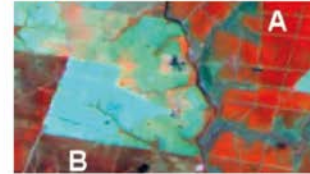
Information system for assessment of the environmental quality in reservoirs and lakes.
Developed by CIMNE

RAMFLOOD



Decision support system (DSS) for risk assessment and managing of floods.
Developed by CIMNE and FLUMEN
www2.cimne.com/ramflood/

GIS+



Web-based interactive Geographic Information System.
Developed by CIMNE

ETESTING



Web-based platform for e-management of experimental tests.
Developed by CIMNE and Aplius

WSNP

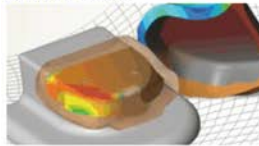


An integrated platform for e-monitoring using wireless sensor network technology.
Developed by CIMNE
www2.cimne.com/wsnp/

SIMULATION SOFTWARE

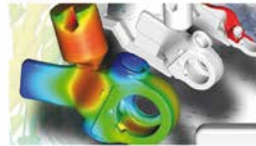
MANUFACTURING PROCESSES

STAMPAK



Sheet metal forming processes.
Developed by Quantech ATZ, SA, in cooperation with CIMNE.
Marketed by Quantech ATZ, SA since 1999
www.quantech.es

VULCAN



Casting and foundry processes.
Developed by Quantech ATZ, SA, in cooperation with CIMNE.
Marketed by Quantech ATZ, SA since 2001
www.quantech.es

WELDPACK



Welding processes.
Developed by CIMNE

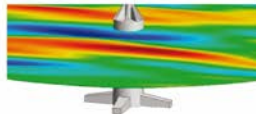
FLUID DYNAMICS

TDYN



Finite element code for analysis of a wide range of multi-physics problems in engineering and applied science (fluid dynamics, heat transfer, fluid-structure interaction, etc.)
Developed by Compass Ingeniería y Sistemas, SA, in cooperation with CIMNE.
Marketed by Compass since 2003
www.compassis.com

SEAFEM



Hydrodynamics and seakeeping analysis of ships and marine structures.
Application for wind tower generators in the sea.
Developed by Compass Ingeniería y Sistemas, SA, in cooperation with CIMNE.
Marketed by Compass since 2011
www.compassis.com

MULTI-PHYSICS

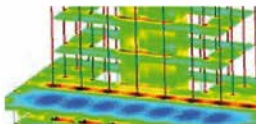
KRATOS



Kratos is an open object-oriented software platform for the development and application of finite element codes for multidisciplinary applications in engineering and applied science.
Developed by CIMNE
www.cimne.com/kratos

STRUCTURAL ENGINEERING

RAMSERIES



Finite element code for analysis of structures in engineering and architecture.
Developed by Compass Ingeniería y Sistemas, SA, in cooperation with CIMNE.
Marketed by Compass Ingeniería y Sistemas, SA, since 2003
www.compassis.com

DEMPACK

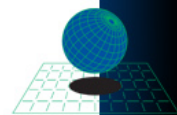


Analysis of granular systems and multifracturing problems in geomechanics and industrial processes using discrete and finite element methods.
Developed by CIMNE
www.cimne.com/dem

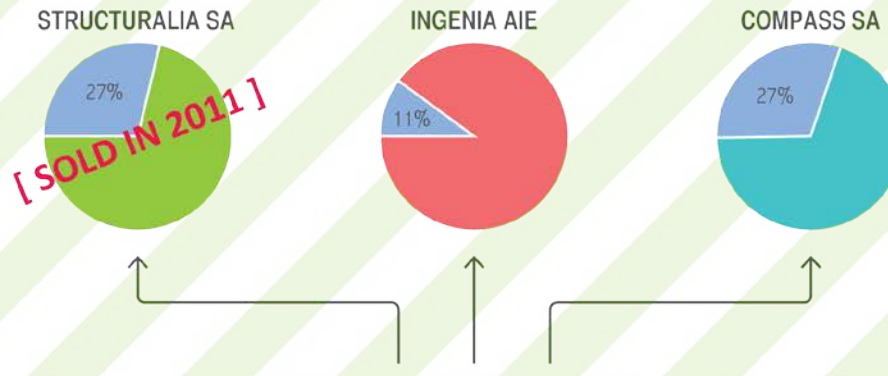
COMET



Finite element code for none linear analysis of thermomechanical problems in solid and structural mechanics accounting for frictional contact situations.
Developed at CIMNE
www.cimne.com/comet



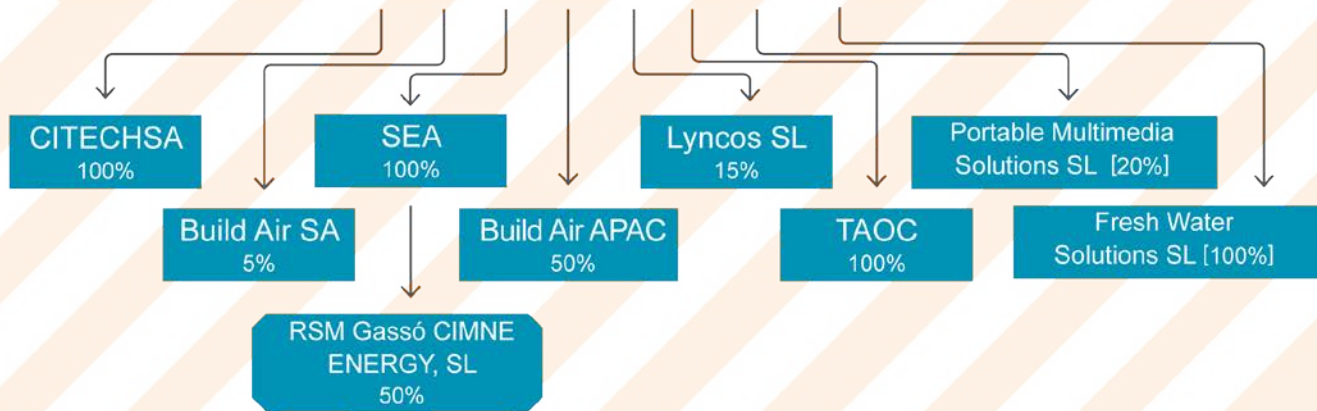
First generation of
CIMNE companies
(2000-2011)



CIMNE

100% CIMNE TECNOLOGÍA SA

SECOND generation of
CIMNE companies
(2011- ...)



Participation in companies (I)



INGENIA AIE (Created in 2004) is a Group of Economic Interest formed by 8 companies and CIMNE. The objective of INGENIA is to promote the participation of its members in projects of industrial size in the aeronautics and space field in cooperation with the main international manufacturers in the sector. The partners in INGENIA are: Applus, Cimsa, Compass, CT Ingenieros, Prae Trade, Quantech ATZ, Rücker Lypsa, Solid Enginyeria and CIMNE. (www.ingenia.aero). CIMNE owns 12% of INGENIA AIE.

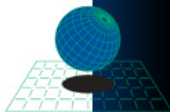


COMPASS INGENIERÍA Y SISTEMA S.A. (Created in 2002) The objective of COMPASS is to develop commercial activities in the application of numerical methods in engineering, with emphasis on civil, naval and maritime engineering. COMPASS offers design and analysis services in engineering, project management, specialized software systems for engineering design, innovative developments in engineering and advanced training courses. (www.compassis.com). CIMNE owns 24% of COMPASS.



STRUCTURALIA S.A. The objective of STRUCTURALIA is to develop training and consulting activities in civil engineering and construction sector via Internet. The company was sold in 2011 to the US company KAPLAN (The Washington Post Group).

SOLD



Participation in companies (II)



CIMNE TECNOLOGÍA SA is a company 100% owned by CIMNE aiming to industrialize and market the products and technology developed at CIMNE. CIMNE Tecnología SA is also an incubator and promoter of new companies. <http://www.cimnetecnologia.com/>
Created in 2011.



TECNOLOGÍAS AVANZADAS PARA EL OCIO SL (TAOC) is a company 100% owned by CIMNE Tecnología SA. It specializes in the development and market of information systems for leisure sectors such as tourism and music. Created in 2012. (www.beaching.com)



BUILD AIR APAC is a subsidiary of Build AIR operating in the Asia-Pacific region from Singapore. CIMNE owns 20% of BUILD AIR APAC. Created in 2012. (www.buildair.com)



SERVICIOS ENERGÉTICOS AVANZADOS SA is a company 100% owned by CIMNE Tecnología SA. It specializes in the development and marketing of services of software products for energy management of public and private buildings in urban areas. Created in 2012.



INERGY (CIMNE-RMS Gassó SL) was created in 2012. This company specializes in the marketing of services and products for energy management of buildings and urban areas. The company is 50% owned by CIMNE Tecnología SA. (www.inerybcn.com)

Participation in companies (III)



BUILDPAIR INGENIERIA Y ARQUITECTURA SA is a company created in 2002 specialized in the development and marketing of inflatable structures for a wide range of applications in engineering and architecture. CIMNE Tecnología SA owns 5% of BUILDPAIR (www.buildair.com).



COMPUTATIONAL AND INFORMATION TECHNOLOGIES SA is a company 100% owned by CIMNE Tecnología SA specialized in the development and application of computational methods and information technology systems in engineering and applied sciences. Created in 2012.



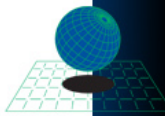
LYNCOS SL is a company specialized in the development, application and marketing of information and communication technologies and devices for a wide range of application in the Internet of Things sector. CIMNE TECNOLOGÍA SA owns 15% of LYN COS SL. Created in 2012. (www.lhings.com)



PORTABLE MULTIMEDIA SOLUTIONS SL (PMS) created in 2013 it is specialized in the development and marketing of mobile pavilion incorporating multimedia technology in the leisure, sport and events sectors, among others.



FRESH WATER SOLUTIONS SL (FWS) created in 2013 and specialized in the development of solutions for obtaining fresh water from desalinization of sea water.





Quantech is Established on Barcelona in 1996 by a group of professors of the UPC and researchers of CIMNE. THE MISSION of this new company is Impulse, develop and distribute simulation software solutions to manufacturing industrial processes.

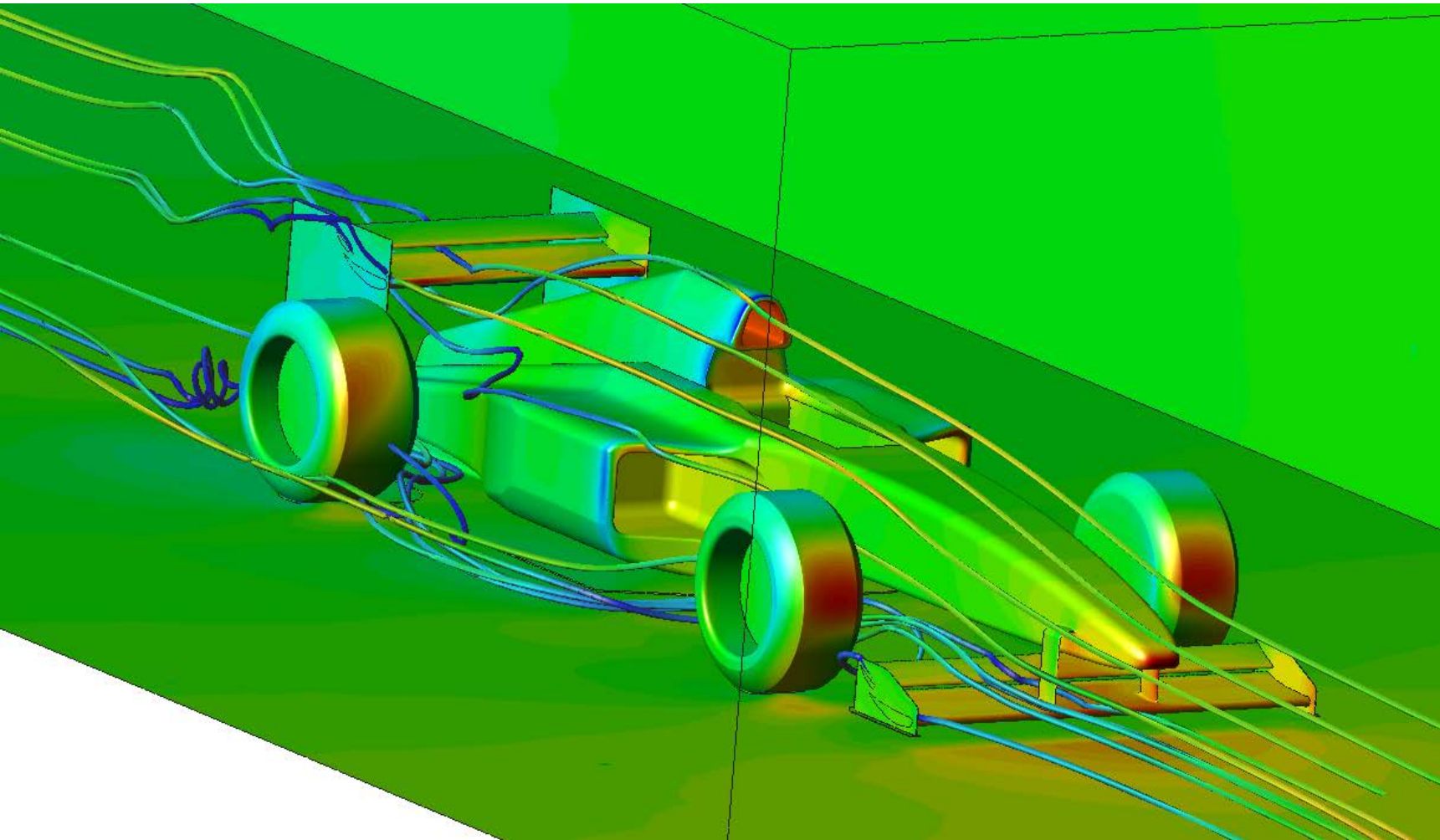




Motivation

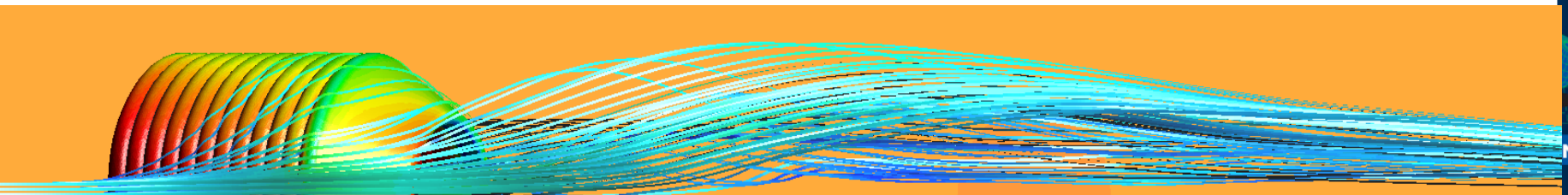
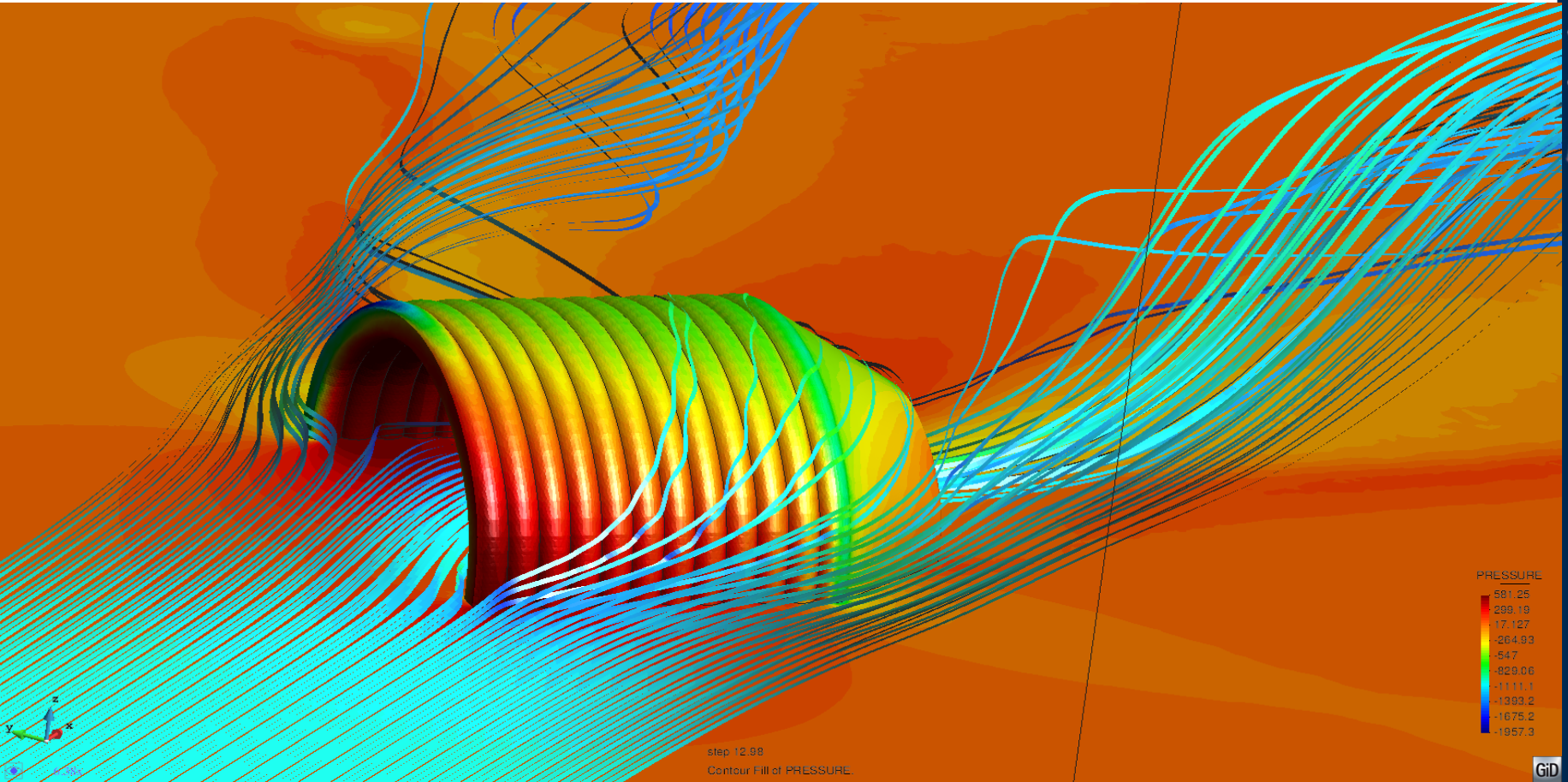
Motivation

Industrial Simulation



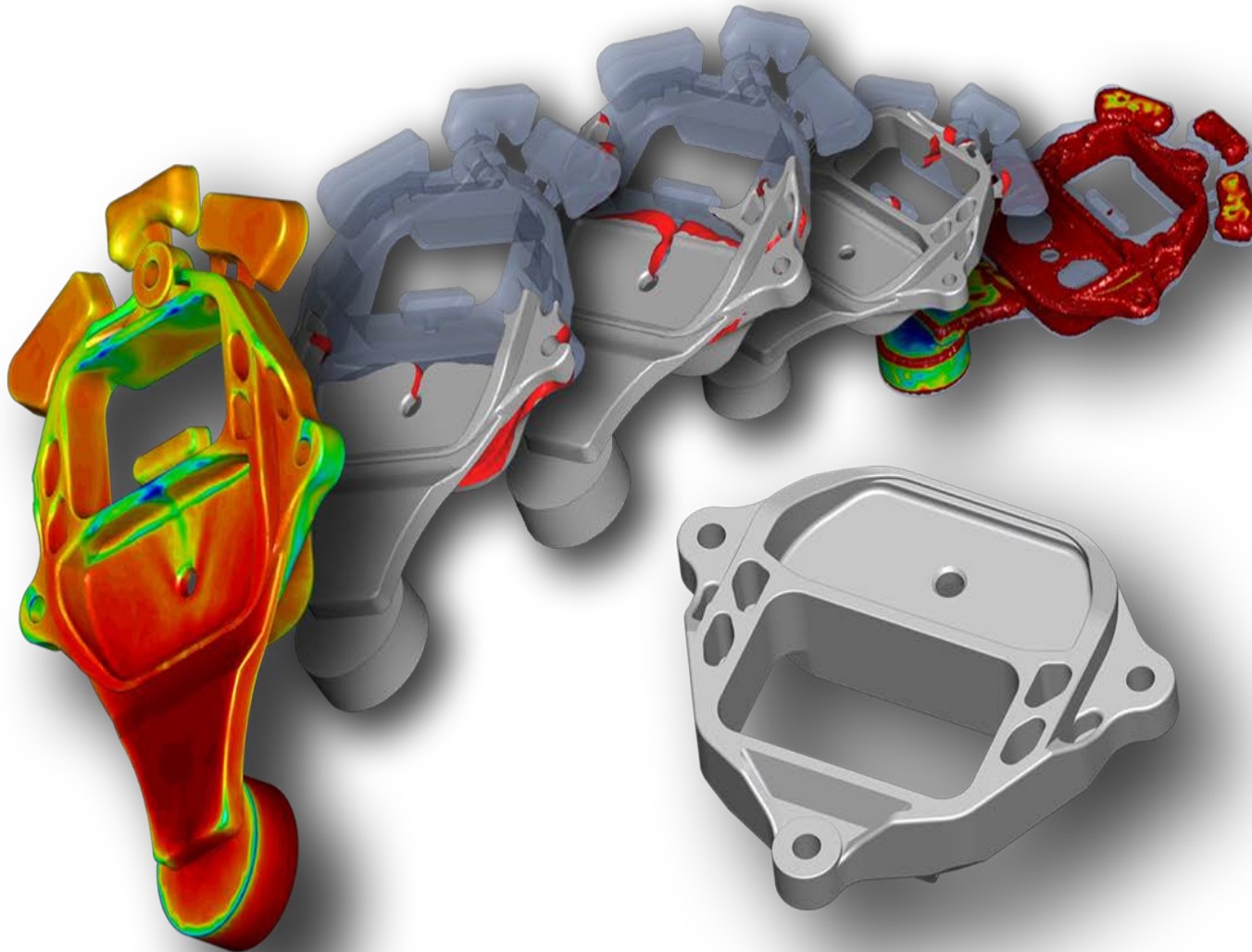
Motivation

Industrial Simulation



Motivation

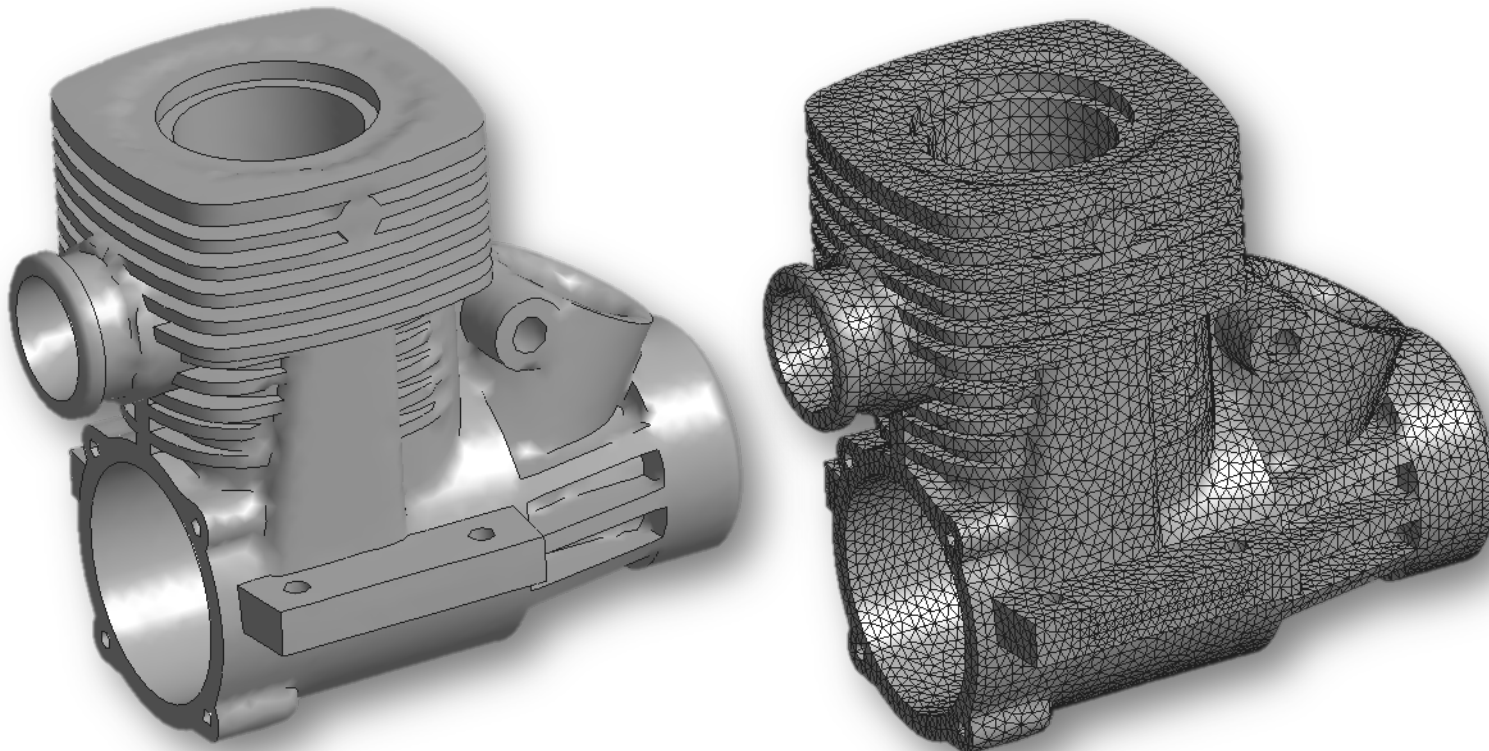
Industrial Simulation



Motivation

Industrial Simulation

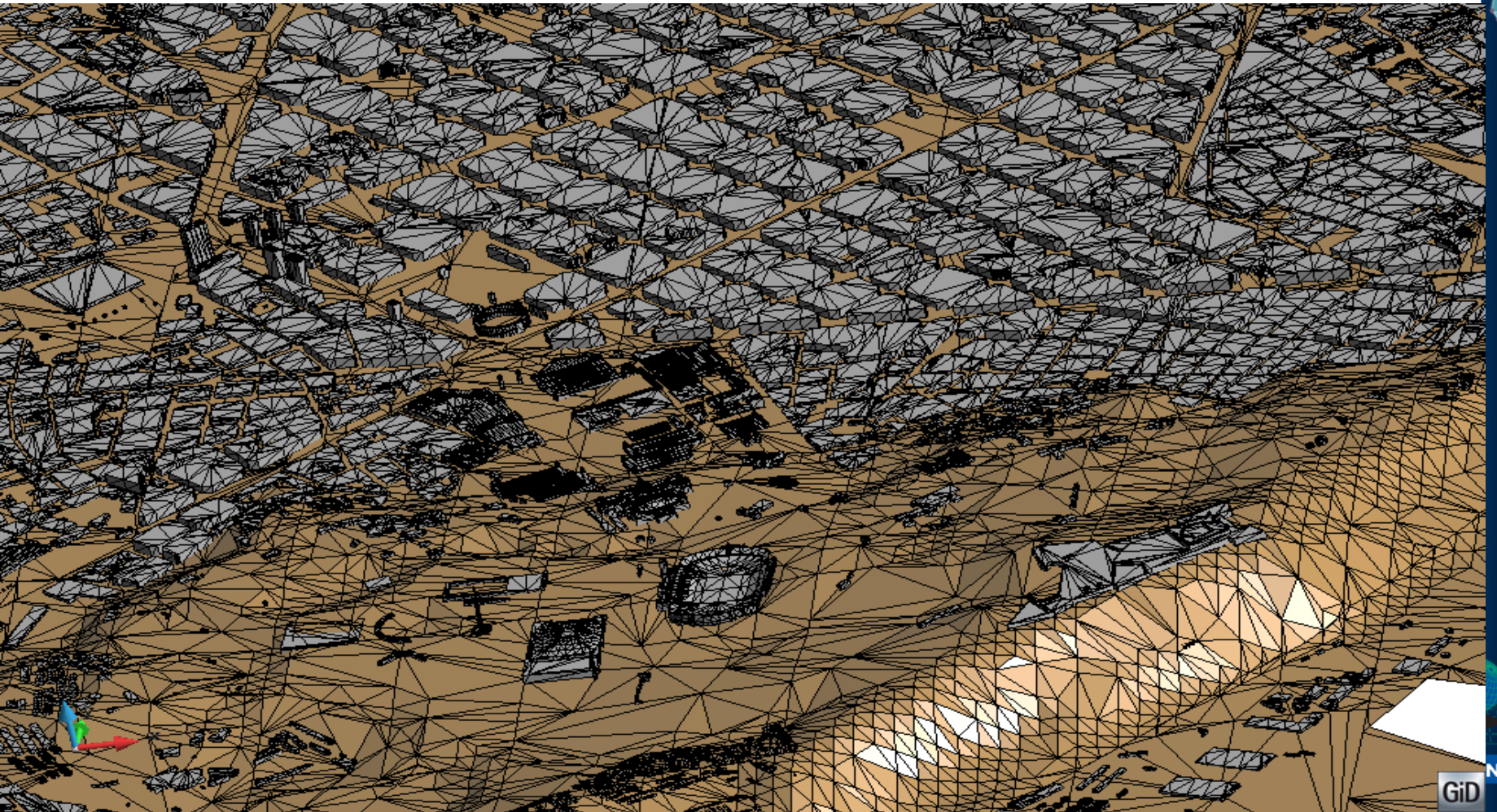
- Reducing calculation time by parallelization
- Modeling and Visualization are the bottleneck



Motivation

Industrial Models

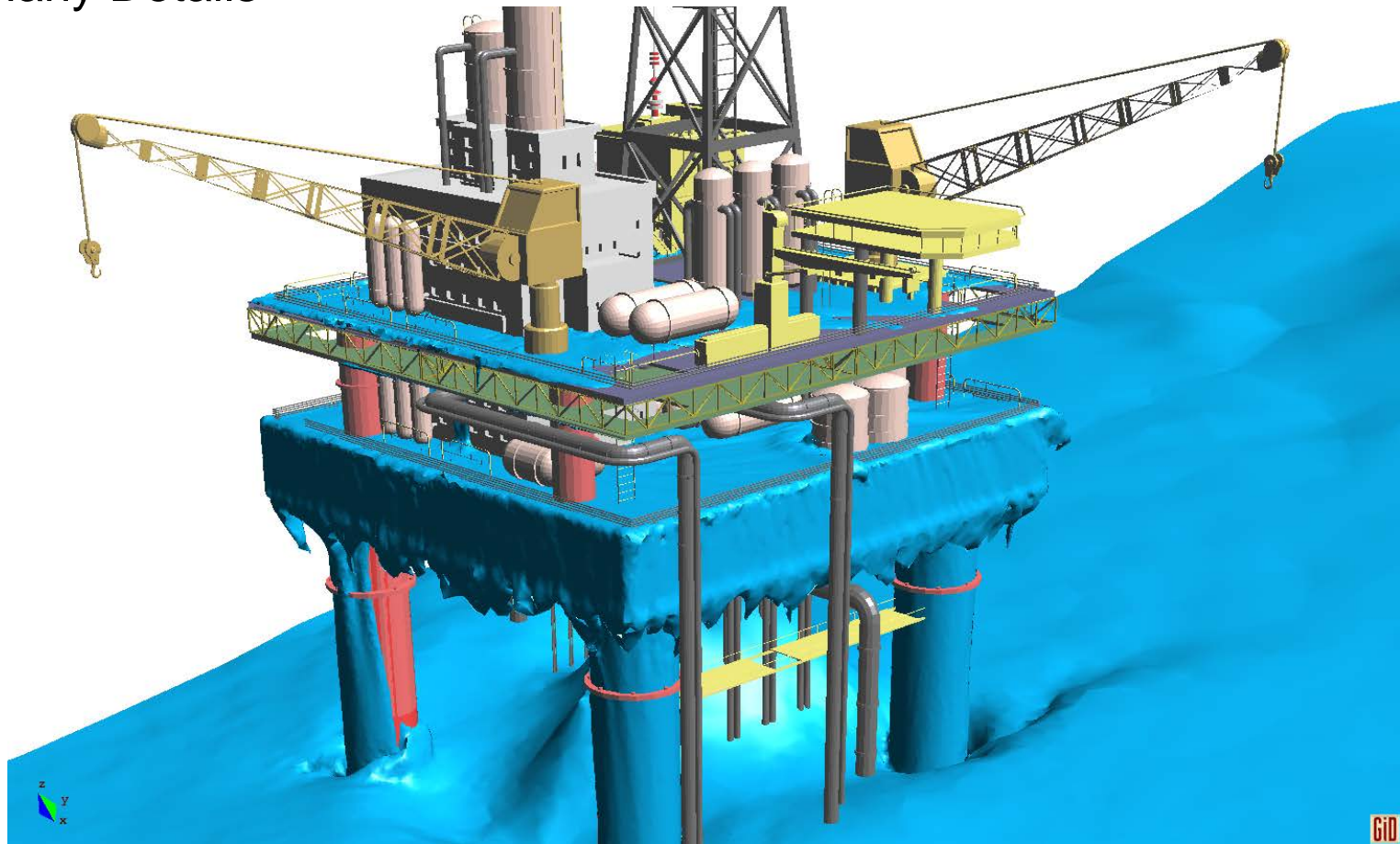
- Large and Complex Models



Motivation

Industrial Models

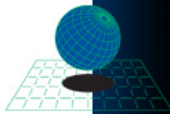
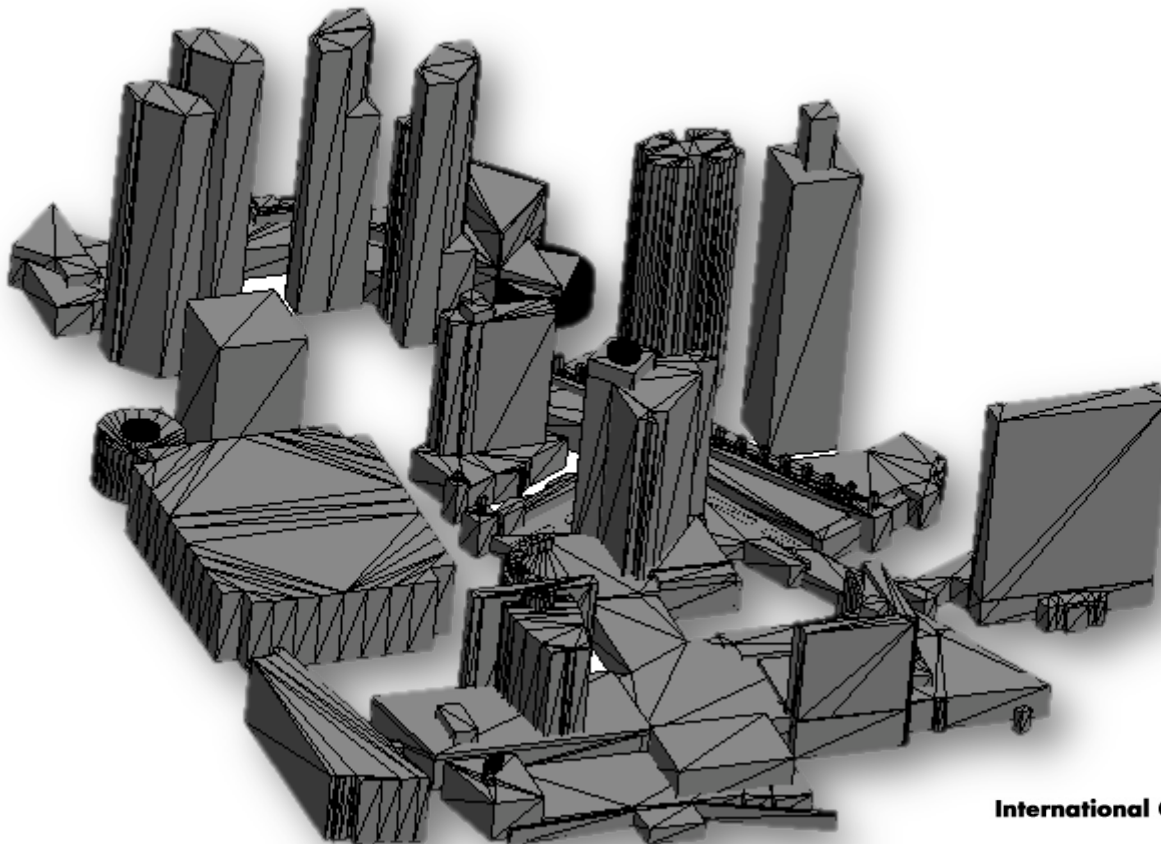
- Many Details



Motivation

Industrial Models

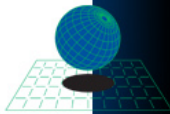
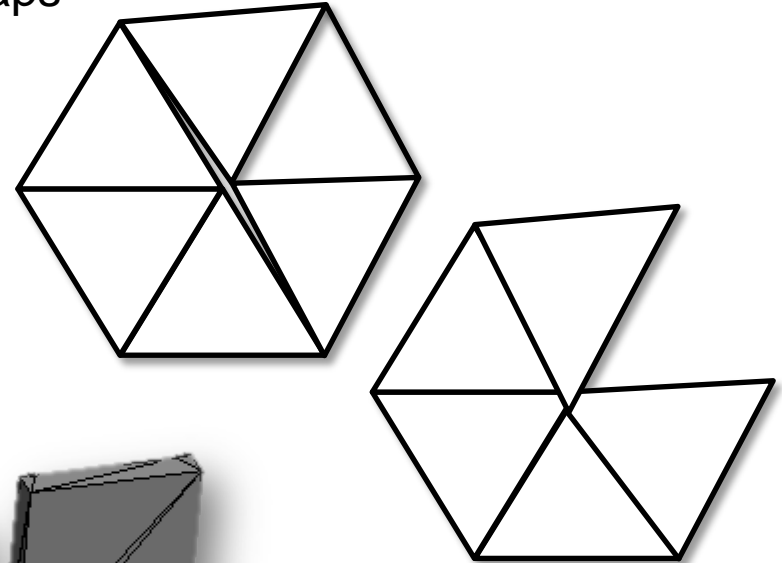
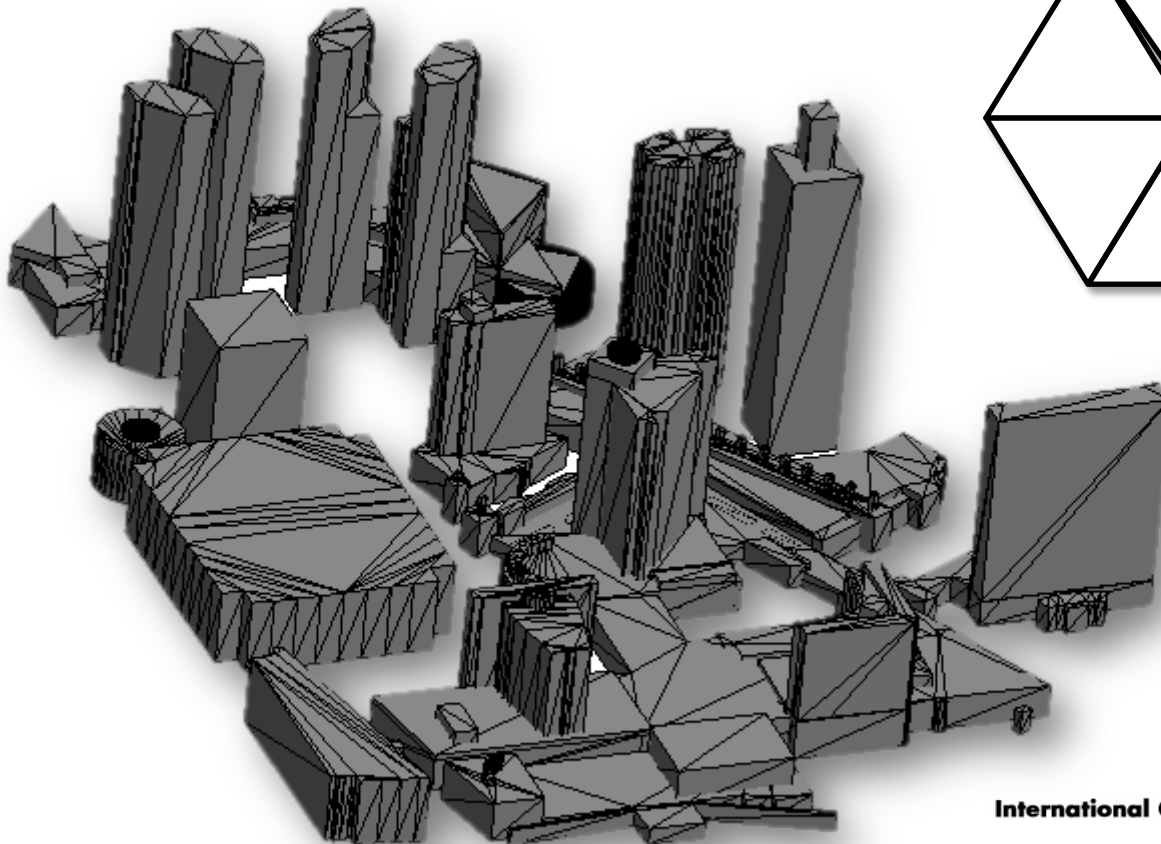
- STL is a common format



Motivation

Industrial Models

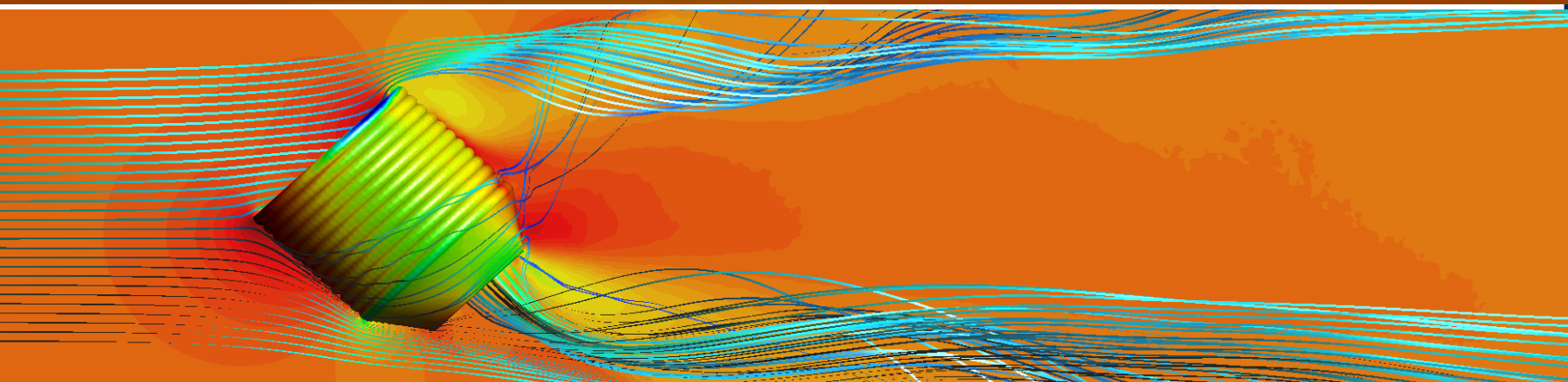
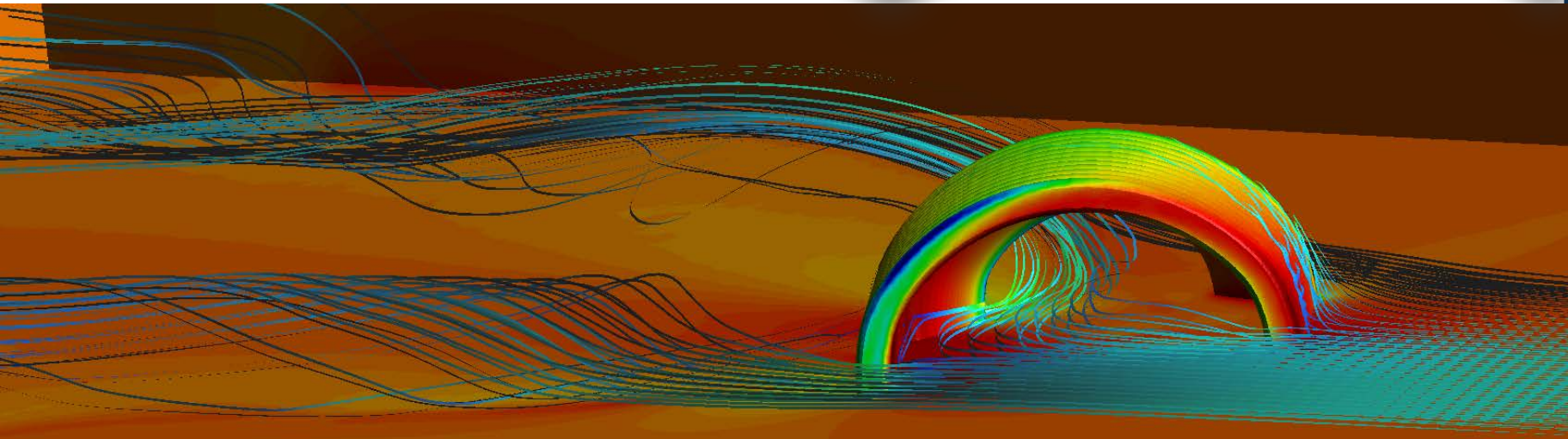
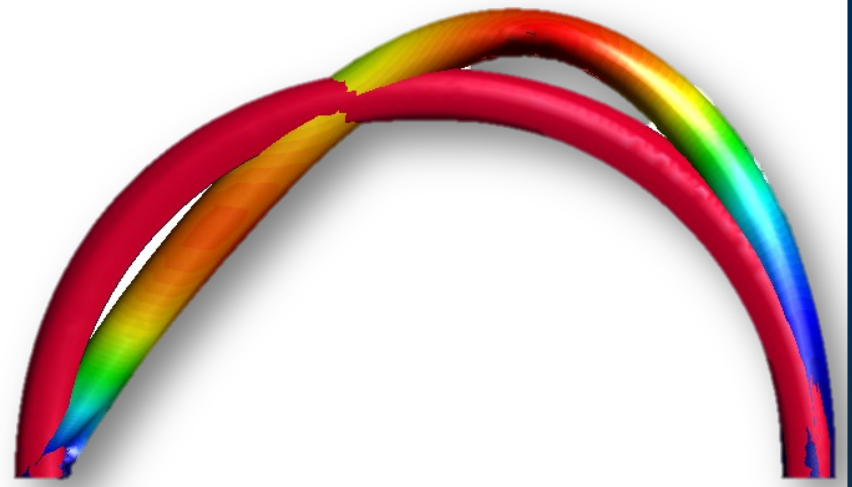
- STL is a common format
- STL files usually have gaps and overlaps



Motivation

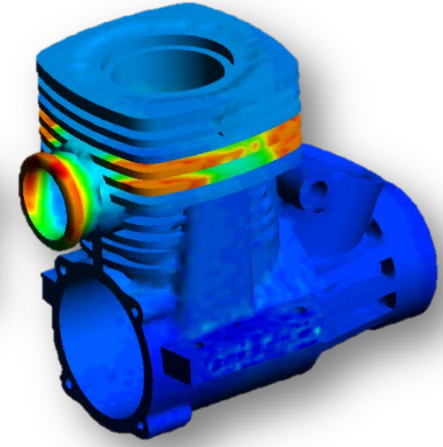
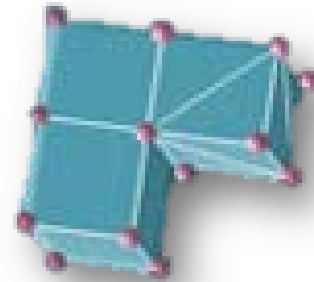
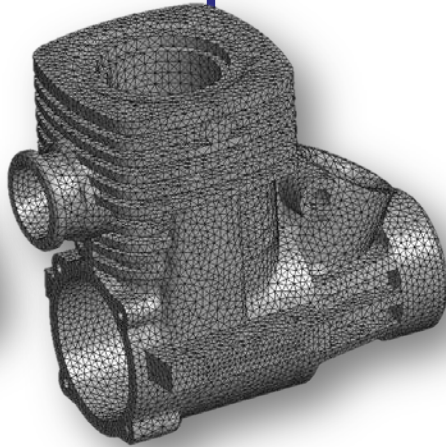
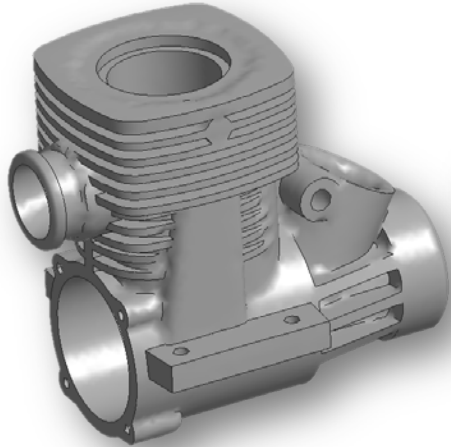
Industrial Models

- Multi-Disciplinary (FSI, etc.)



Motivation

Simulation Pipeline



Modeling

- Not Clean Geometry
- Complex Models

Meshing

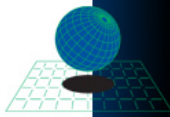
- Robustness
- Not Scalable

Analysis

- Scalability
- Efficiency
- Complexity
 - FSI
- Heterogeneous Machines

Visualization

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



What is C2C

SIMULATION SOFTWARE FOR METAL CASTING

CLICK2CAST

GEOMETRY MESH PARAMETERS CALCULATE RESULTS REPORT

Part Material
Group: Aluminium
Type: ASi/Mg
Temperature [°C]: 700

Mold Material
Steel-140CrMoV5-m
Temperature [°C]: 150

Process params
Gravity direction:
Distance [mm]: 150.0

T [ms]	P [bar]
100.0	100.0
5000.0	250.0
10000.0	300.0

Low Pressure

BACK NEXT

Define material and process parameters.

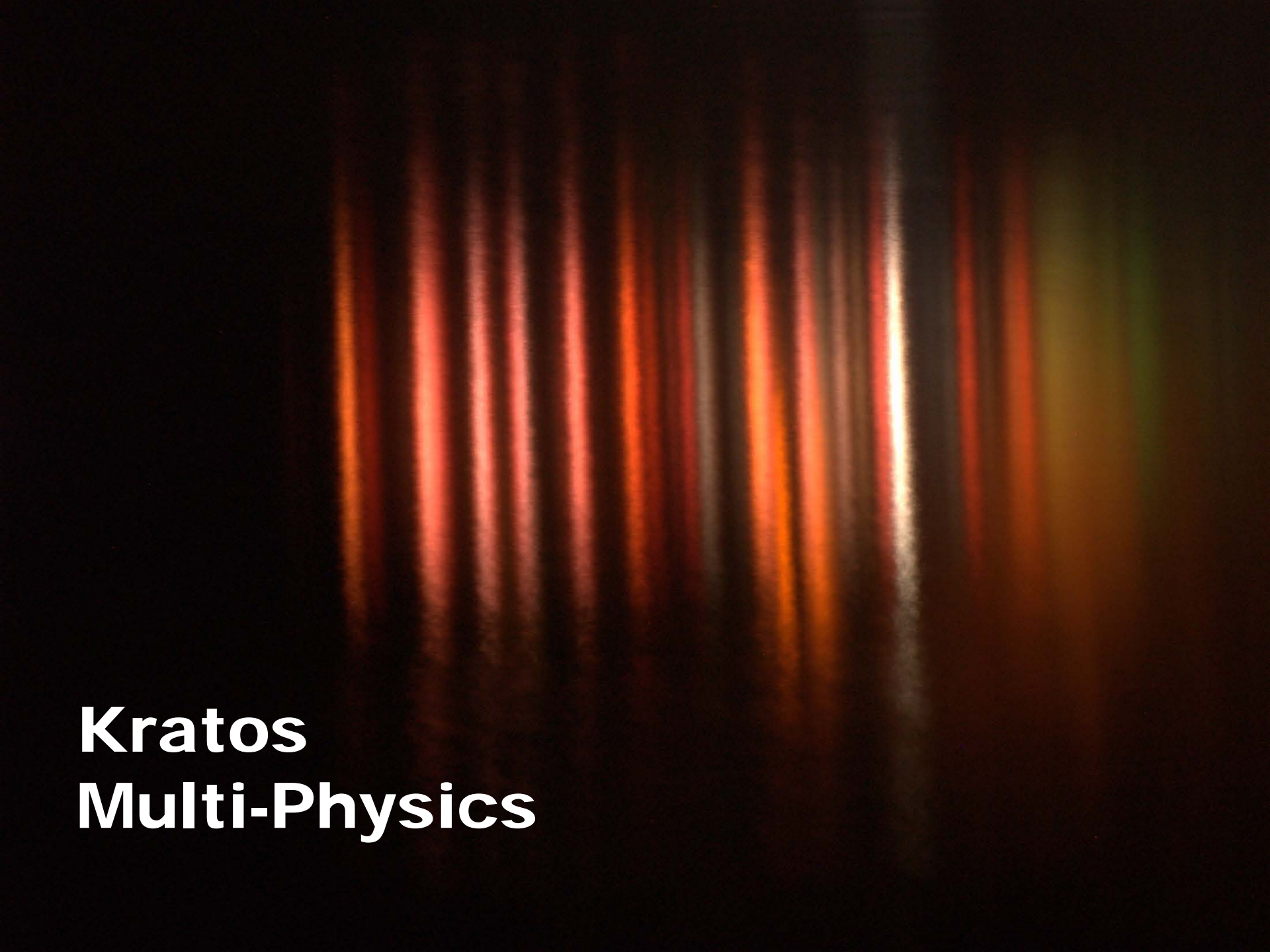
XY XZ YZ Iso

HPDC – LPDC

GRAVITY SAND

PERMANENT MOLD CASTING



A vertical streak of light is centered in the upper half of the image. It starts with a bright orange-red at the top, transitions through yellow, and ends in a soft green at the bottom. The background is dark, with some faint, blurry light patterns.

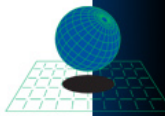
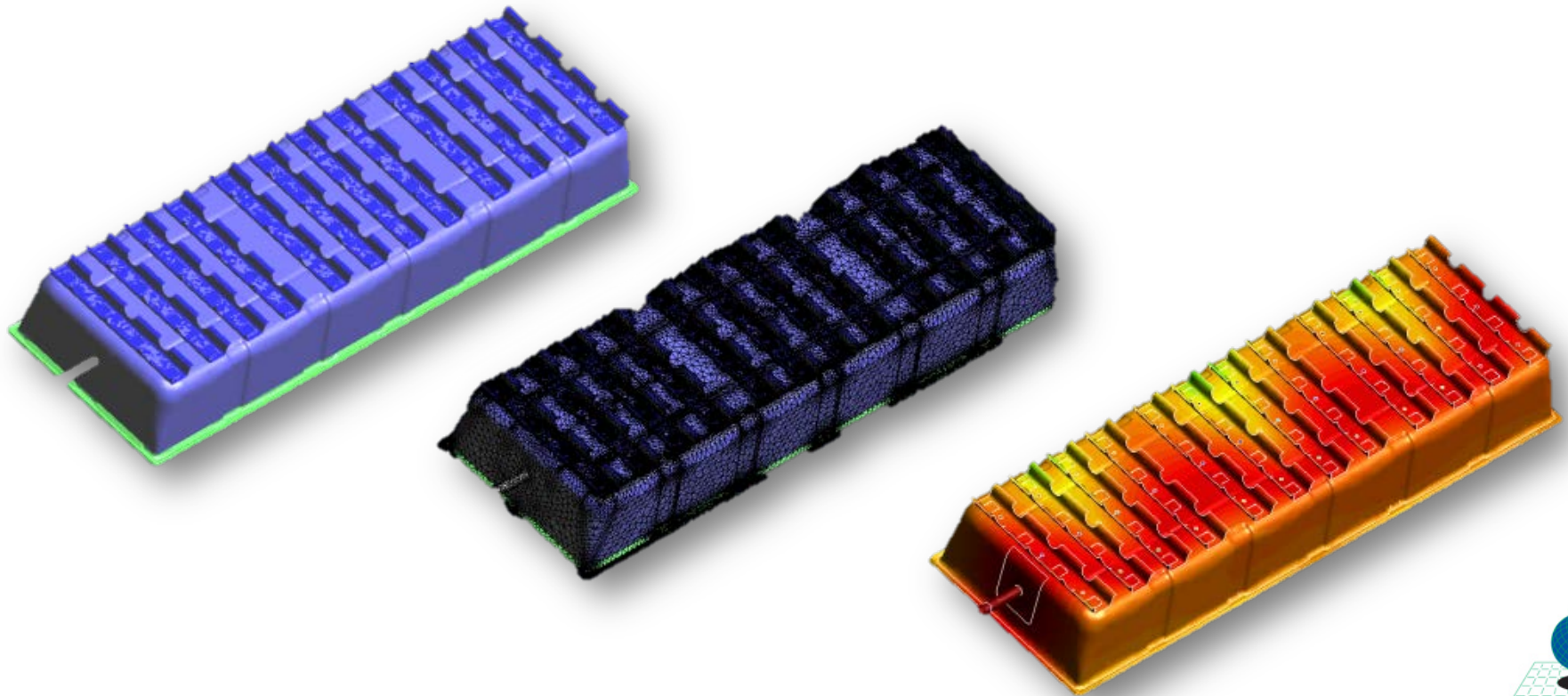
Kratos Multi-Physics

Kratos

What is?

A Program for Engineering Calculation

Engineers



Kratos

What is?

A Program for Engineering Calculation

Engineers

Framework for parallel Multi-physics
programs development

Developers

Kratos

What is?

A Program for Engineering Calculation

Engineers

Framework for parallel Multi-physics
programs development

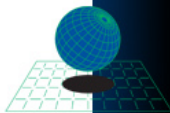
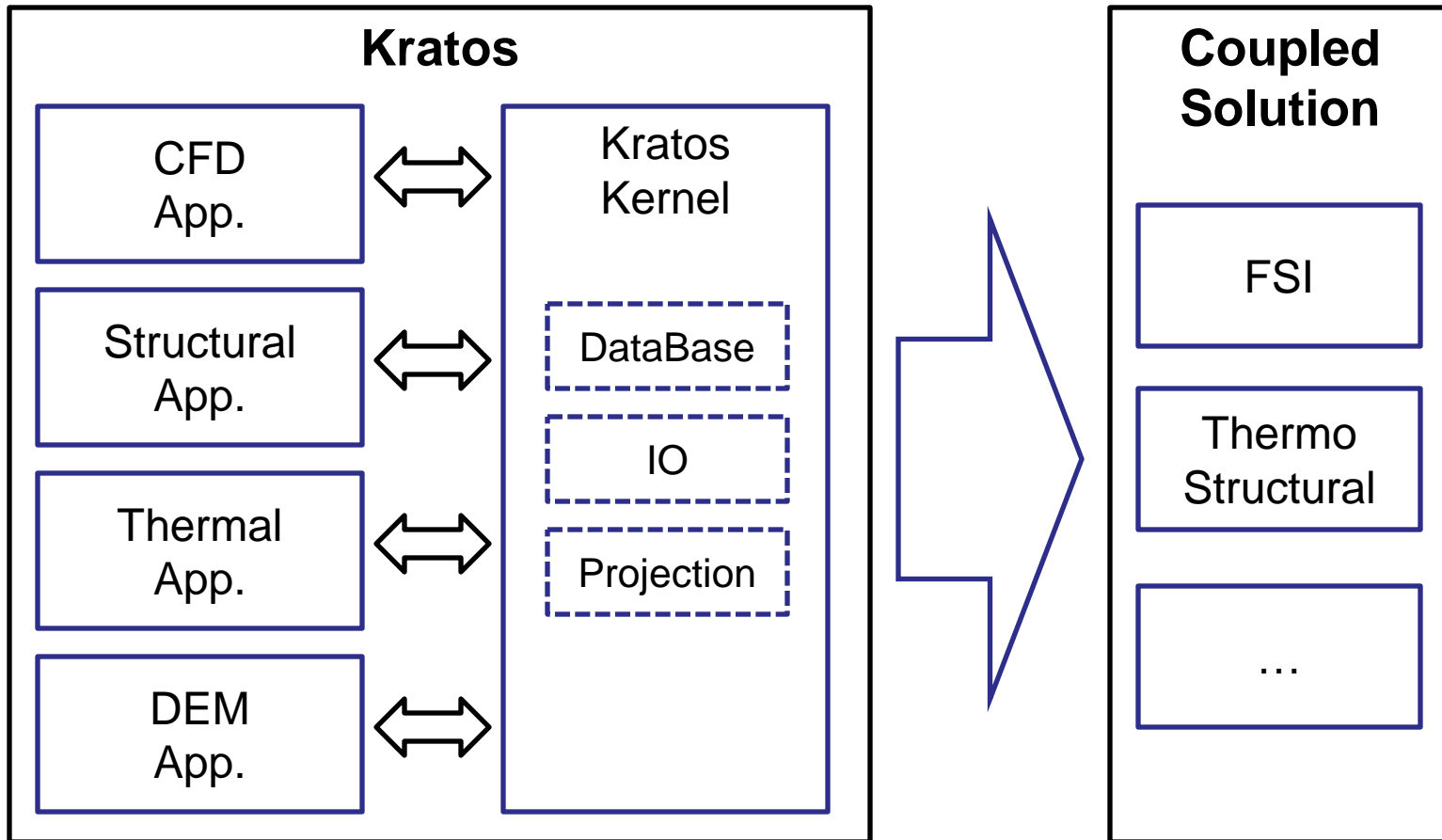
Developers

OPEN SOURCE and FREE (BSD Licence)

Everyone

Kratos

What is?



Kratos

What can do?

Solid Mechanics

DEM

Fluid Dynamics

Thermal

Kratos

What can do?

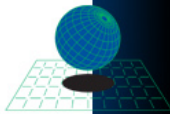
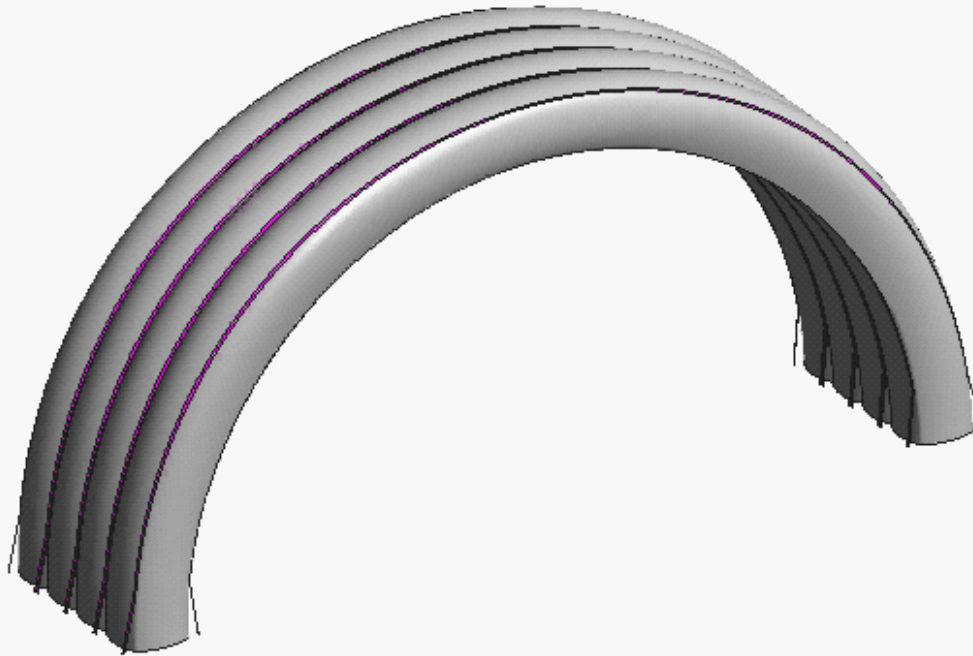
Solid Mechanics

Solid, Shell,
Membrane, Beam

Static, Dynamic

Linear, Non-linear

Small and Large
Deformation



Kratos

What can do?

Solid Mechanics

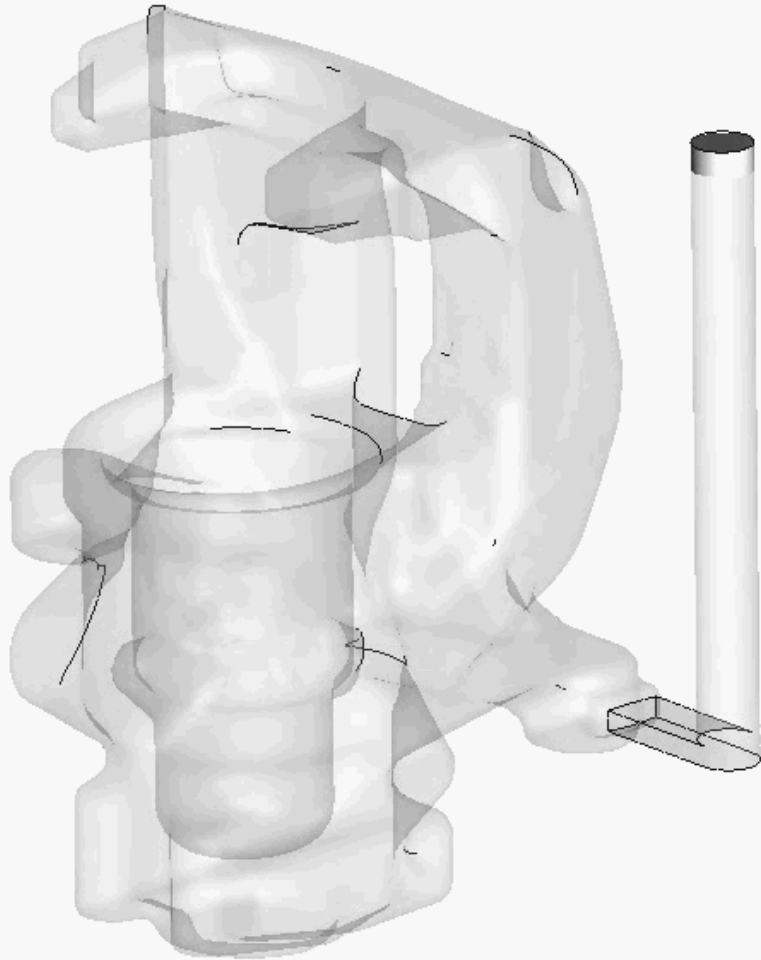
DEM

Fluid Dynamics

Thermal

Kratos

What can do?



step 0.0086197

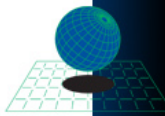
Contour Fill of DISTANCE.

Fluid Dynamics

Incompressible
Fluid

Free Surface

Turbulence



Kratos

What can do?

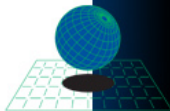
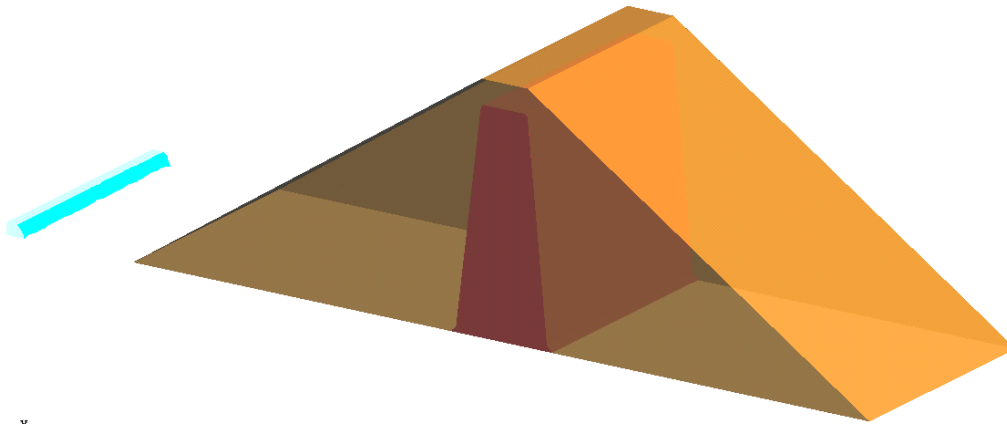
Fluid Dynamics

Incompressible
Fluid

Free Surface

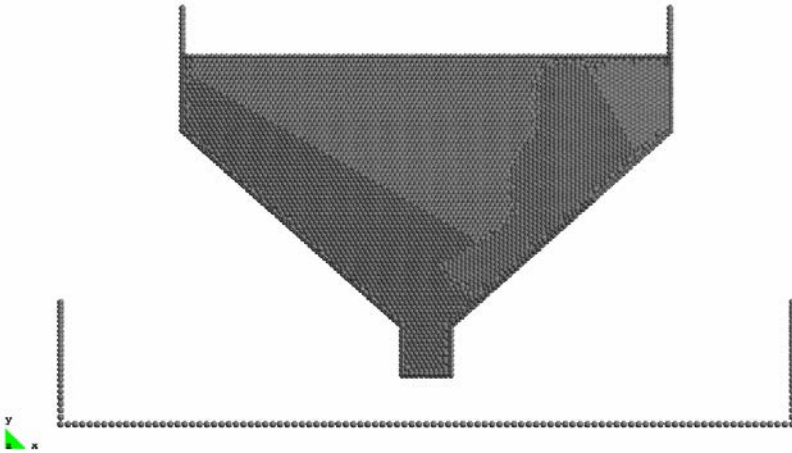
Turbulence

Porous Media

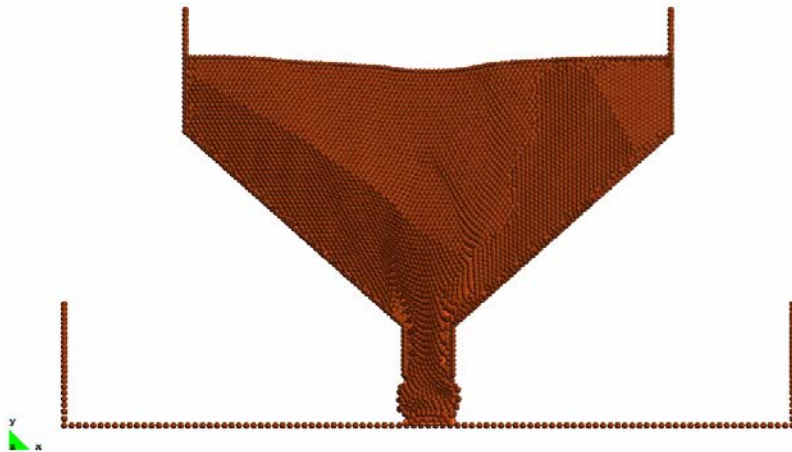


Kratos

What can do?



BINGHAM



**VARIABLE
YIELD**

Fluid Dynamics

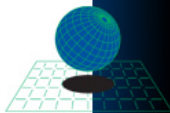
Incompressible
Fluid

Free Surface

Turbulence

Porous Media

Non-Newtonian



Kratos

What can do?

Solid Mechanics

DEM

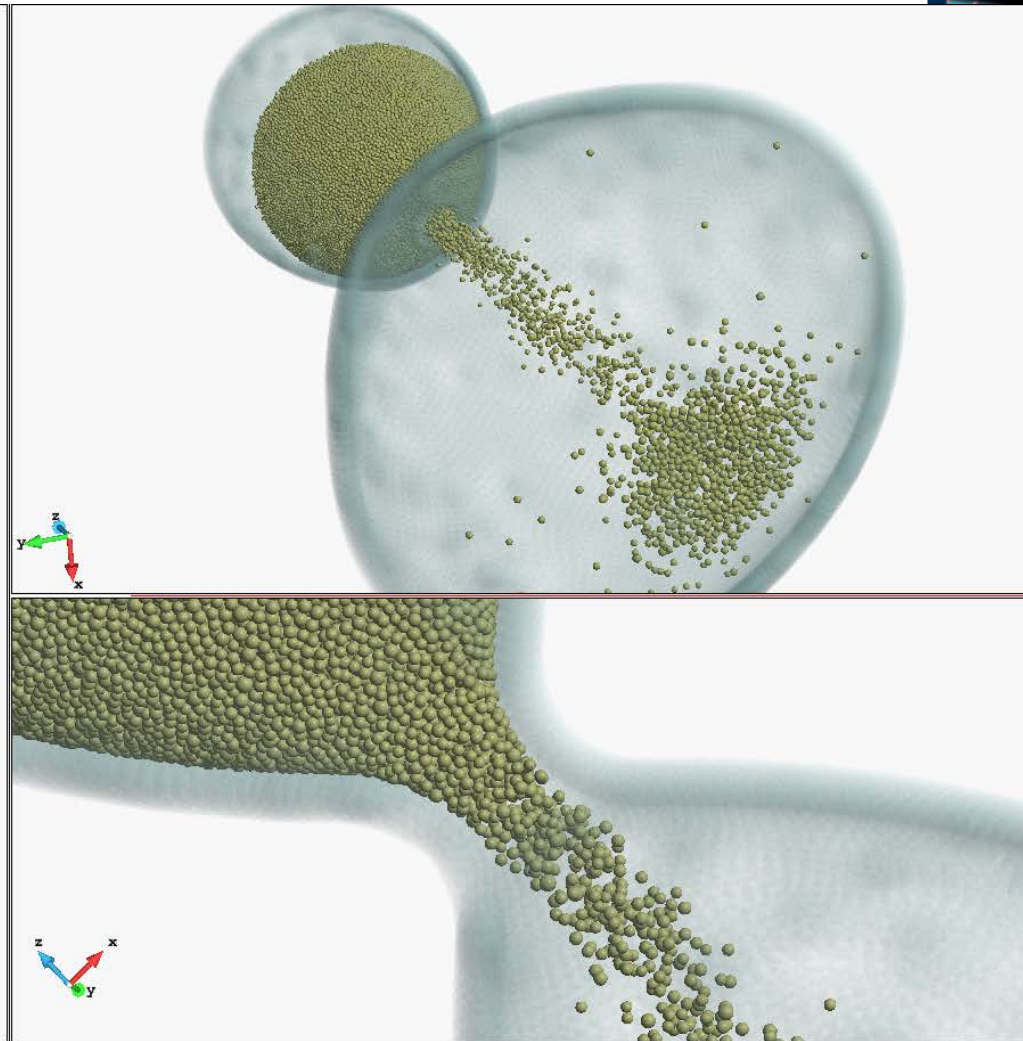
Fluid Dynamics

Thermal

Kratos

What can do?

DEM



Kratos

What can do?

Solid Mechanics

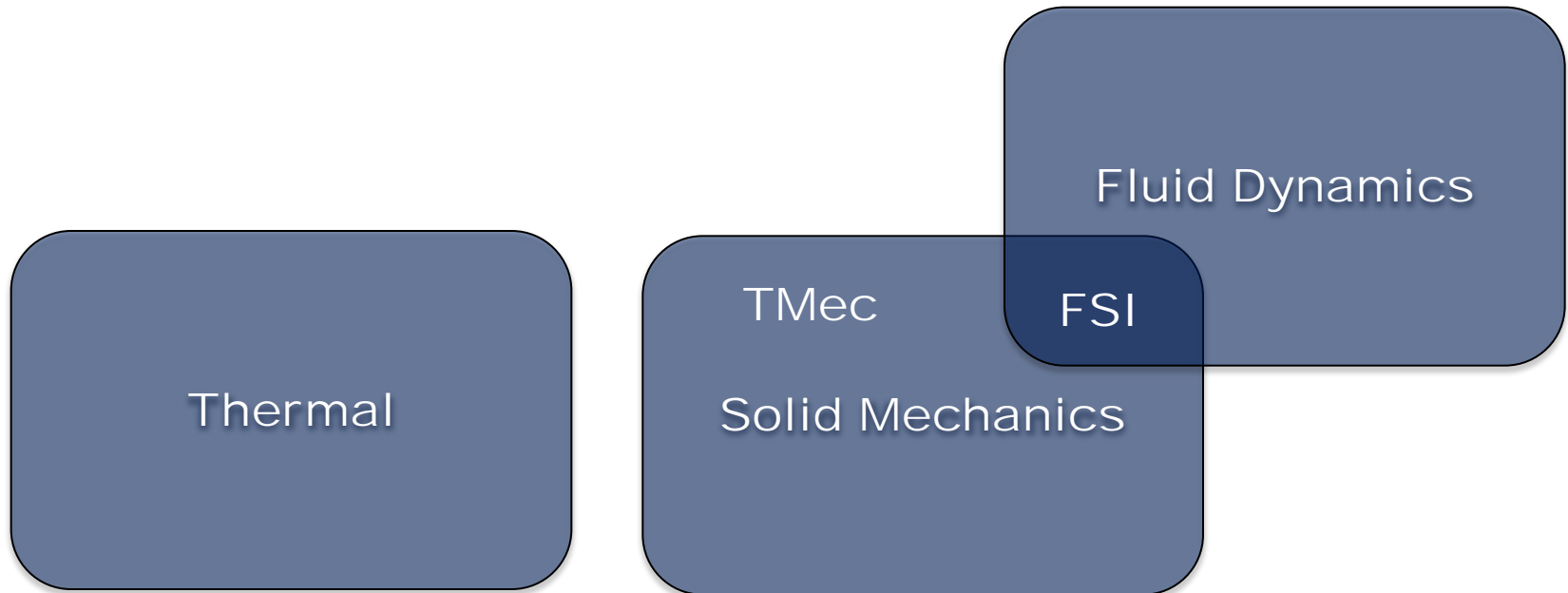
DEM

Fluid Dynamics

Thermal

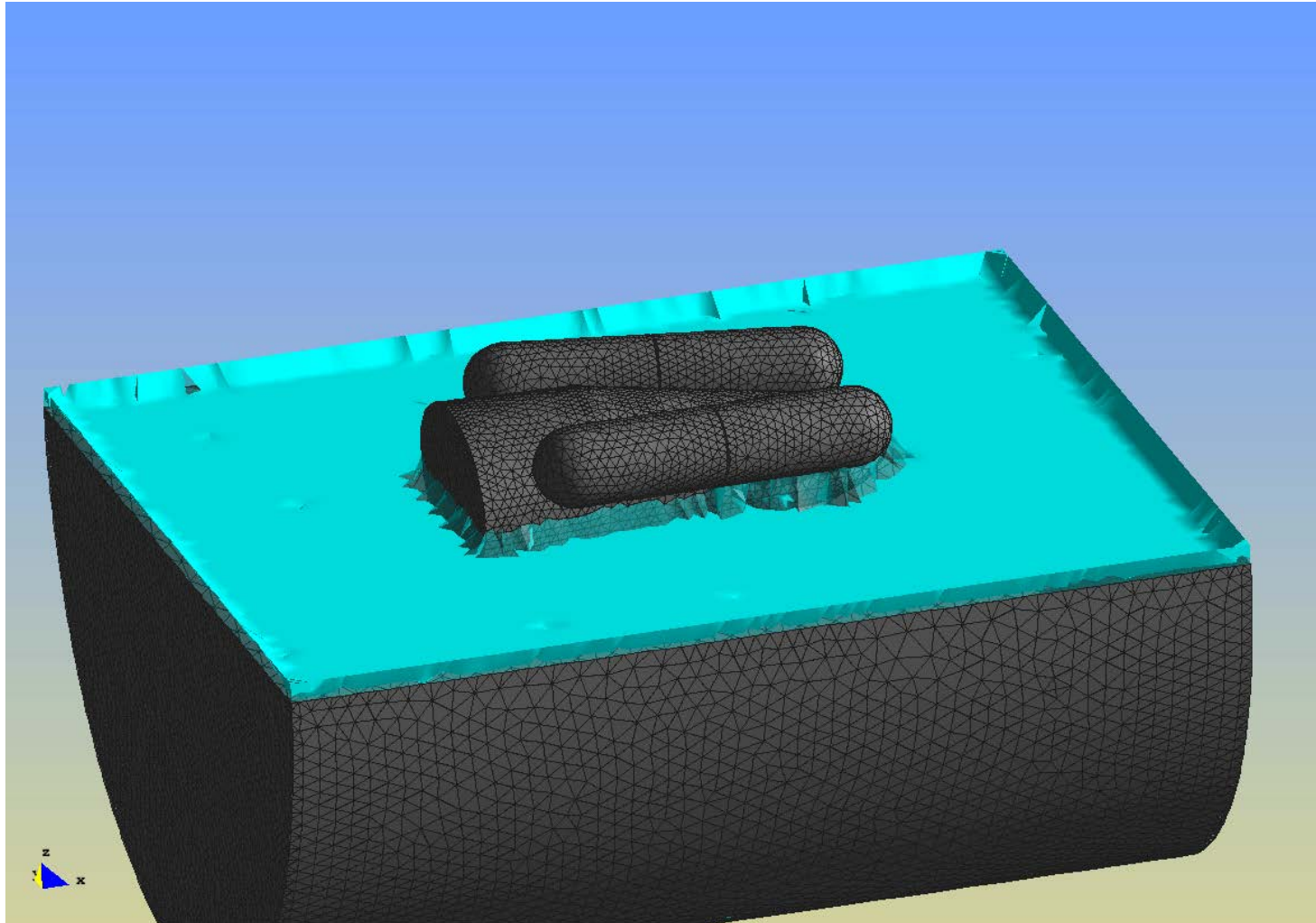
Kratos

What can do?



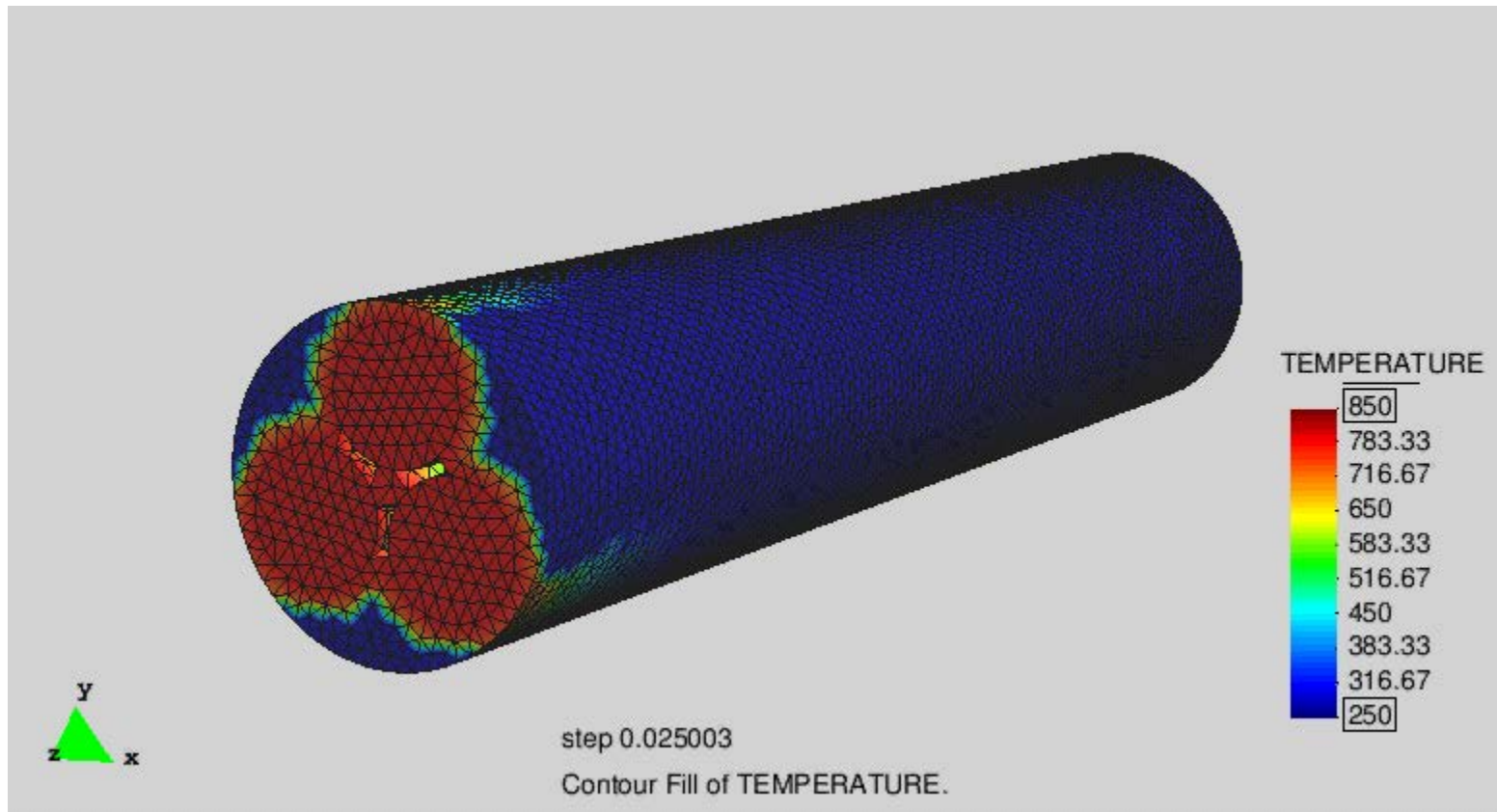
Kratos

What can do?



Kratos

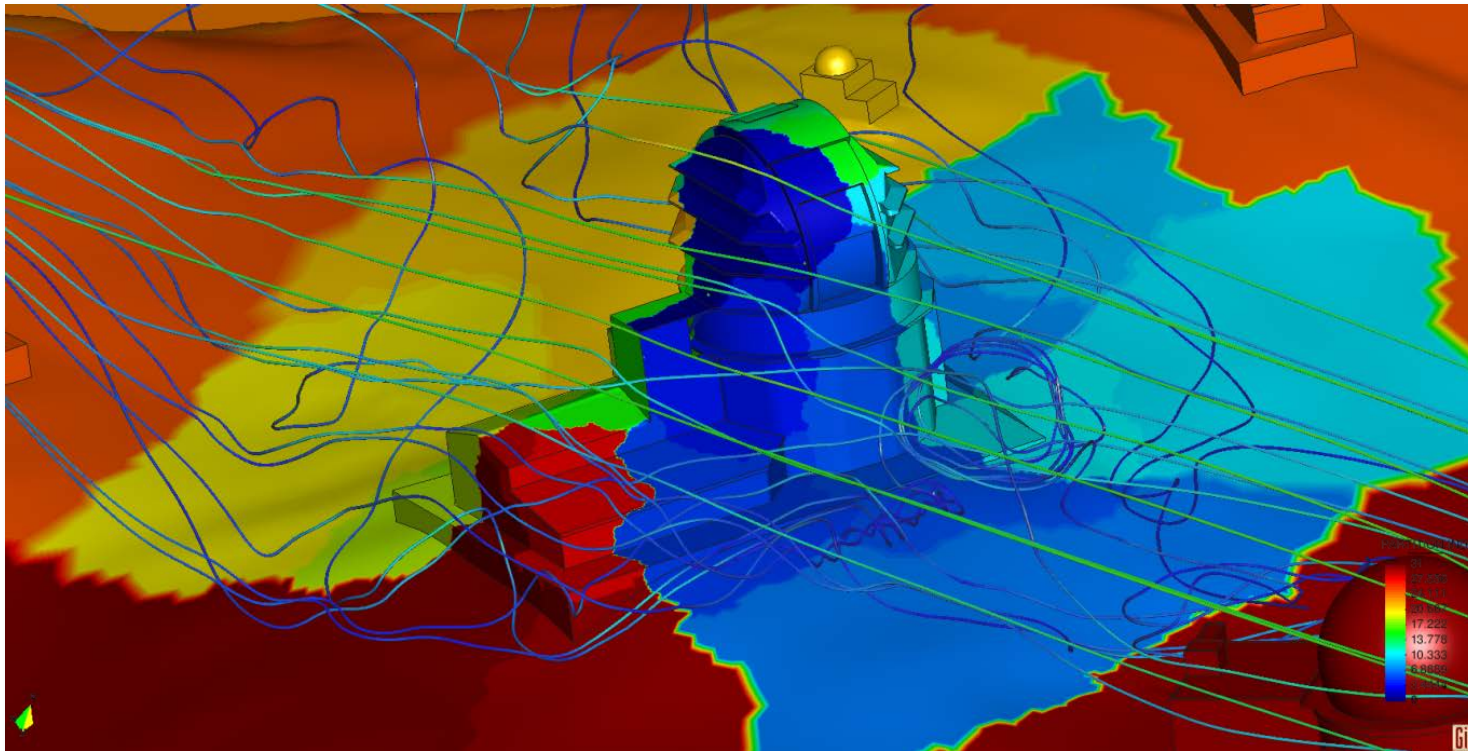
What can do?



Kratos

HPC

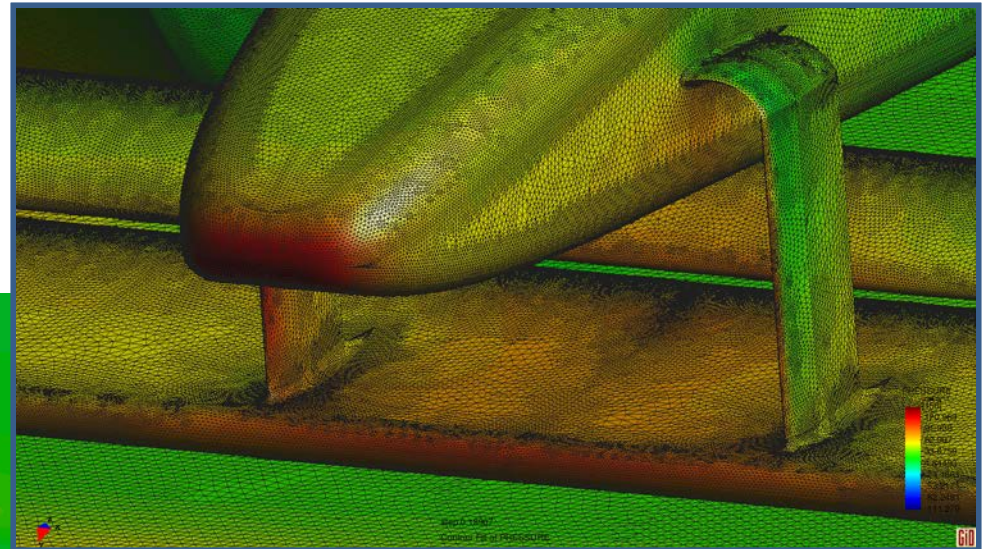
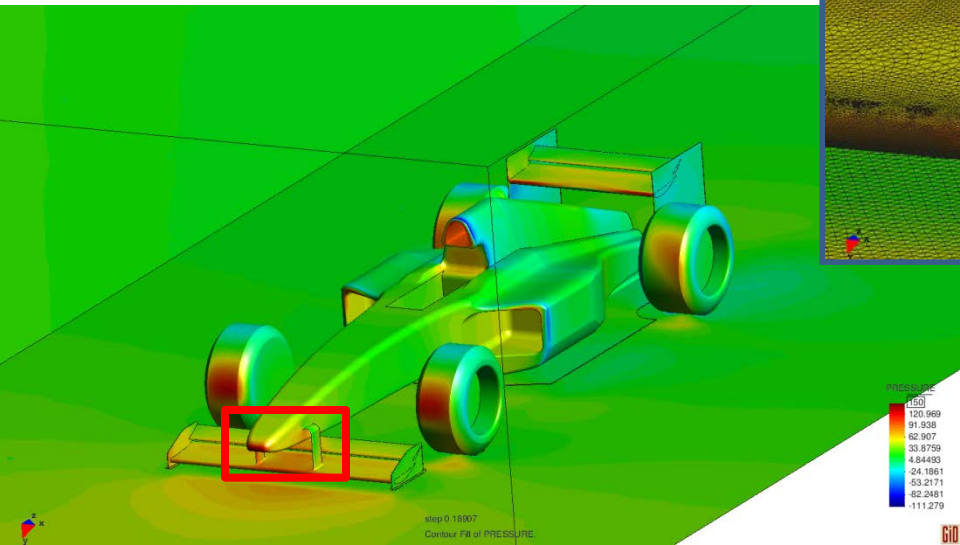
- Shared Memory
- Clusters
- GPU support



Experiences

HPC

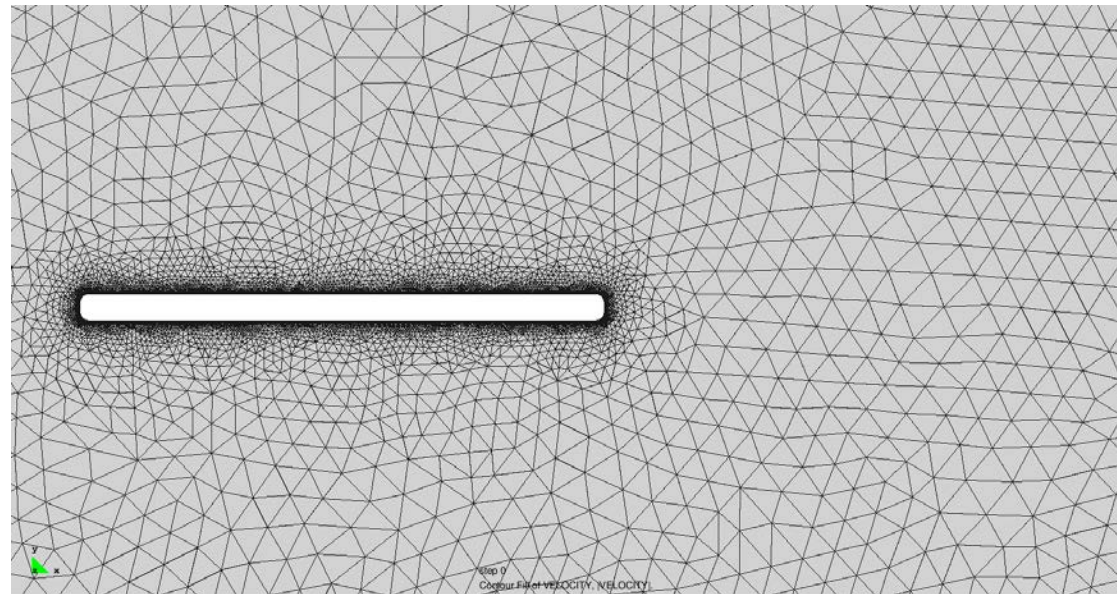
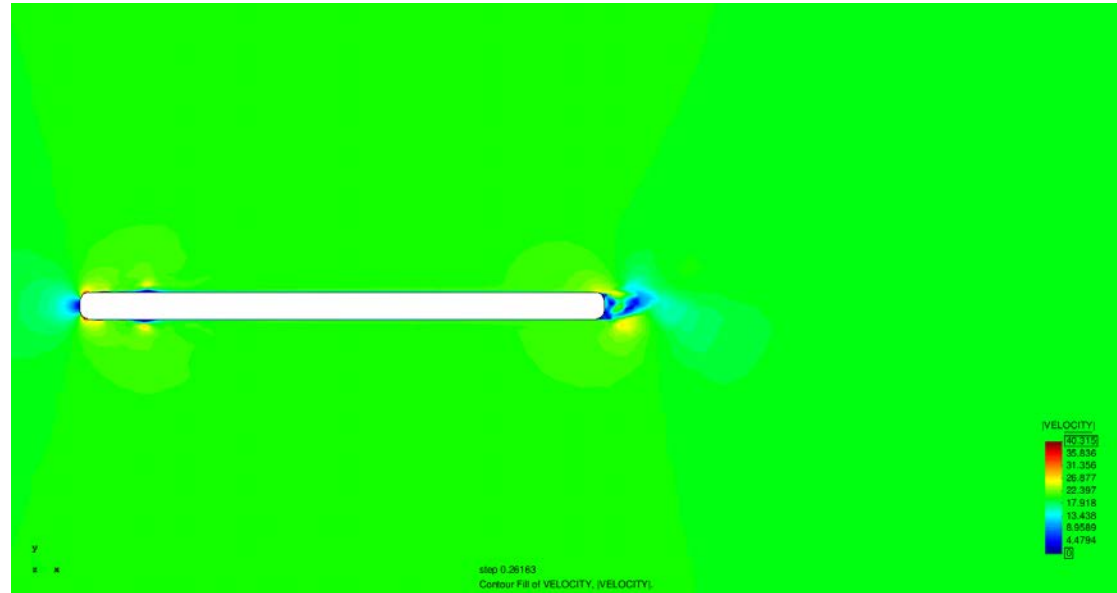
- Working with large models



Kratos

Mesh
Refinement
2D and 3D

MPI support

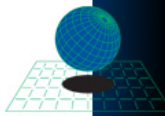
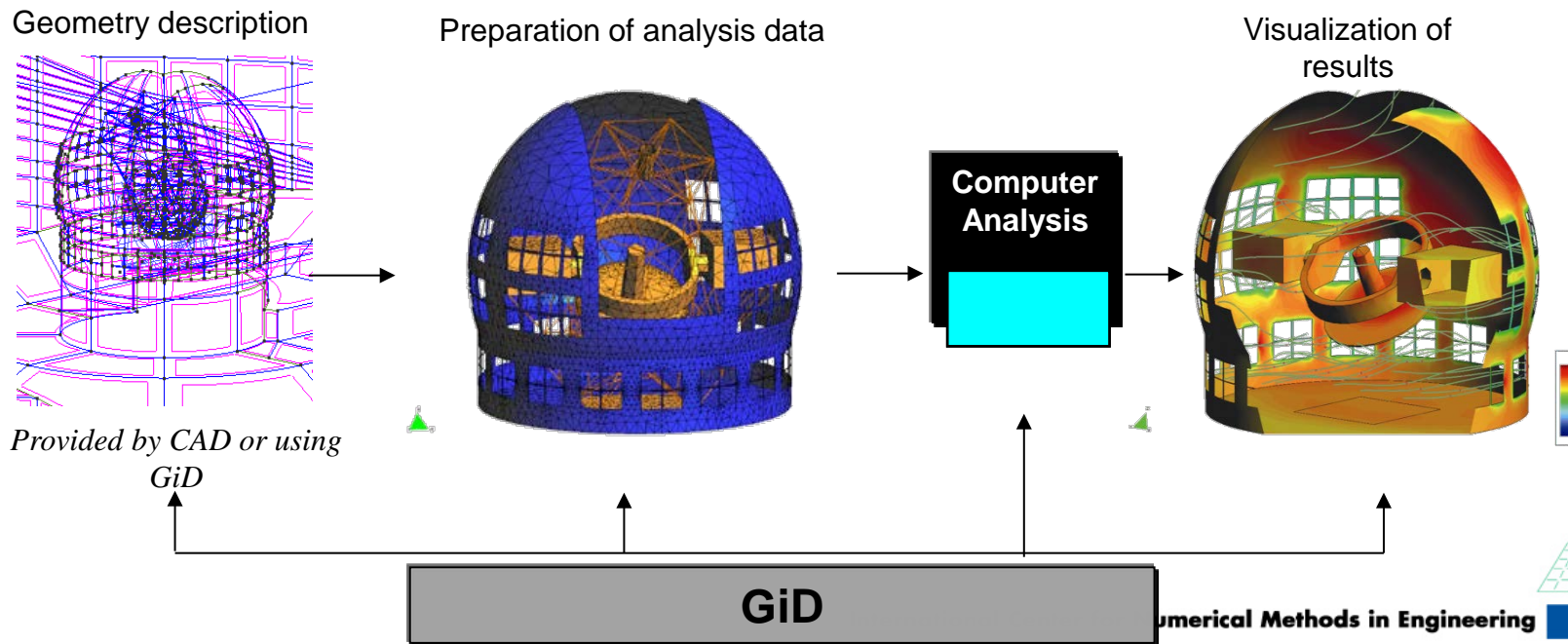




GiD
Pre & Post-processor

What's GiD

- A graphic pre and postprocessor
- Motivation: several research groups and same needs
- CAD systems, mesh generator, connection to solvers and visualization of results
- Advanced visualization tools

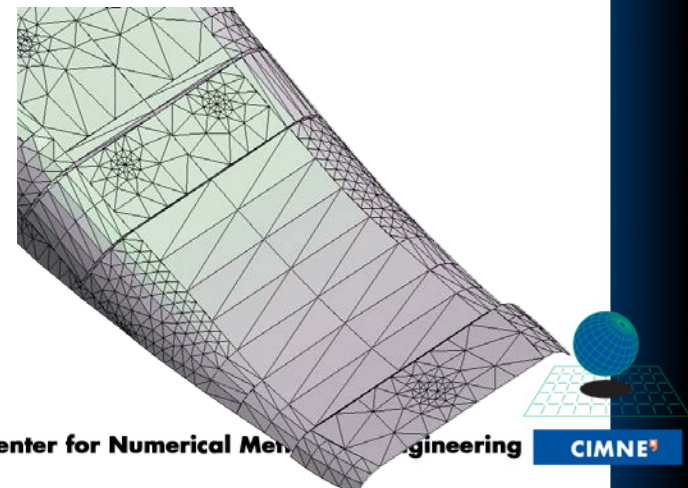
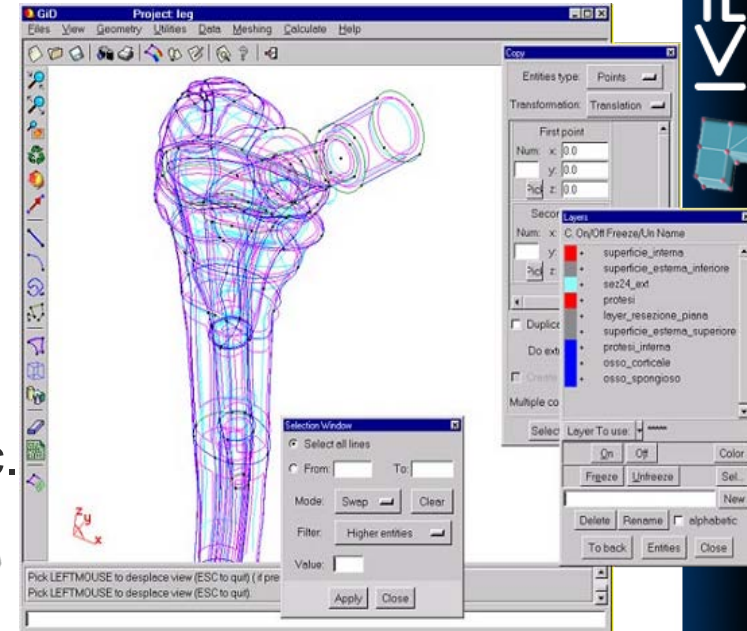
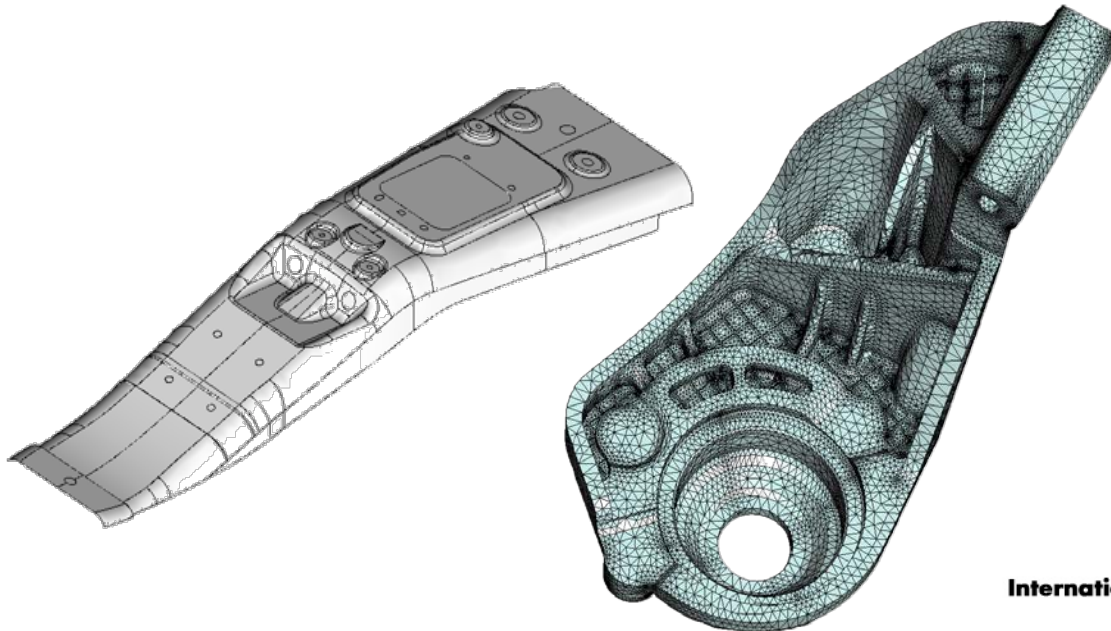


GiD

Pre Processing

Analysis Data generation

- Read in and correct CAD data
- Assignment of boundary conditions
- Definitions of analysis parameters
- Generation of analysis data
- Assignment of material properties, etc.

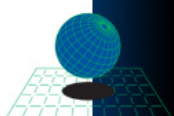
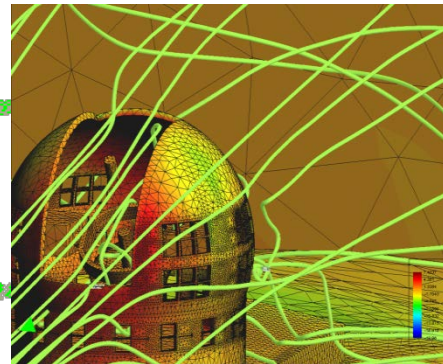
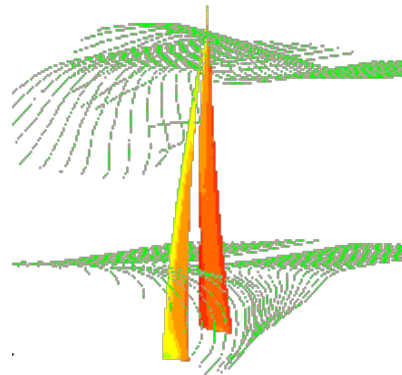
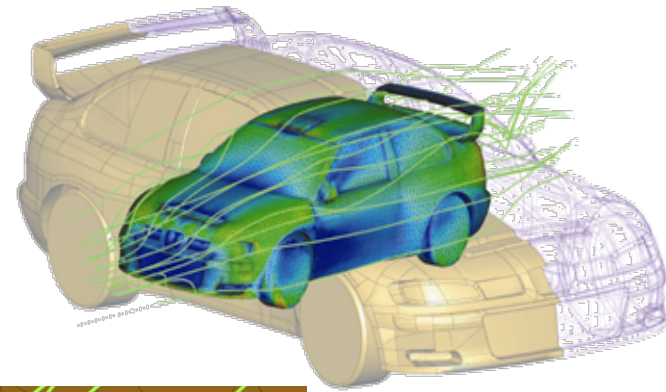


GiD

Post Processing

Visualization of Numerical Results

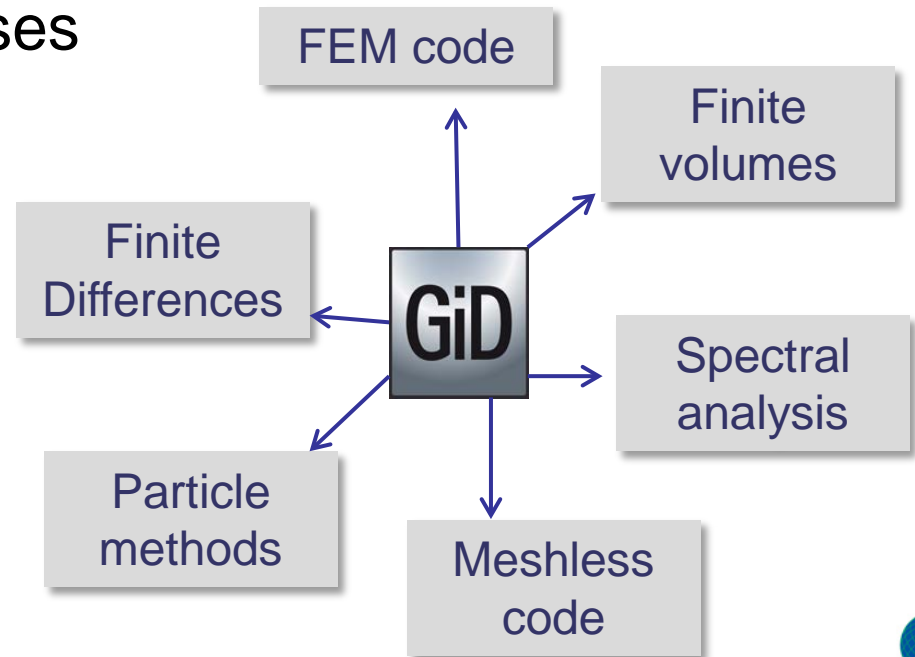
- Deformed shapes, temperature distributions, pressures, etc.
- Vector, contour plots, graphs, line diagrams, results surfaces
- Animated sequences
- Particle line flow diagrams
- Simple user-definable interface
- User-customisable menus



GiD

Applications

- Structural analysis
- Computation fluid mechanics (CFD)
- Geomechanics
- Industrial forming processes
- Electromagnetics
- Acoustics
- Bio-medical engineering
- Coupled problems
- Earth sciences

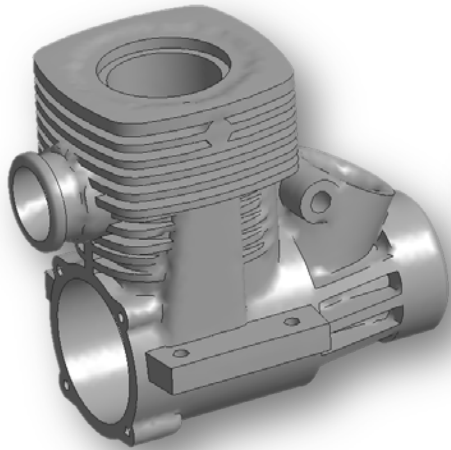




Industrial Exascale Challenges

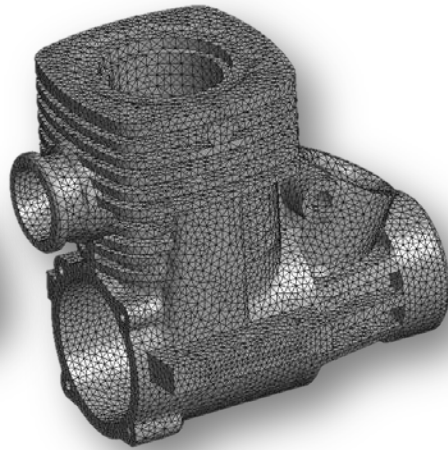
Challenges

Simulation Pipeline



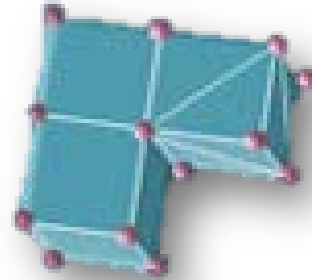
Modeling

- Cleaning
- Applying Conditions



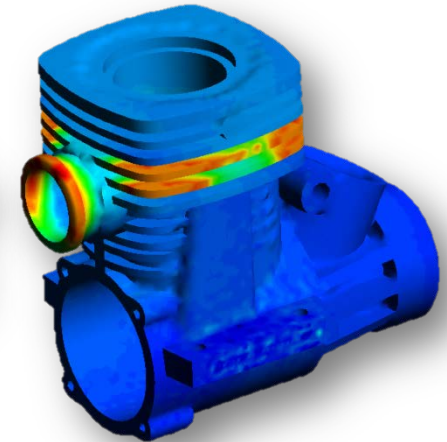
Meshing

- Scalability
- Memory



Analysis

- Scalability
- Efficiency
- Complexity
 - FSI

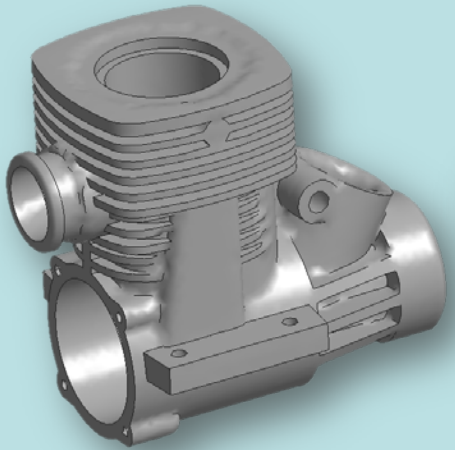


Visualization

- Data mining
- Simplification
- In-situ post-processing

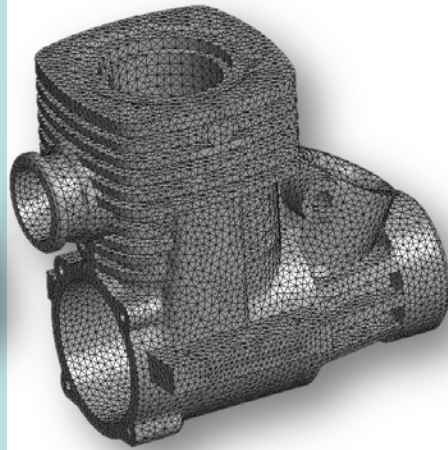
Challenges

Simulation Pipeline



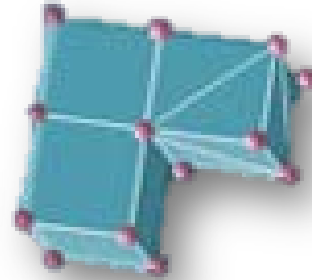
Modeling

- Cleaning
- Applying Conditions



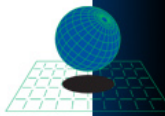
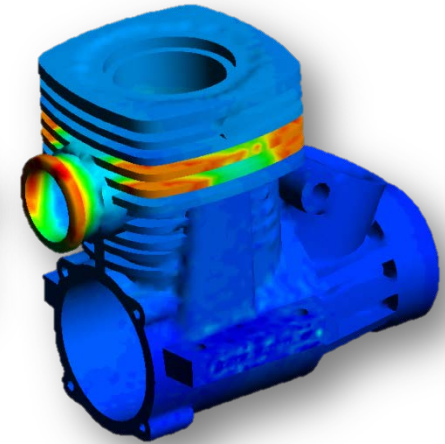
Cleaning

- Automatic In/Out
- Embedded Approaches



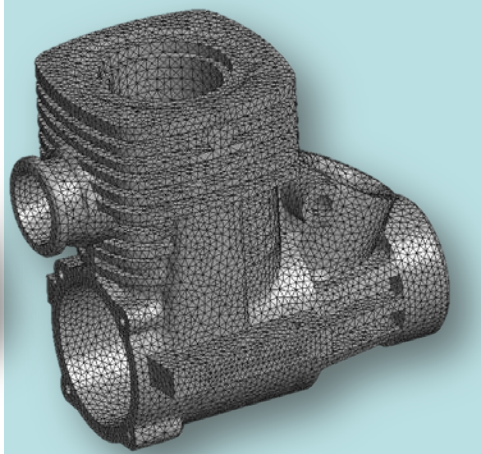
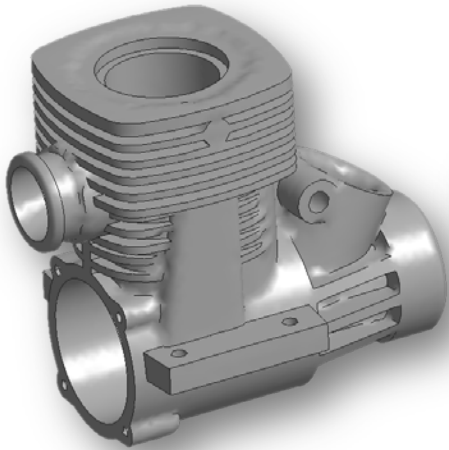
Applying Conditions

- GUI
- Scripting



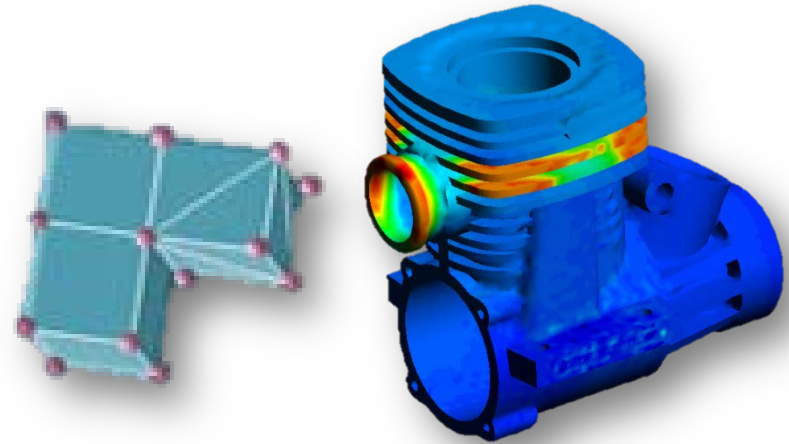
Challenges

Simulation Pipeline



Meshing

- Robustness
- Scalability



Octree Mesher

- Robust
- Fast and scalable
- Tradeoff between structure and unstructured mesh

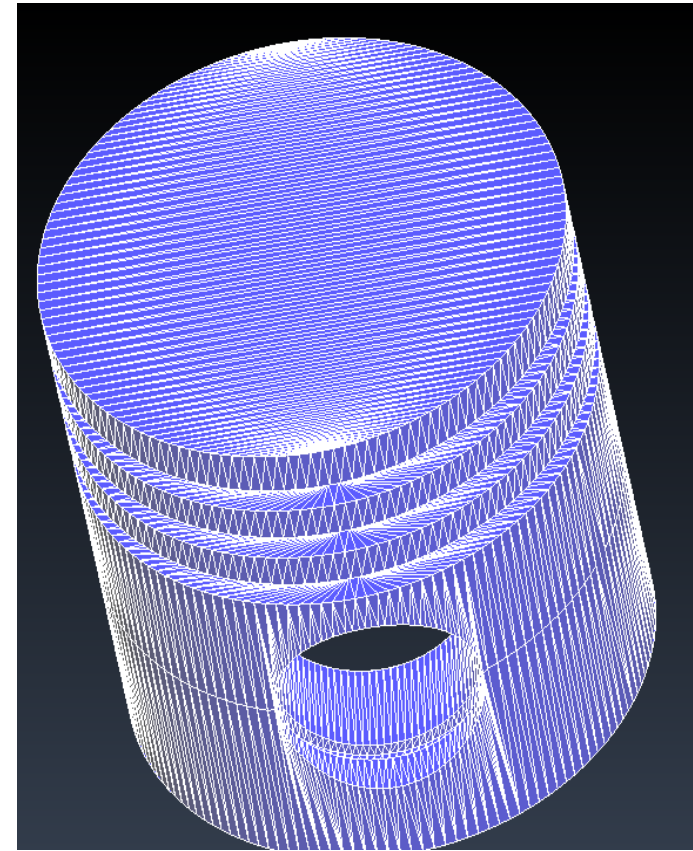
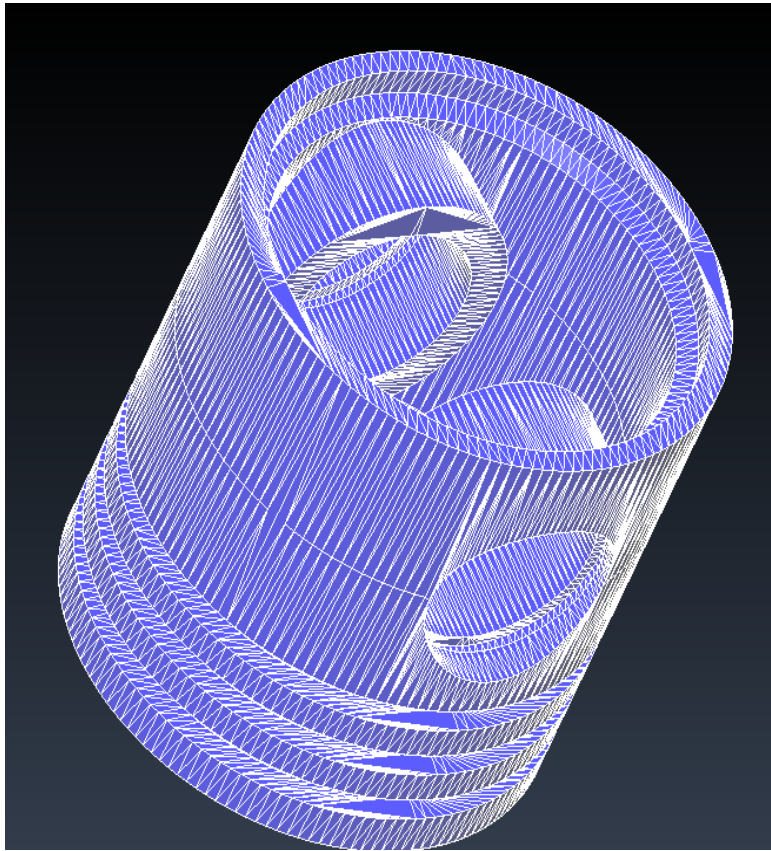
Parallel Refinement

- For larger meshes

Challenges

Simulation Pipeline

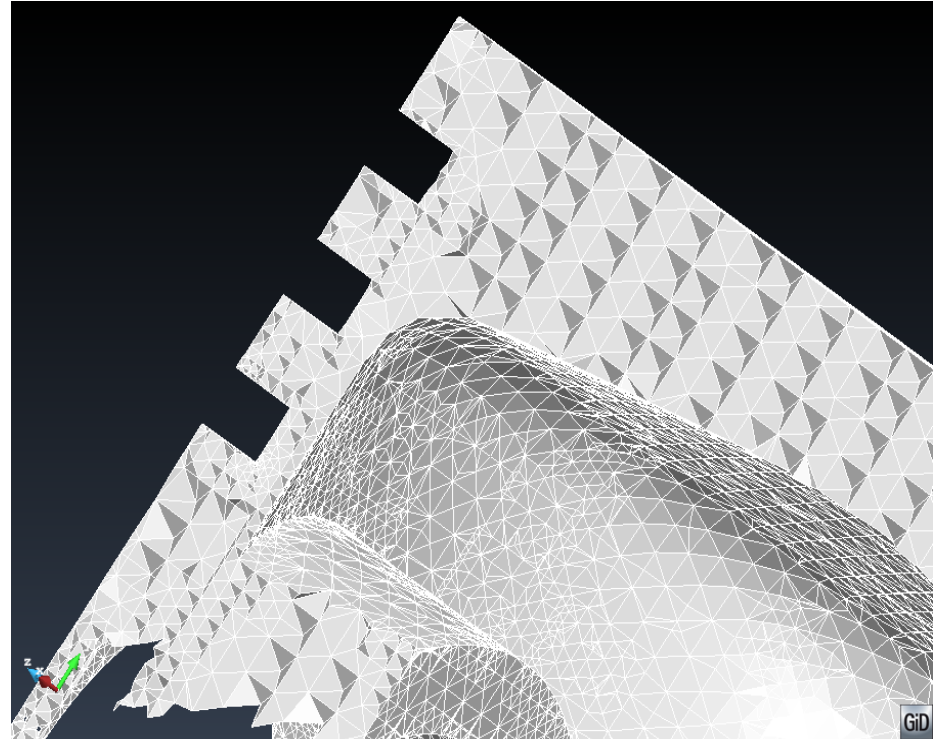
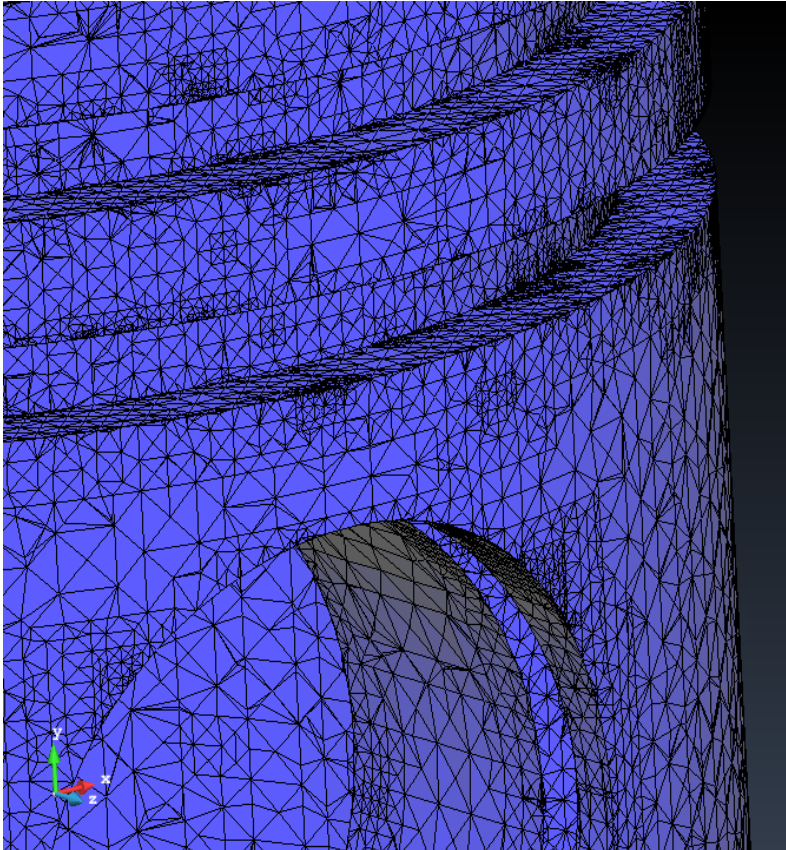
- STL as input boundary



Challenges

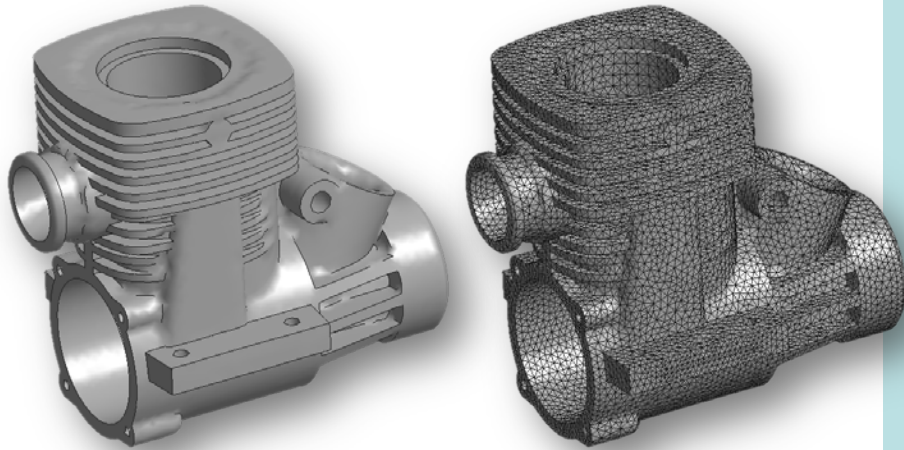
Simulation Pipeline

- Resulting mesh:



Challenges

Simulation Pipeline

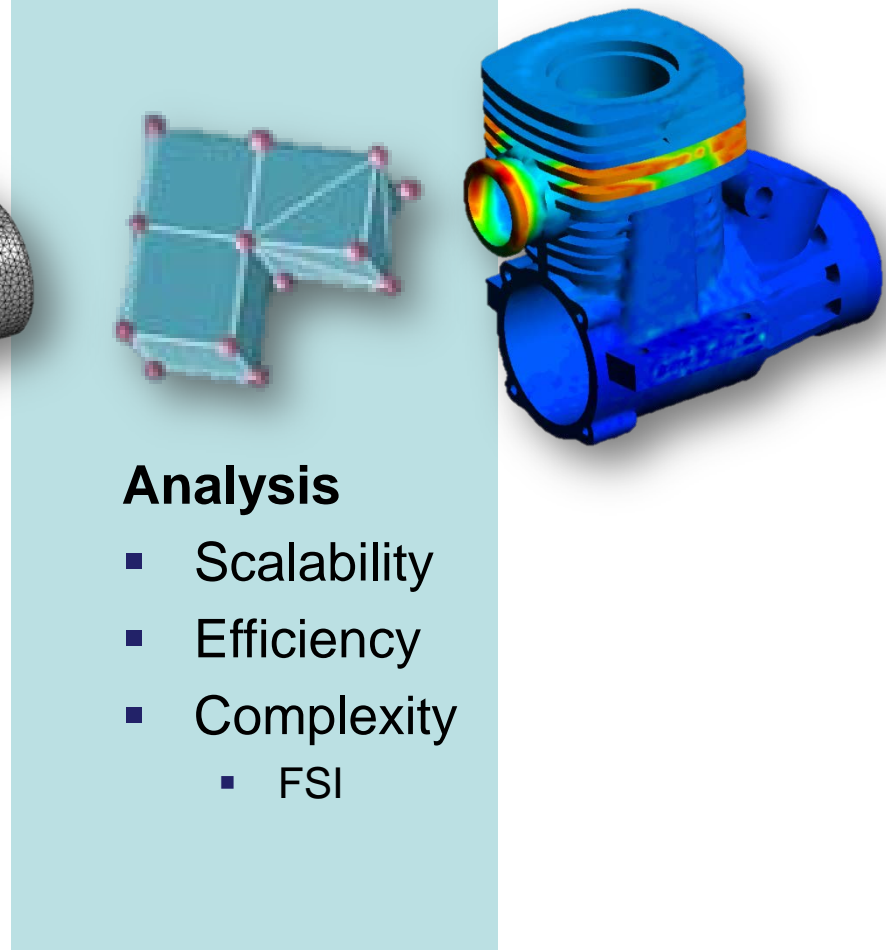


New Formulations

- To ensure more locality
- Decrease memory access
- Fixed mesh methods
- Multi Scale

Heterogeneous Machines

- Non-uniform Load Balance
- Different paradigms
- Hybrid approaches

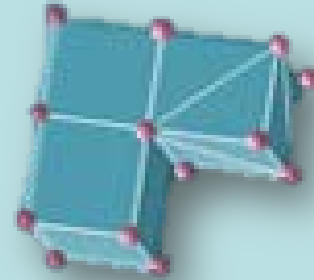
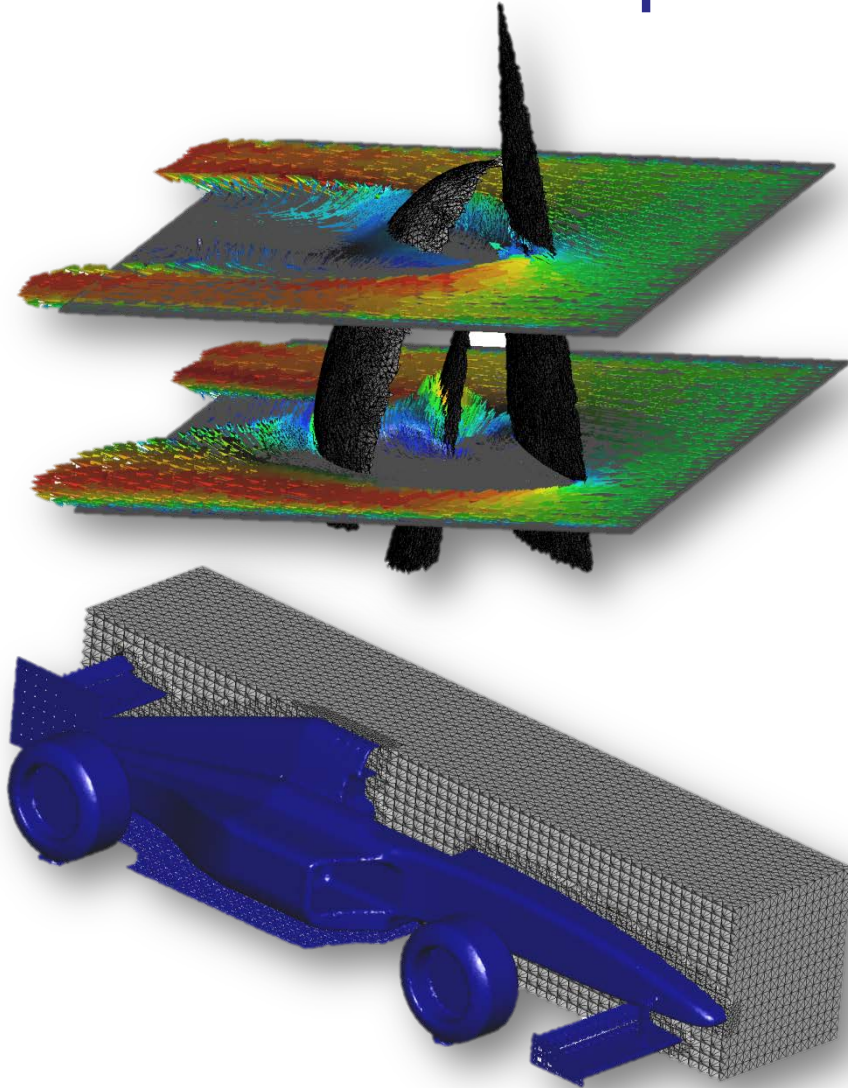


Analysis

- Scalability
- Efficiency
- Complexity
 - FSI

Challenges

Simulation Pipeline

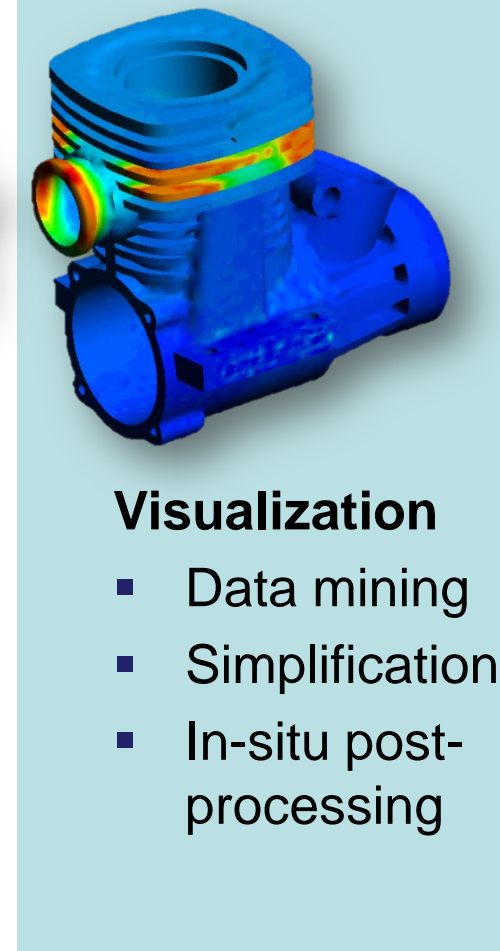
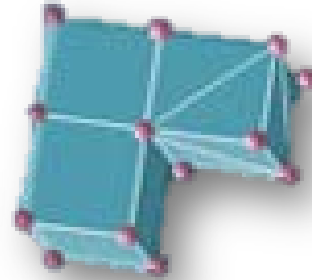
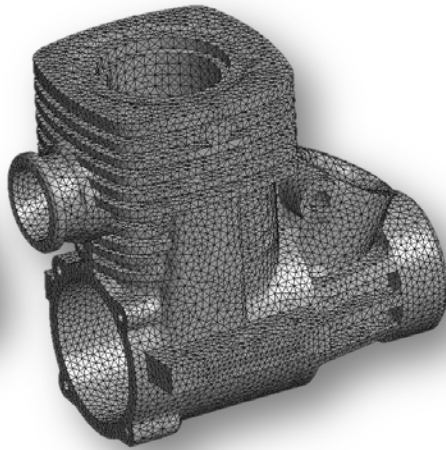
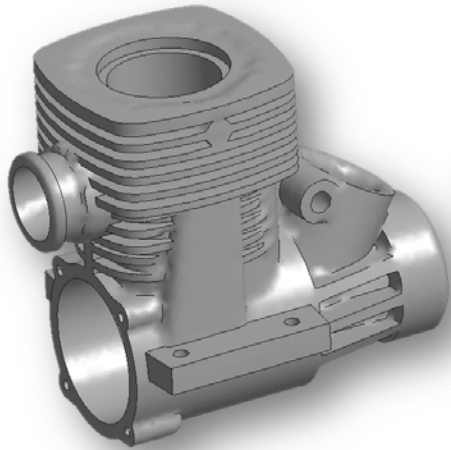


Analysis

- Scalability
- Efficiency
- Complexity
 - FSI

Challenges

Simulation Pipeline



In-situ Post-Processing

- Sensors
- Cuts
- Iso-surfaces

Simplification

- Geometry Based
- Result Based

Data Mining

- Sensors
- Cuts
- Iso-surfaces

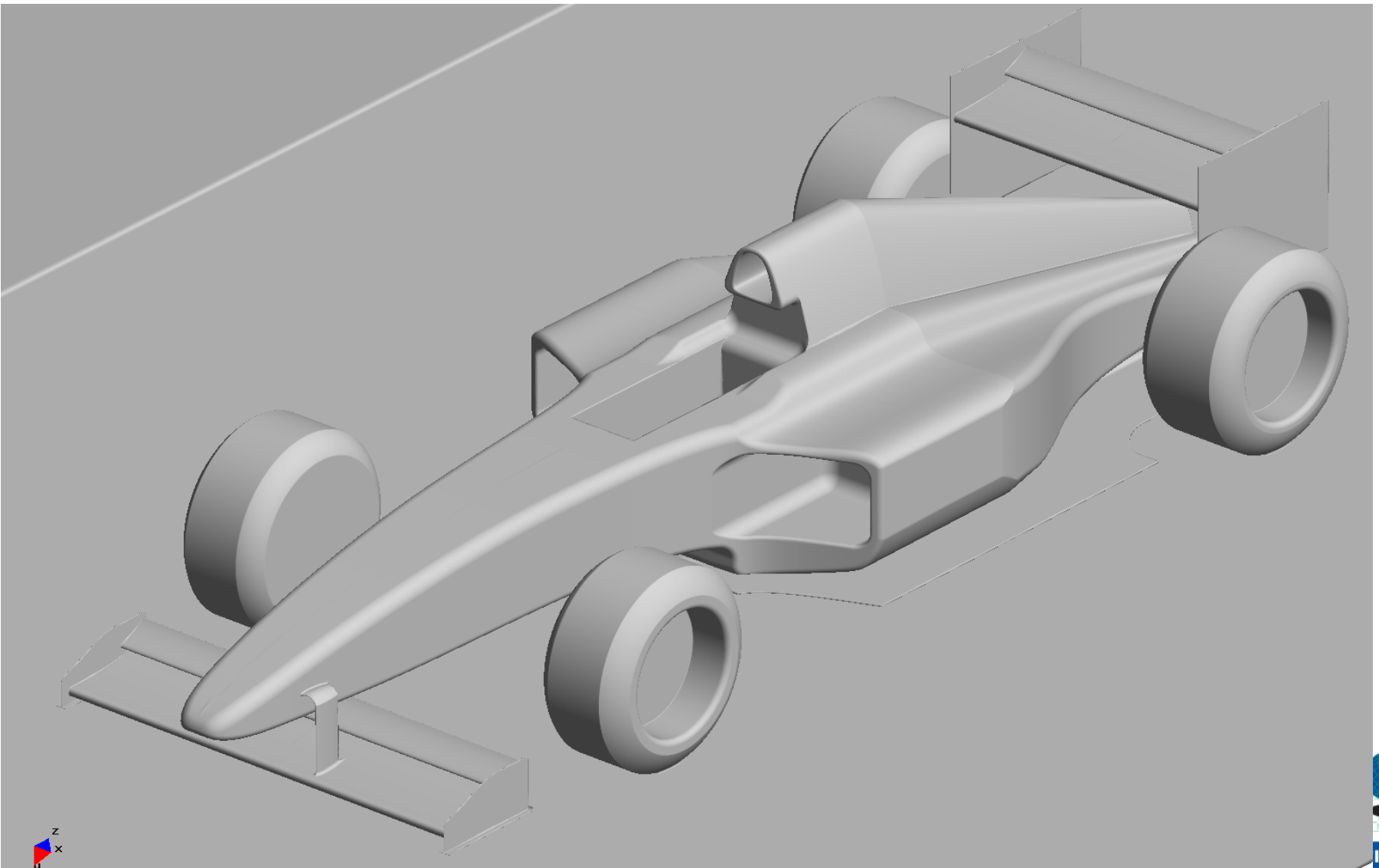
Visualization

- Data mining
- Simplification
- In-situ post-processing

Challenges

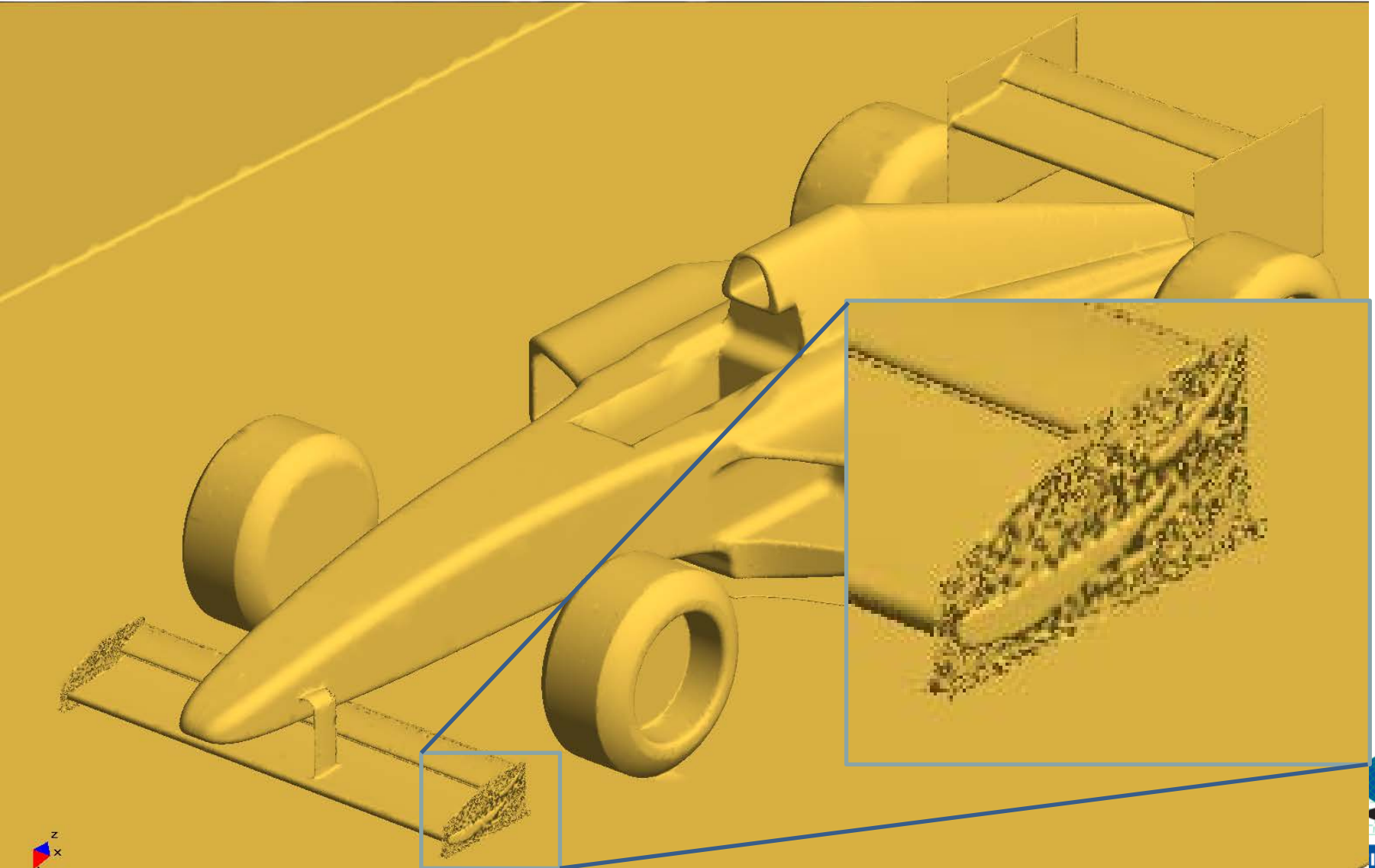
Simulation Pipeline

Original model: 6 M triangles



Challenges

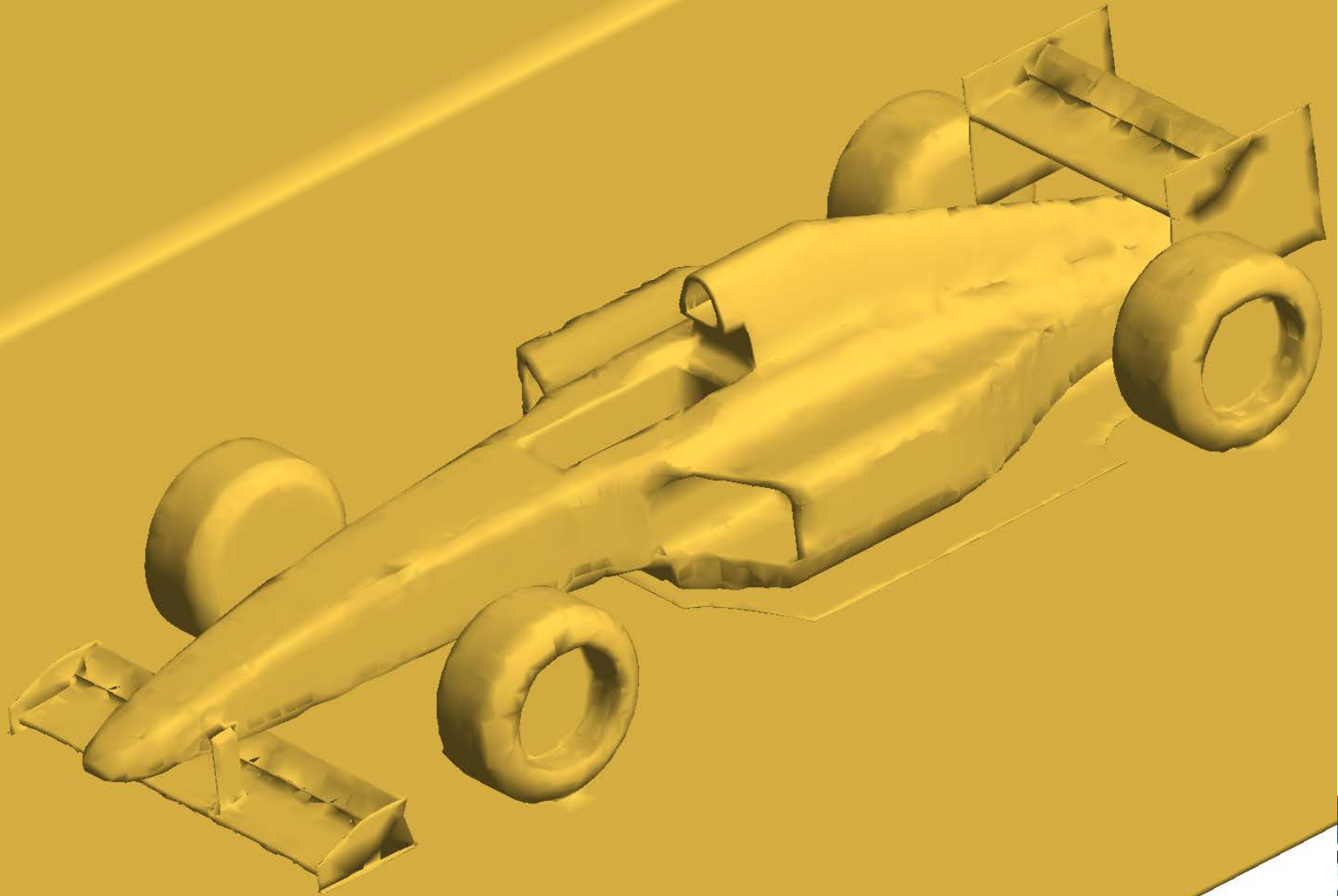
Octree($13 - 8192^3$) $< 1e-7$: 1.4 M triangles (23 % original)



Challenges

Simulation Pipeline

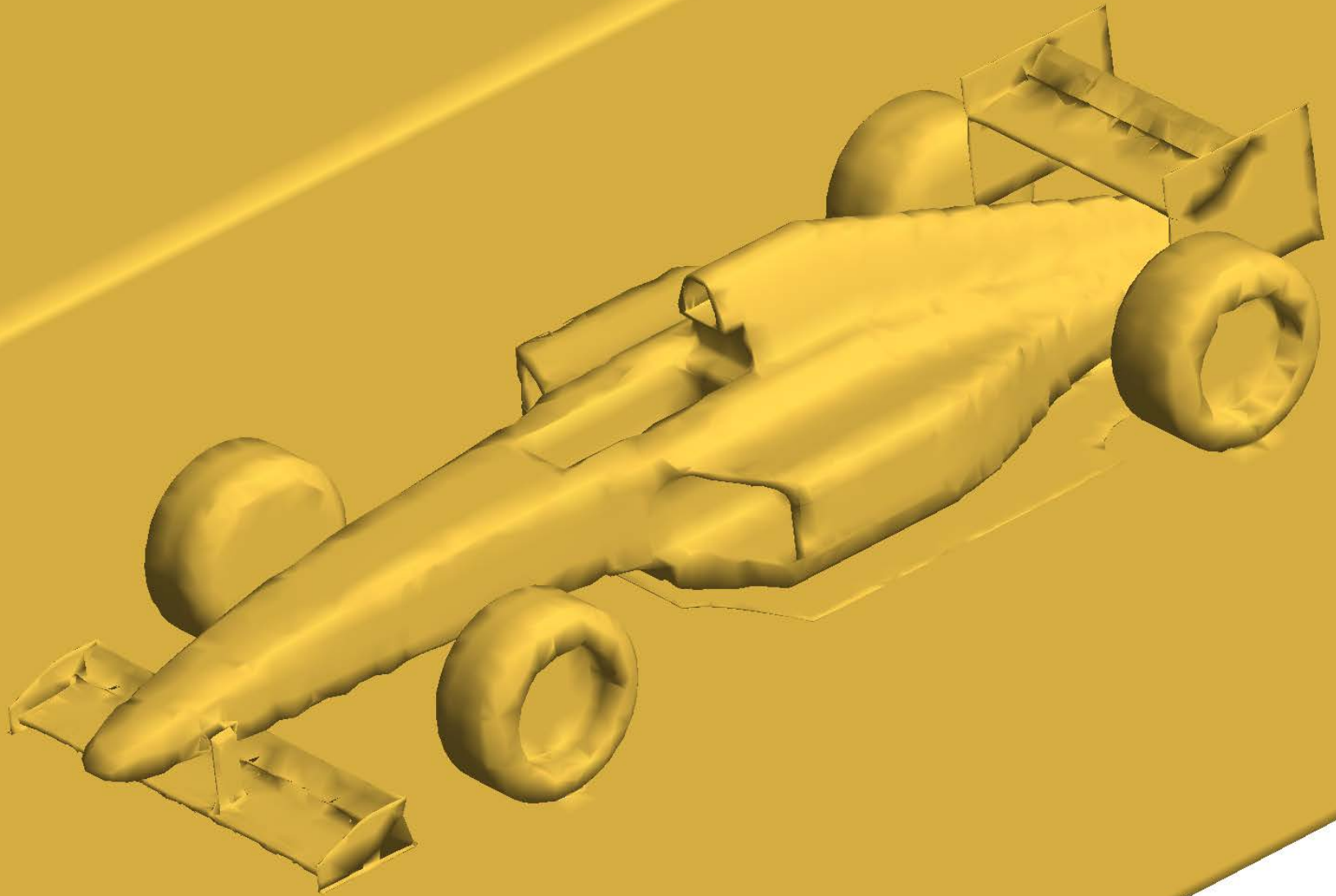
Normal subdivision: 203 K triangles (3.1 %)



Challenges

Simulation Pipeline

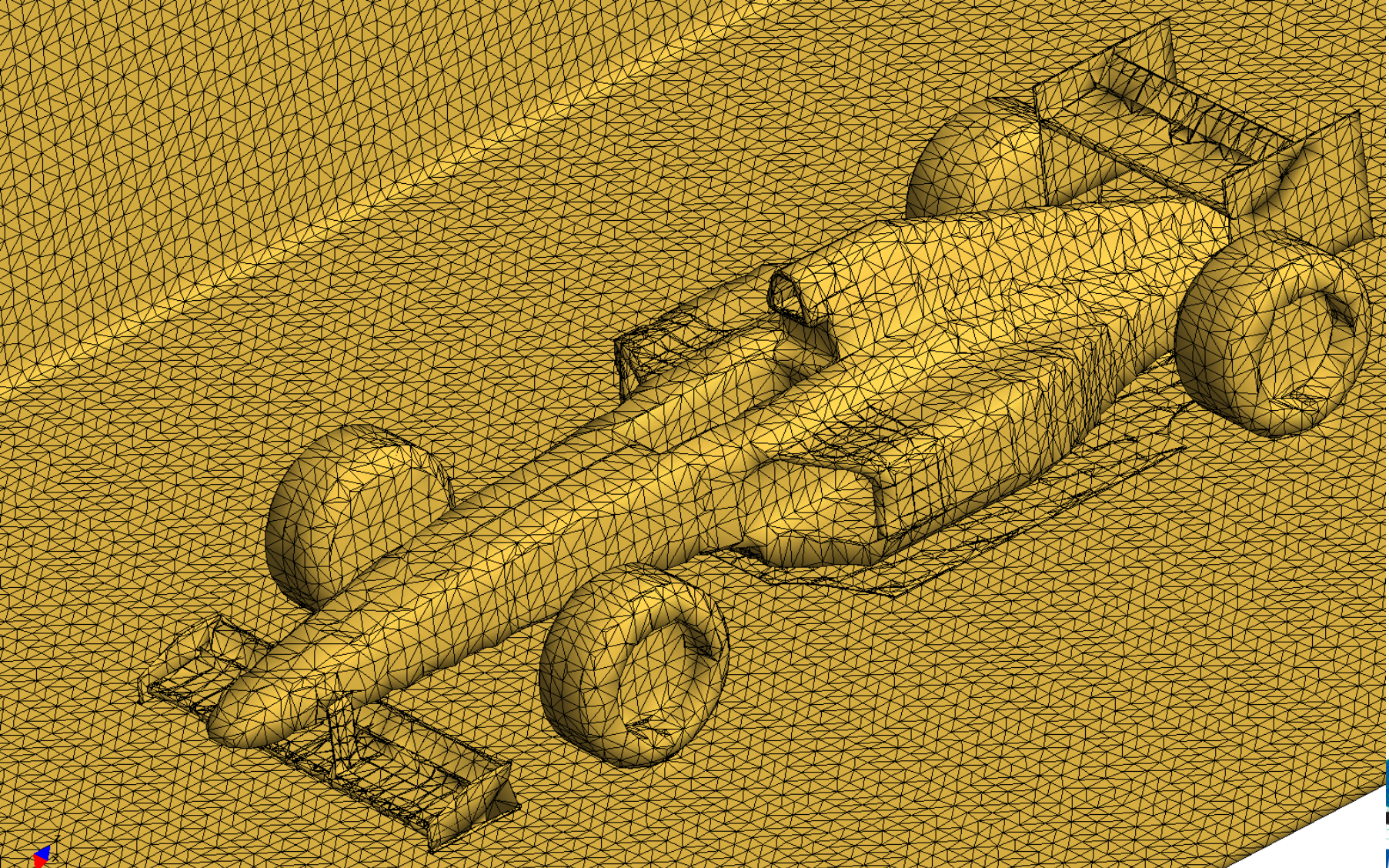
Normal cone filter: 181 K triangles (2.9 %)



Challenges

Simulation Pipeline

Normal cone filter: 181 K triangles (2.9 %)



Challenges

Simulation Pipeline

Grid 2^3

8 Points

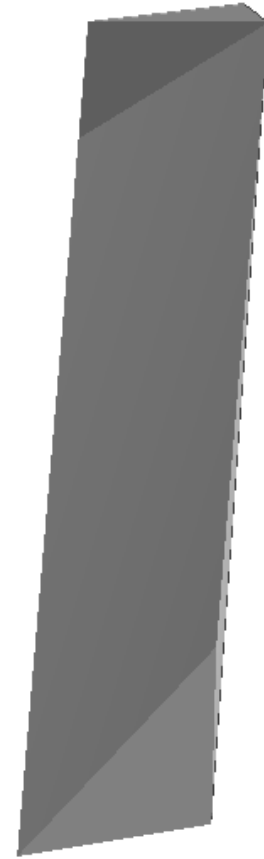
14 Triangles

0 Lines

< 0,0001 %

62 s. con HashUC

62 s. con FullUC



Challenges Projects



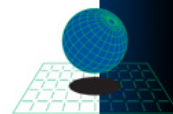
- **NUMEXAS:**

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

<http://www.numexas.eu/>

- **VELaSSCo:**

**Visual Analysis for Extremely Large-Scale Scientific
Computing**

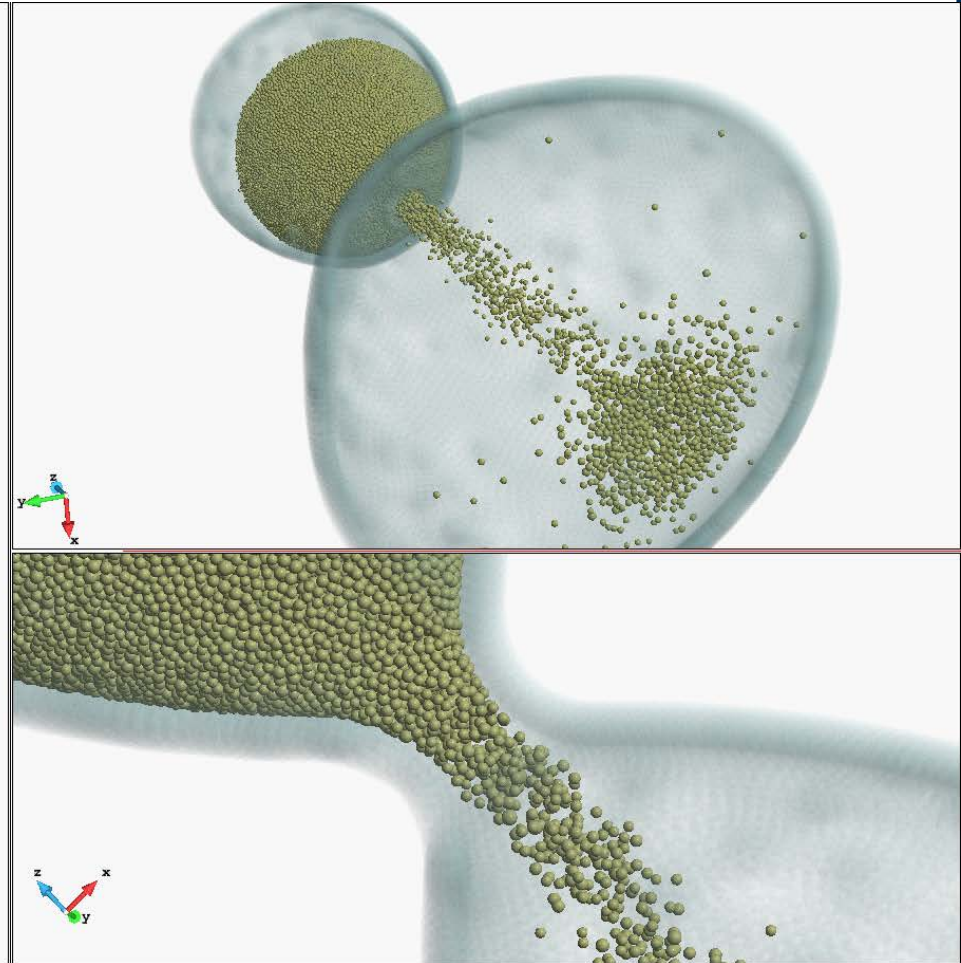


Challenges

Horizon



谢谢！



<http://www.cimne.com>

<http://www.gidhome.com/>

<http://www.cimne.com/kratos>

