

# **NUMEXAS project Team & Objectives**

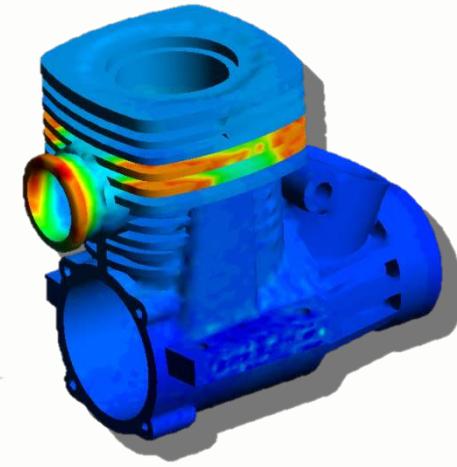
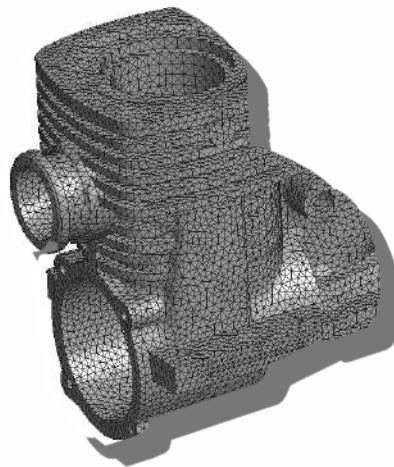
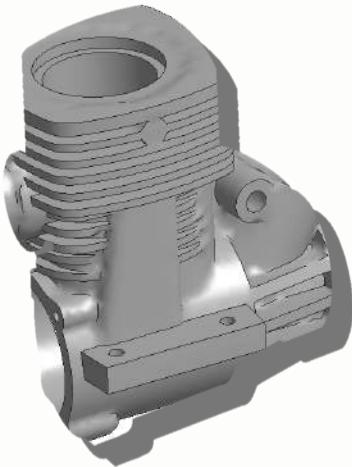
**Dr. Riccardo Rossi**

**Dr. Cecilia Soriano**

**Dr. Pooyan  
Dadvand**

# Objectives (in my words): Solve **Engineering Problems** on EXASCALE architectures

## Challenges Simulation Pipeline



### Modeling

- Cleaning
- Applying Conditions

### Meshing

- Scalability
- Memory

### Analysis

- Scalability
- Efficiency
- Complexity
- FSI

### Visualization

- Data mining
- Simplification
- In-situ

# “Today’s” Objectives:

## GENERAL OBJECTIVES

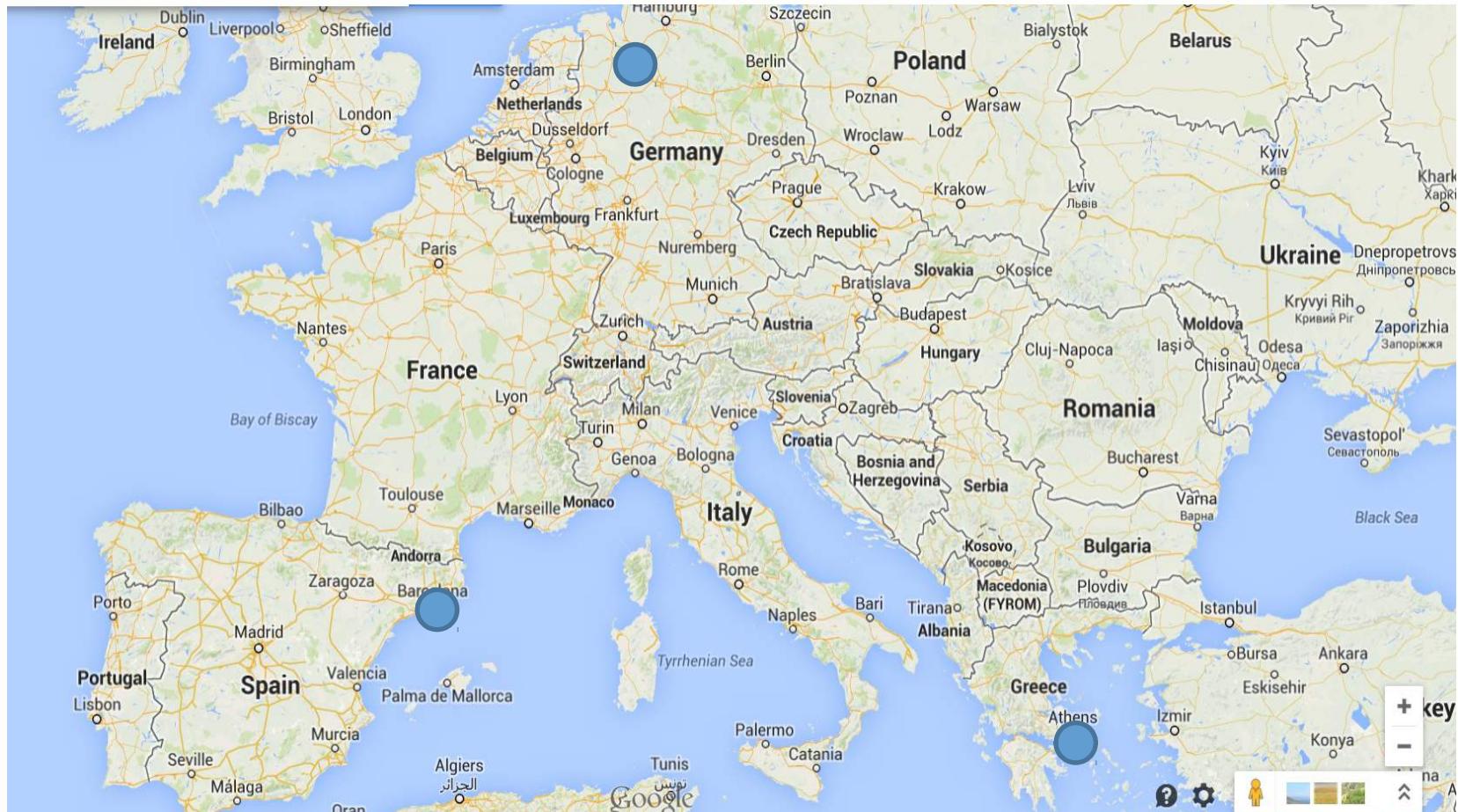
- Meet parallel efforts in the towards exascale Race
- Syncronize if possible with the efforts of the other groups

## SPECIFIC OBJECTIVES

- **PROVIDE A USER FEEDBACK in the hope it can be taken into account in future developments in the HPC area.** □ PLEASE INCREASE MEMORY BANDWIDTH not just FLOPs!!!
- Quest for simple profiling tools
- Check suitability of new programming paradigms (needs industrial-grade compiler support, portability, Open Standard Definition, etc...)
- Make a few questions on current hardware/compiler directions.

# Members of the team:

HANNOVER



BARCELONA

ATHENS



# In Hannover



Institut für  
Kontinuumsmechanik  
Prof. Dr.-Ing. P. Wriggers  
Dr. B. Avci

# Institute of Continuum Mechanics

## Leibniz University of Hannover



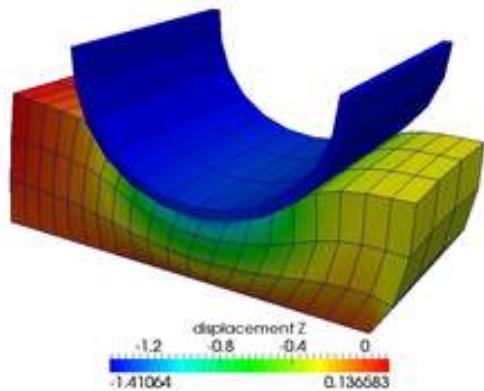
Director: Prof. Dr.-Ing. P. Wriggers

Research Team: 30 Phd Students, 7 Postdoc  
Researcher

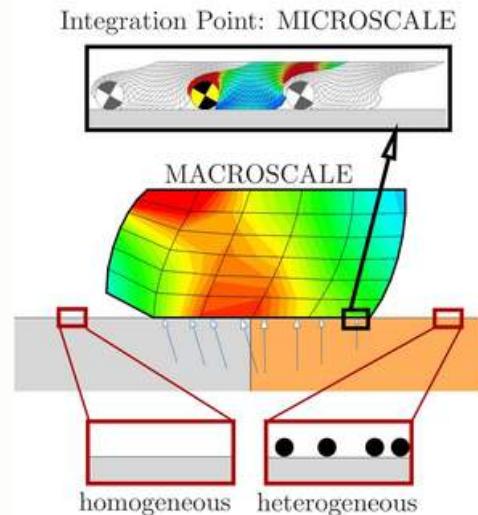
Research: Contact Mechanics, XFEM, DEM, SPH,  
Fluid- Particle Interaction, Crystal  
Plasticity, Multiscale Methods, ...



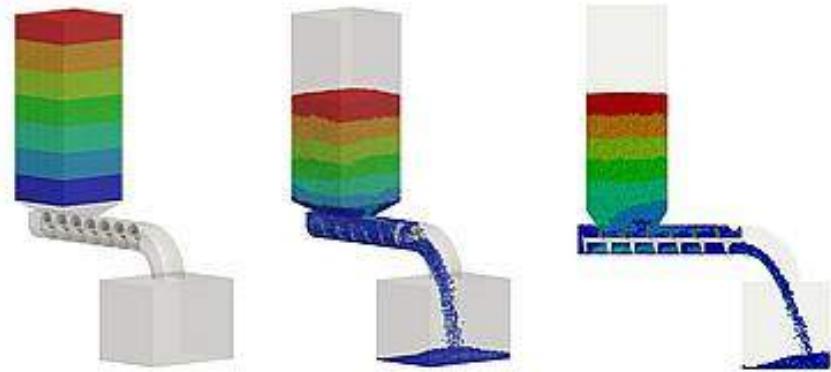
## Contact Mechanics



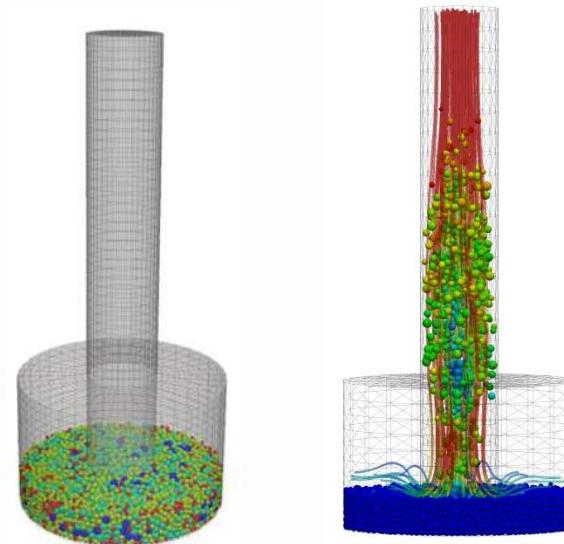
## Multiscale Contact Homogenization of Granular Material



## Discrete Element Methods



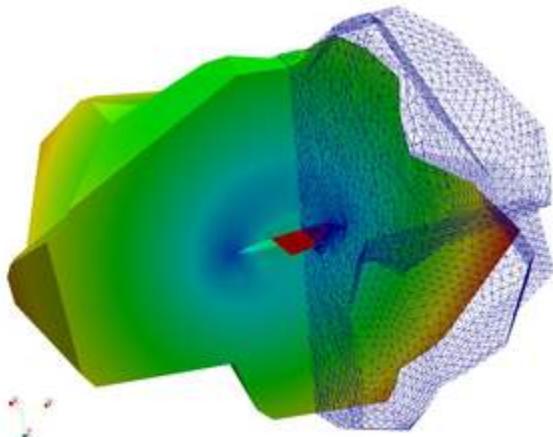
## Fluid-Particle Interaction



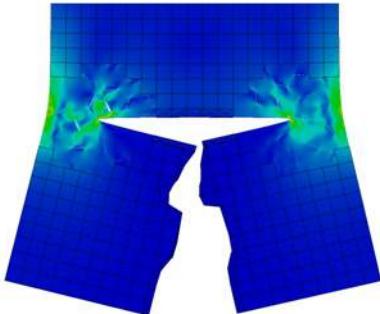
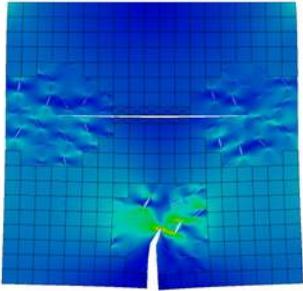


Institut für  
Kontinuumsmechanik  
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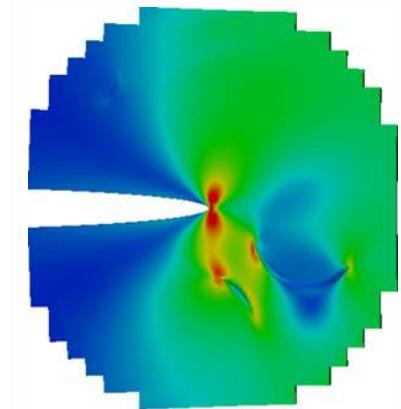
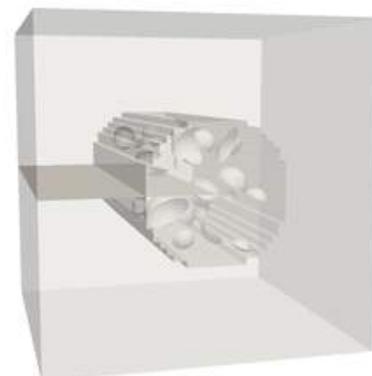
## Micro Crack Modeling at Polycrystal Level Using XFEM



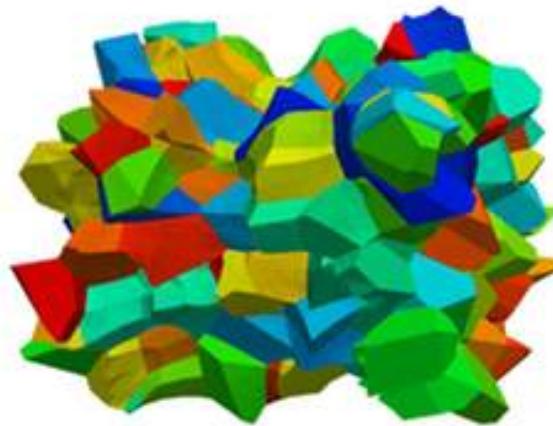
## Modeling of Crack Propagation in a Multiscale Framework using XFEM



## Multiscale Methods for Fracturing Solids



## Crystal Plasticity at Large Strains



Haga clic para modificar el estilo de texto del patrón

Segundo nivel

Leibniz  
Universität

Tercer nivel  
Cuarto nivel

Hannover  
Quinto nivel

Haga clic para modificar el estilo de texto del patrón

Segundo nivel

Tercer nivel  
Cuarto nivel

Quinto nivel



- Team members:

- Dr. Steffen Schulze-Kremer  
*Management*
- Dr. Mohammad Siahatgar  
*Project collaborator*
- Dr. Gerd Brand  
*Support*
- Dr. Holger Naundorf  
*Support*

- Contributions:

- Providing up-to-date HPC hw/sw tools  
*HLRN-III (Cray XC30), JUQUEEN (BG/Q)*
- Support for sw in WPs 3-7  
*KRATOS*
- Benchmarking, Scalability Testing  
*Epetra, HPCG*
- Towards Exascales resources scaling *FEMPAR on JUQUEEN*



# In Athens - NTUA

# solverize<sup>∞</sup>

- Solverize is a software suite that supports various types of simulation methods, like the Finite Element Method (FEM), Element-Free Galerkin methods and Isogeometric Analysis. *Solverize* exploits parallelism in CPU as well as GPUs, for bulk calculations such as those needed for large-scale problems in simulation-based sciences and engineering.
- Core developers (in alphabetical order):
  - - Karatarakis Alexander
  - - Manitaras Theofilos
  - - Stavroulakis George

A graphic element on the left side of the slide, consisting of overlapping triangles in shades of orange, red, and dark blue.

# In Barcelona (Consortium Leader)

## **TEAM LEADERS @ CIMNE:**

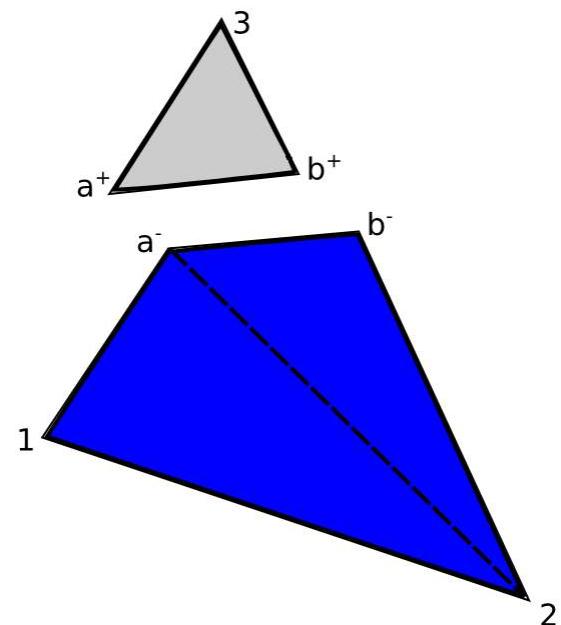
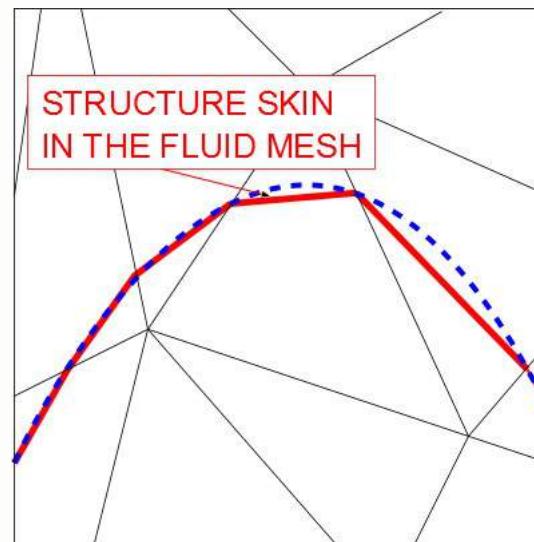
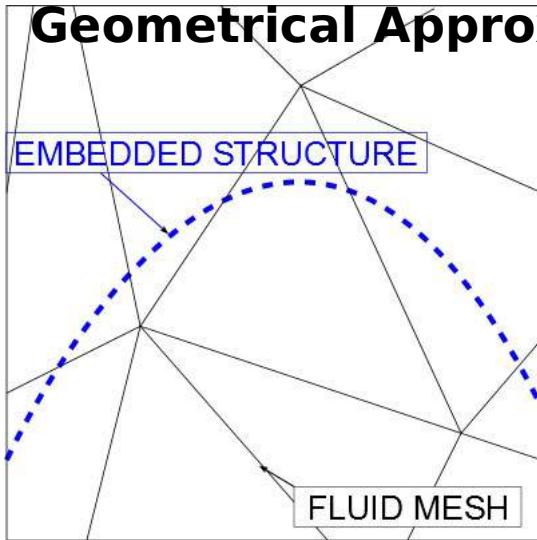
**Prof. Eugenio Oñate** - ERC Advanced Grant Holder

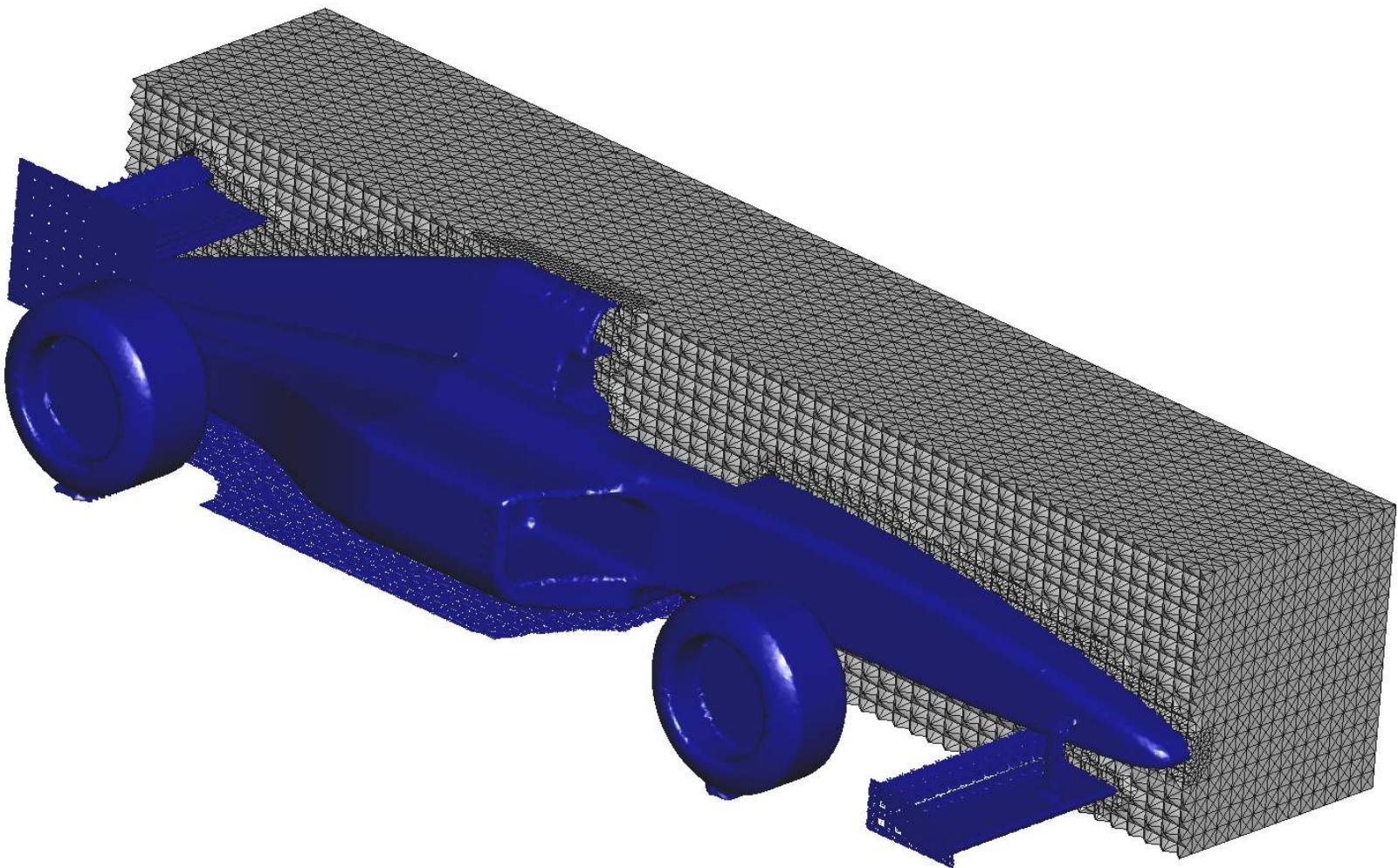
**Prof. Sergio Idelsohn** - ERC Advanced Grant Holder

**Prof. Santiago Badia** - ERC Starting Grant Holder

# EMBEDDED METHODS to go large-scale

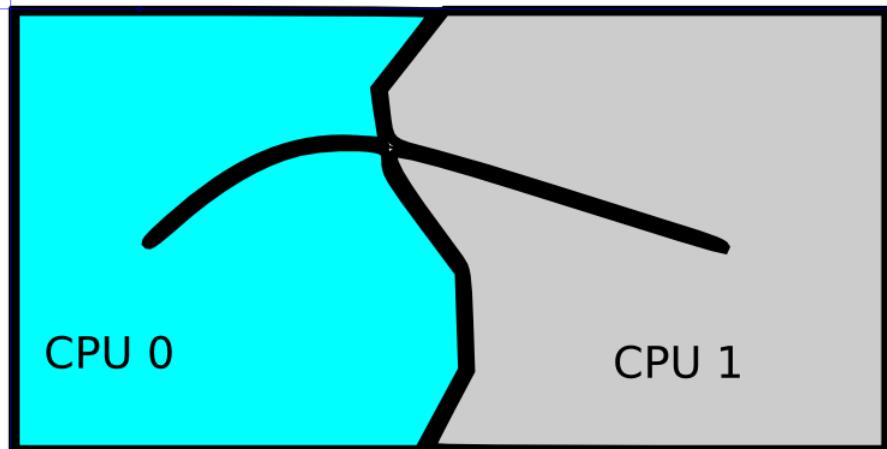
## Geometrical Approximation process



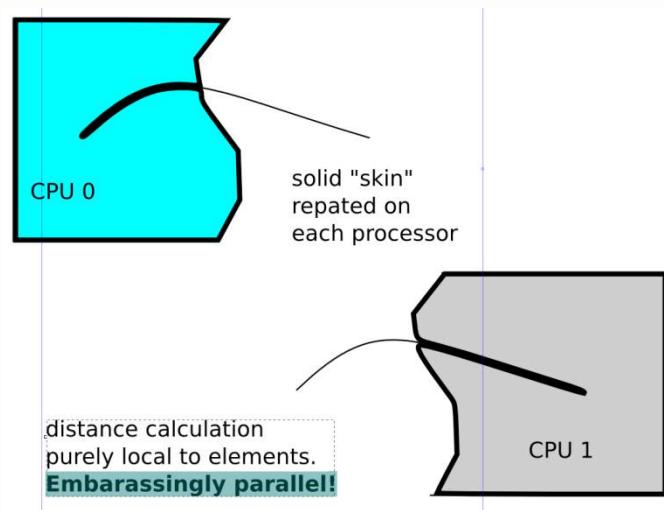


Parallel mesh adaptivity to reproduce the geometry

## MPI PARALLELIZATION:

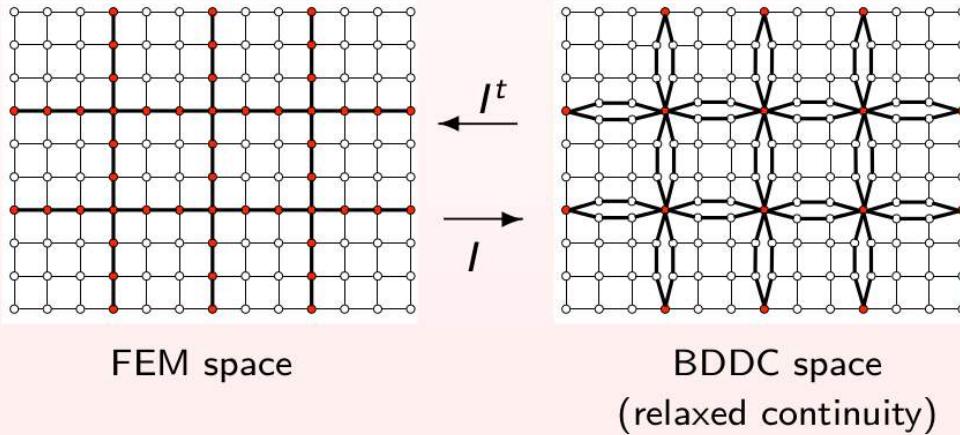


“a view” of the structural model is replicated in all of the mpi domains



Development of **FEMPAR**: Finite Element Multiphysics and massively PARallel scientific software for the numerical simulation of complex physical phenomena governed by PDEs

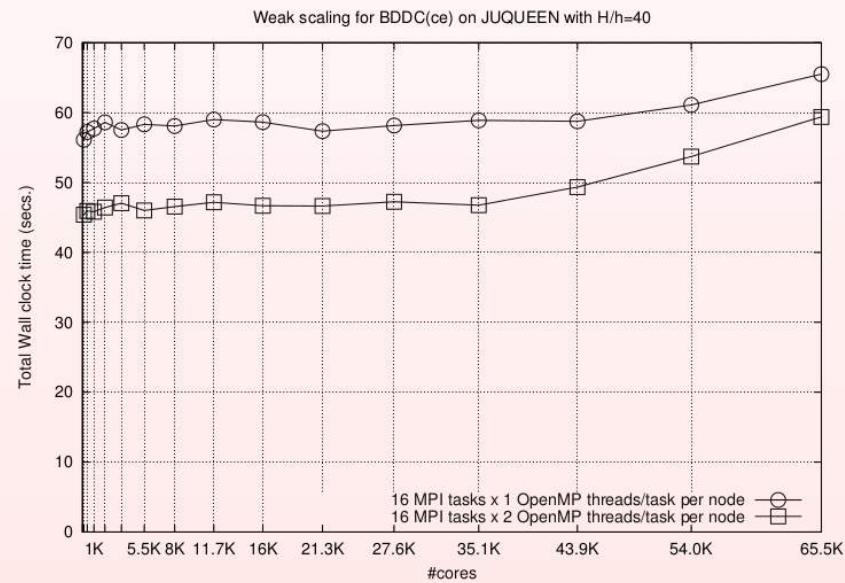
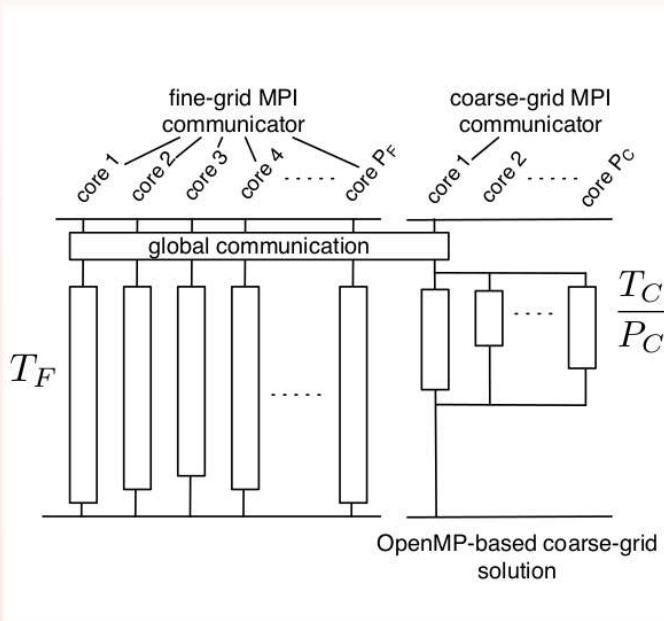
- Massively parallel solvers for one-physics problems (e.g., Poisson or Elasticity) ground on **Balancing Domain Decomposition by Constraints** preconditioning ideas
- **BDDC** correction based on the solution of the original problem in a **modified space**



- $P_{BDDC}^{-1} = P_o^{-1} + P_\bullet^{-1}$
- $P_o^{-1}$ : fine-grid (local subdomain corrections, highly parallel)
- $P_\bullet^{-1}$ : coarse-grid (global correction, “small” Schur complement)

- Multi-physics solvers (MHD, fluid, FSI, etc.) tackle the fully-coupled, implicit linear system via **inexact recursive block LU factorization** + BDDC preconditioners

- Hybrid MPI+threads via OpenMP-based subdomain local/global coarse-grid solvers
- Hybrid direct/iterative (AMG) subdomain local/global coarse-grid solvers
- Scalability: excellent up-to **65,536 cores** on IBM BG/Q (JUQUEEN)
- On-going multilevel extension (**MLBDDC**), potential to scale up-to  $\mathcal{O}(10^5\text{--}6)$  cores



S. Badia, A. F. Martín and J. Principe. A highly scalable parallel implementation of balancing domain decomposition by constraints. SIAM SISC. In press, 2014.

# GiD - interactive rates to manipulate big models

Coarsening: Vertex clustering with detail-preserving techniques

		Remote vis.	Entry-level laptop
	Num. triangles	Contour fill	Contour fill
Original model	6 M	0.25 fps	0.40 fps
Simplified model	179 K	2.8 fps	12 fps

## Remote visualization:

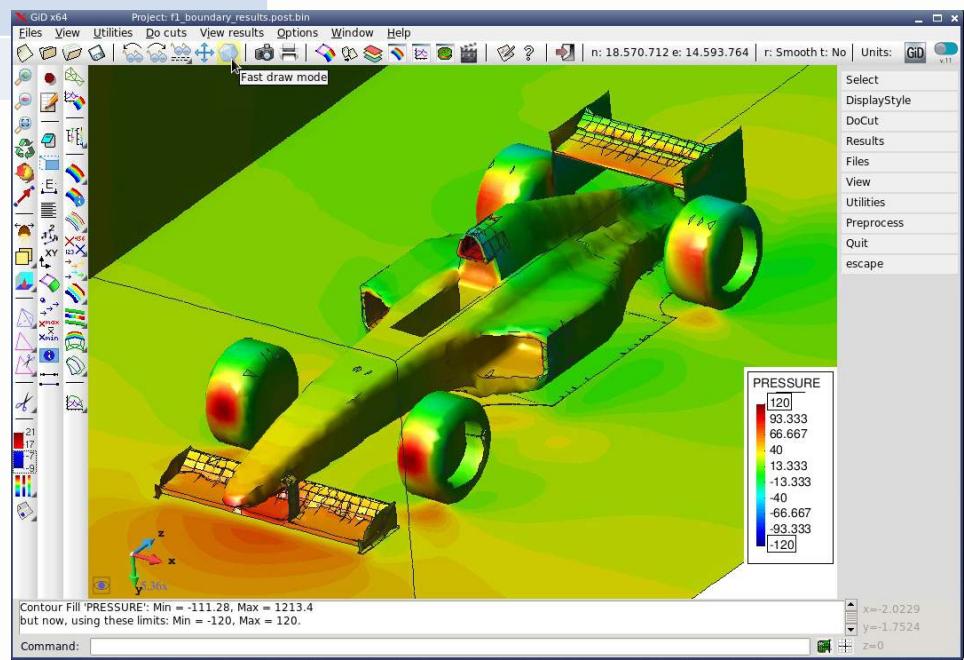
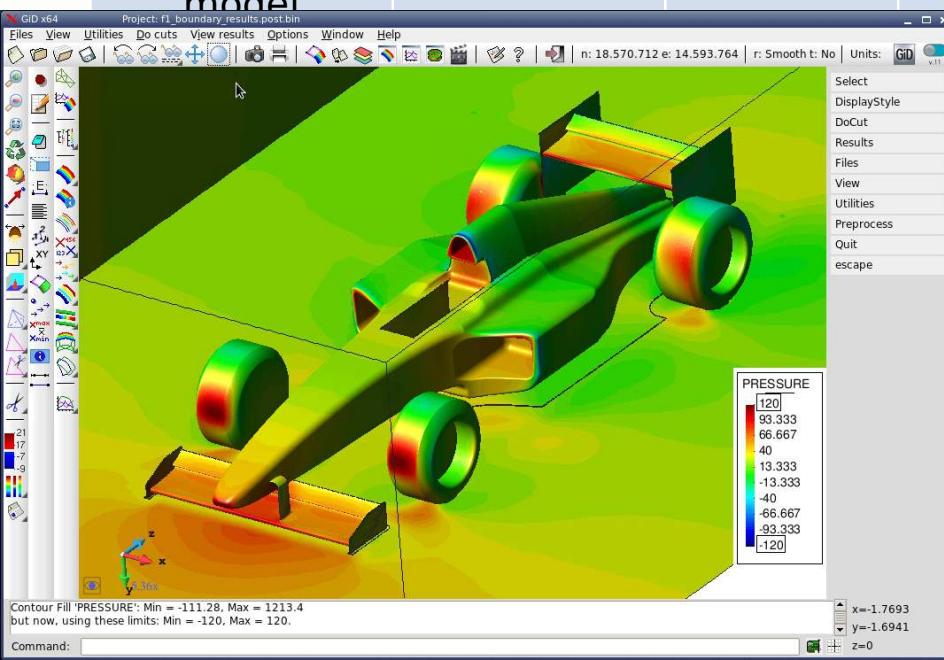
server: Node with 2xQuad Xeon E5410

client: Quad Q9550 MS Windows 7, x64 bits

## Entry-level laptop:

network: 100 Mbps  
ULV Dual Pentium SU4100 @ 1.30GHz,

Intel graphics, MS Windows 7 x64

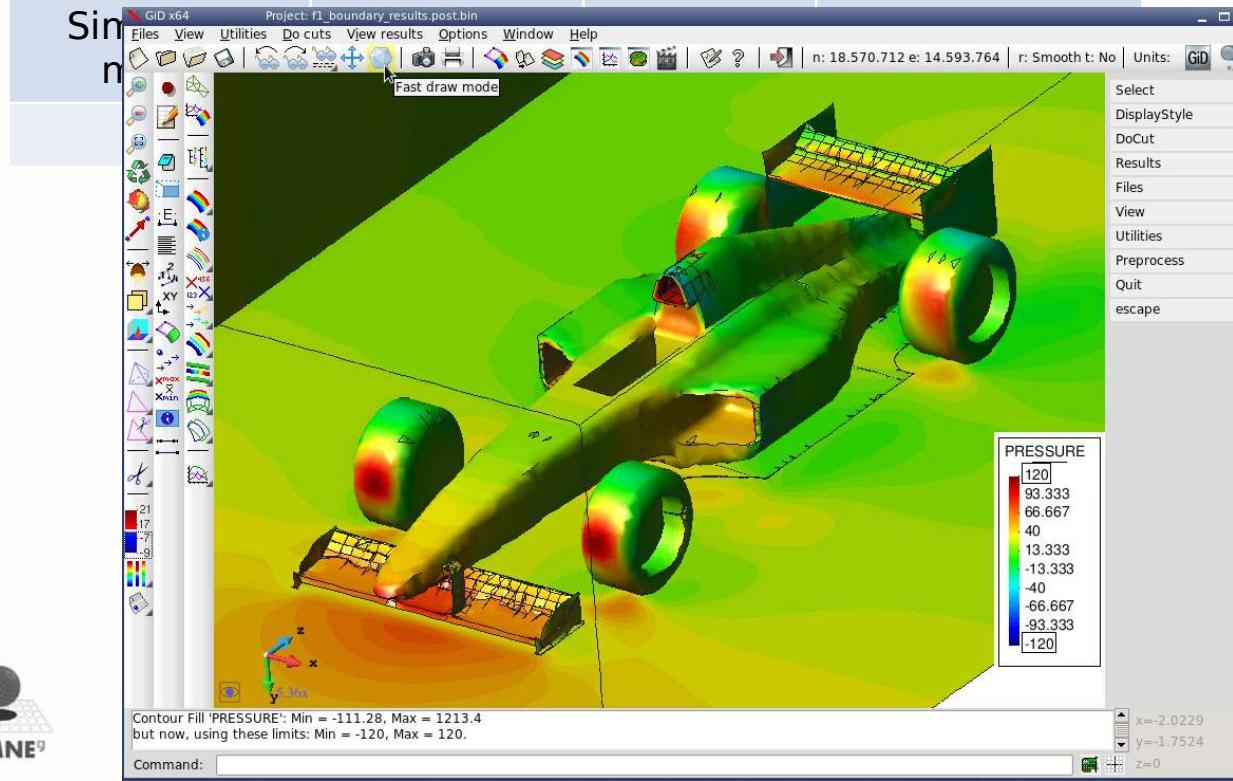


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Original F1 racing car model  
with 6 million triangles:  
0.25 fps remote  
visualization

Simplified model with 179  
thousand triangles:  
2.8 fps remote  
visualization  
12 fps very modest  
laptop



# Industrial Applications

# “Click2Cast”



Commercial software, developed by  
Quantech ATZ ☐ **Industrial Partner**

[www.click2cast.com](http://www.click2cast.com)

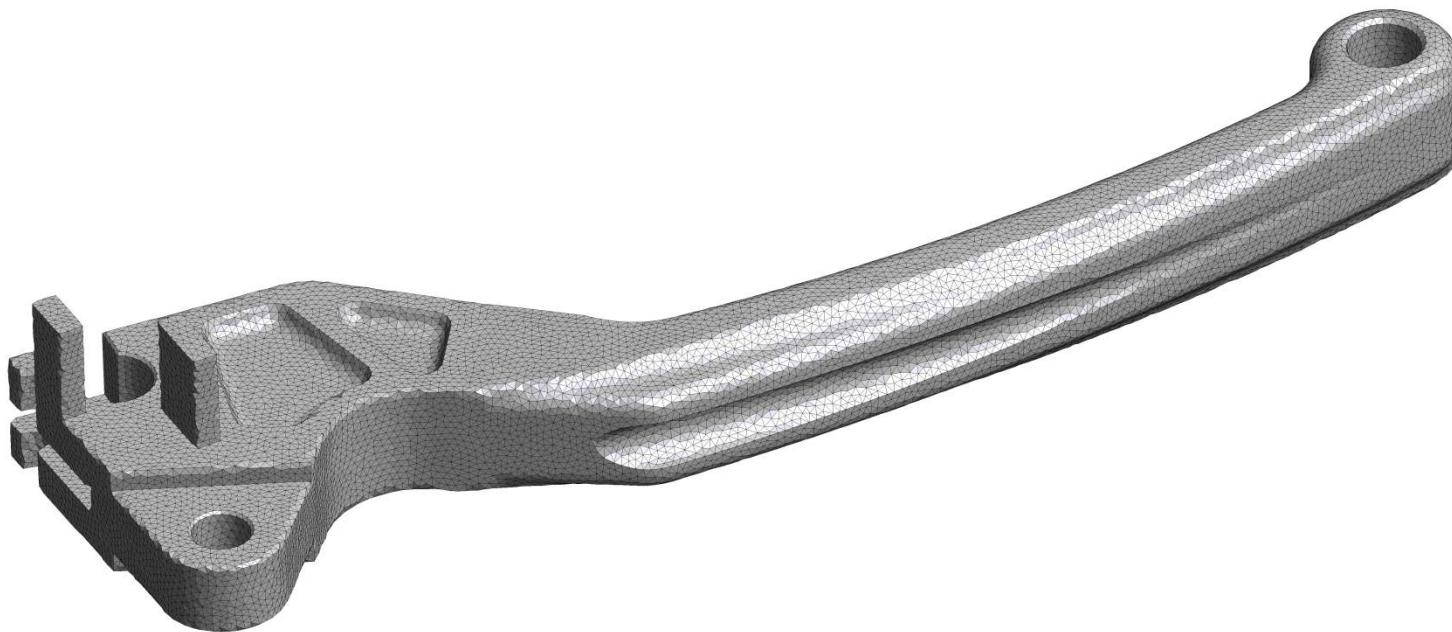
- Streamlined interface – very controlled work environment
- Very advanced stl meshing capabilities

FE solver hidden behind the interface

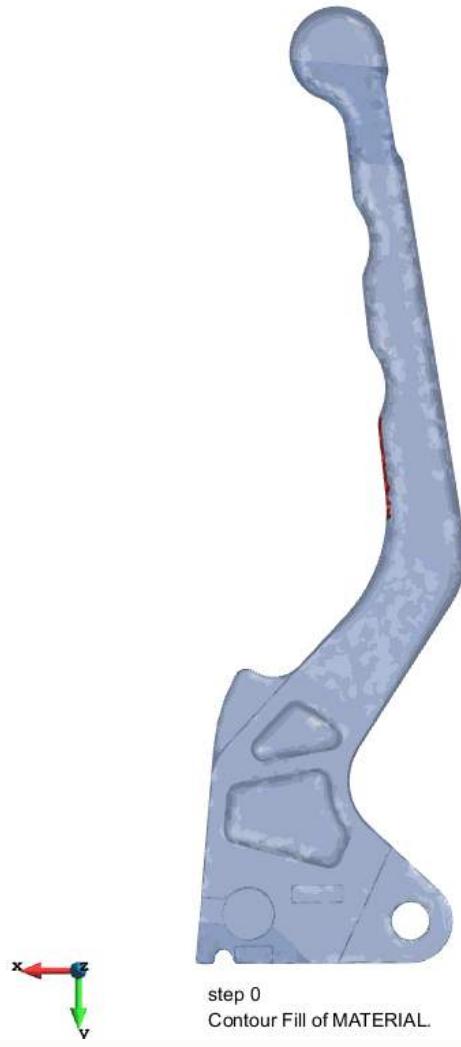
# INPUT - STL MESH



# OUTPUT- NICE VOLUME MESH



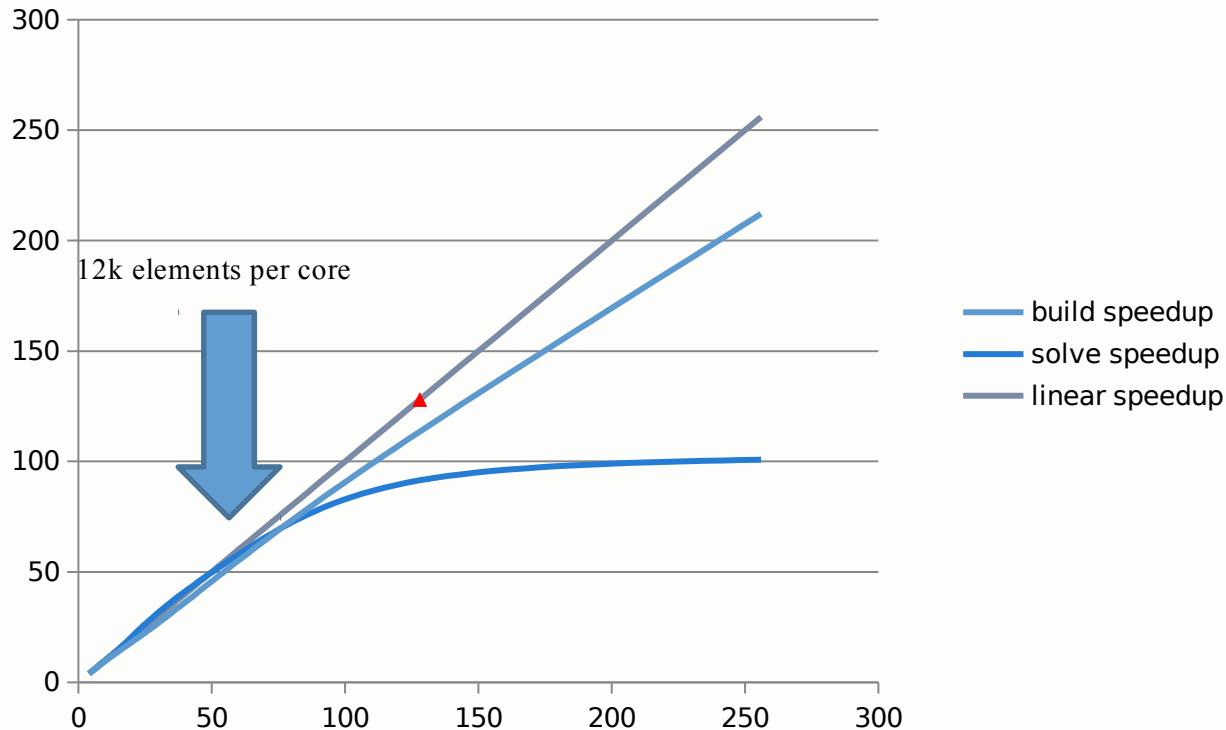
# RESULT:



step 0  
Contour Fill of MATERIAL.

# MPI SCALABILITY

## 800k elements, gravity flow

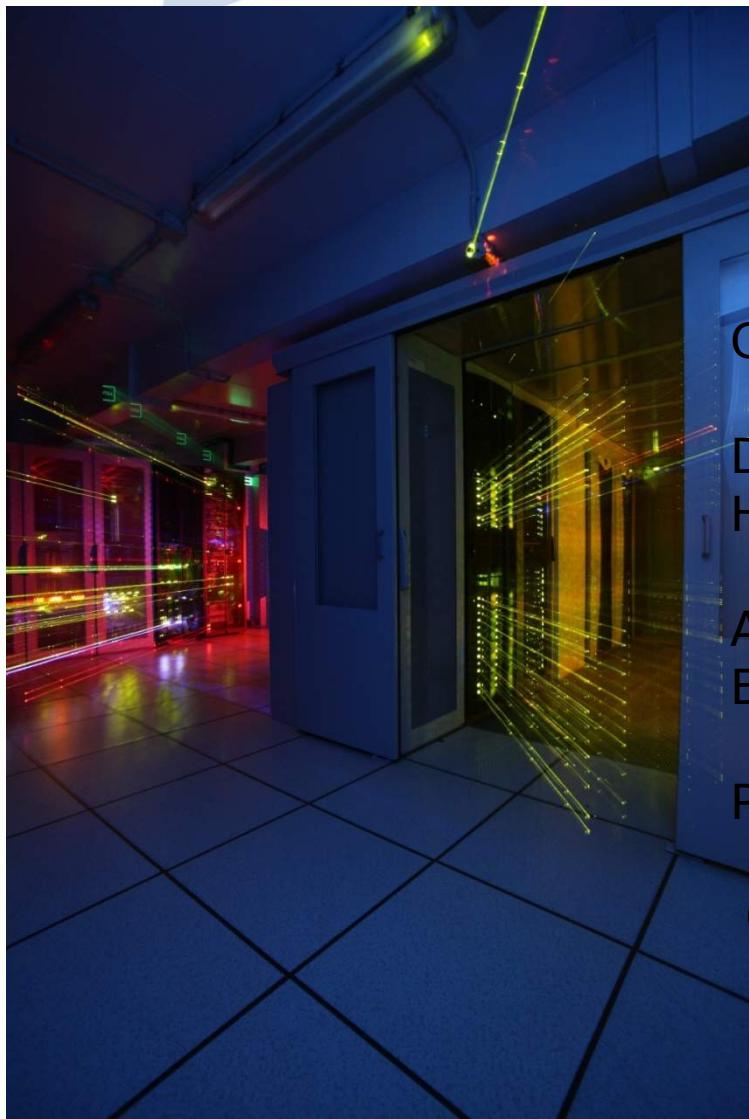




**CSUC (former CESCA)**

**provides supercomputing infrastructure**

## Description of the team



Consorci de  
Serveis Universitaris  
de Catalunya

Gorka Roldan: Project manager)

David Tur: HPC Scientist and coordinator of the HPC team

Alfred Gil: HPC Scientist, Benchmarking&Profiling Expert

Pere Puigdomènech: HPC Engineering Support.

Cristian Gomollon: HPC Support Scientist