Global Research and Development

ArcelorMittal

How numerical simulation can accelerate knowledge and product design in the steel industry?

June 28th 2017

Astrid PERLADE, Thierry IUNG
with the contribution of C. ALBA, N. DE ABAJO, M. ARIAS, S. ALLAIN, J. DEQUEKER, R. JACOLOT, D. HUIN, A. PACHON, N. D. HASENPOUTH…

Teratec 2017 Forum
Big data for materials sciences

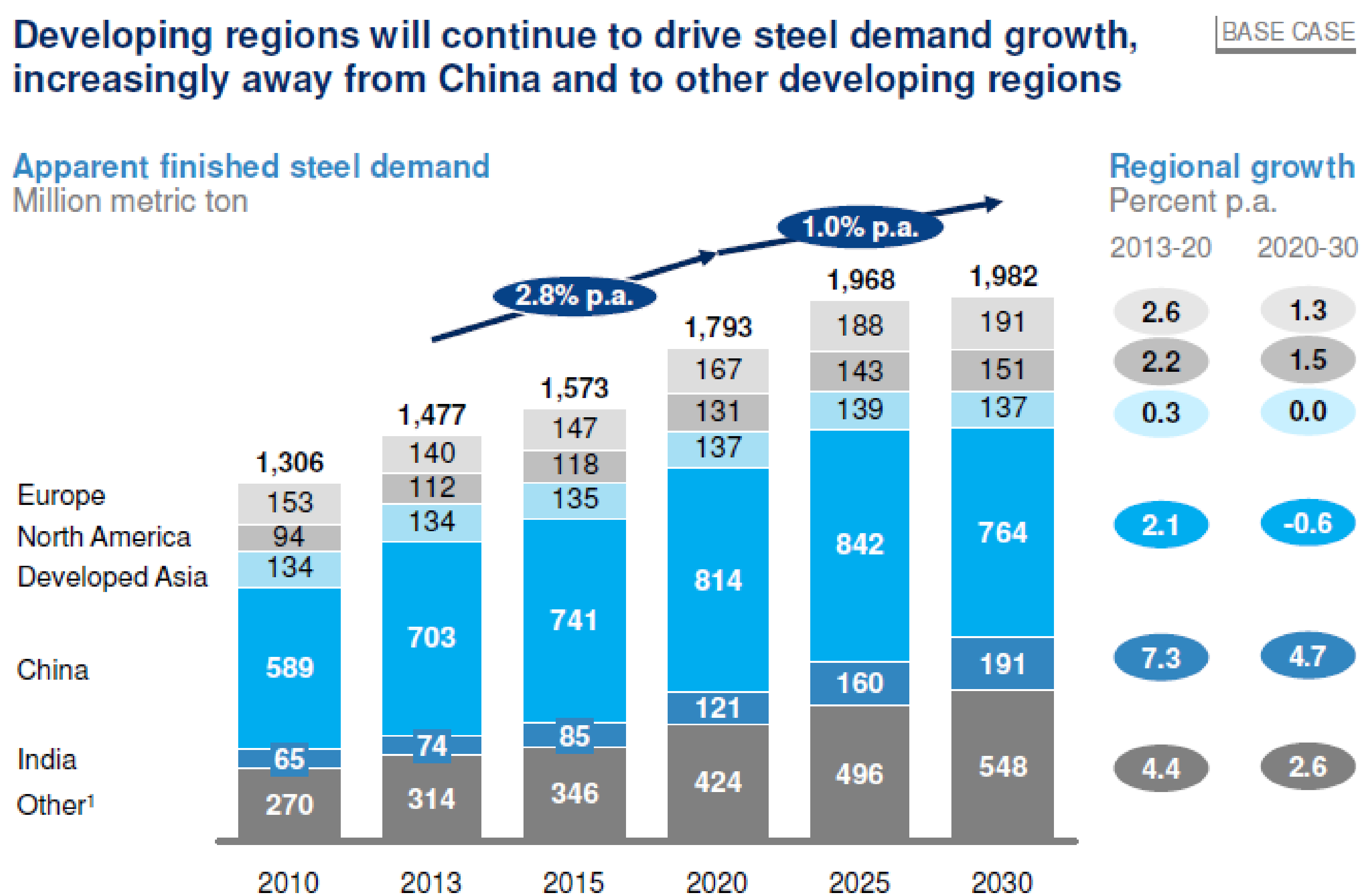
The right formula
for the steels of the future

Outline

- Introduction
  - Brief presentation of ArcelorMittal and main markets
- How numerical solutions can accelerate product knowledge development and design?
- How numerical solutions can promote steel solutions at the customers?
- How numerical solutions can support steel production?

For sure, presentation will not be exhaustive
Purpose is to present few examples of applications of simulations in the steel industry

Steel is by far the largest material in use



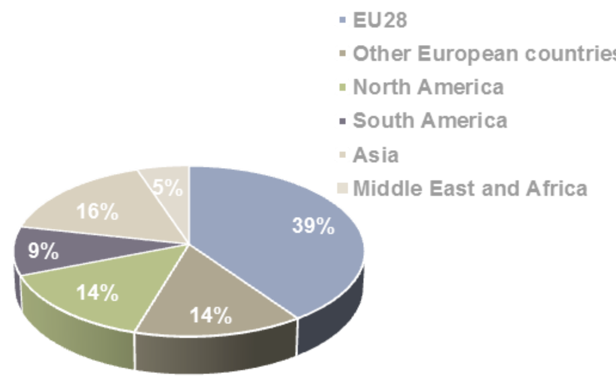
World steel production
Reference in 1973 : around 600Mt

ArcelorMittal : Key figures

	2015	2014	2013
Sales (US$ billion)	63.6	79.3	79.4
Ebitda (US$ billion)	5.2	7.2	6.9
Operating income / (loss) (US$ billion)	(4.2)	3.0	1.2
Net income / (loss) (US$ billion)	(7.9)	(1.1)	(2.5)
Steel shipments (million tonnes)	84.6	85.1	82.6
Crude steel production (million tonnes)	92.5	93.1	91.2
Own iron ore production (million tonnes)*	62.8	63.9	58.4

*Own iron ore and coal production excluding strategic long-term contracts.

Allocation of employees in 2015 according to geographic location (full-time equivalent)

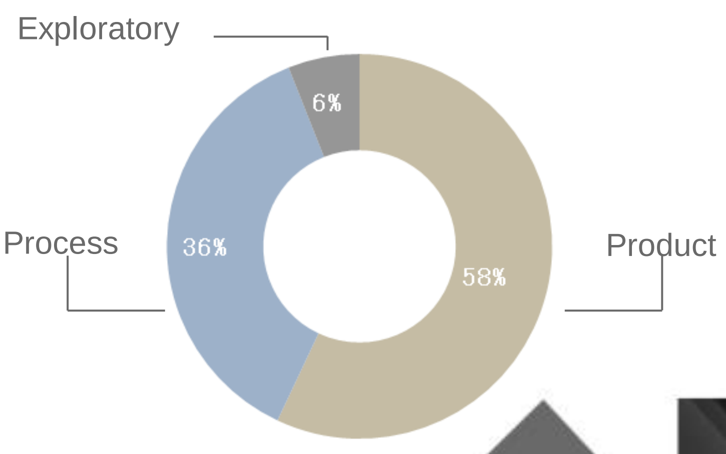


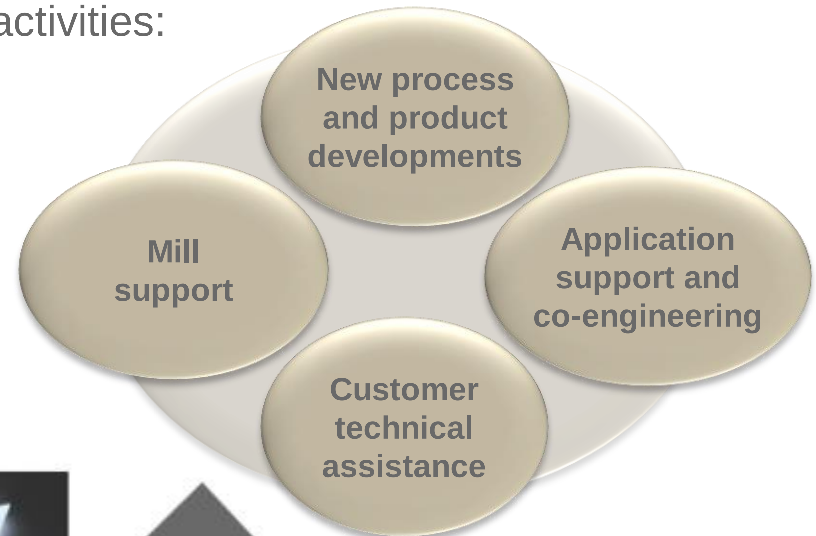
Around 210,000 employees in more than 60 countries

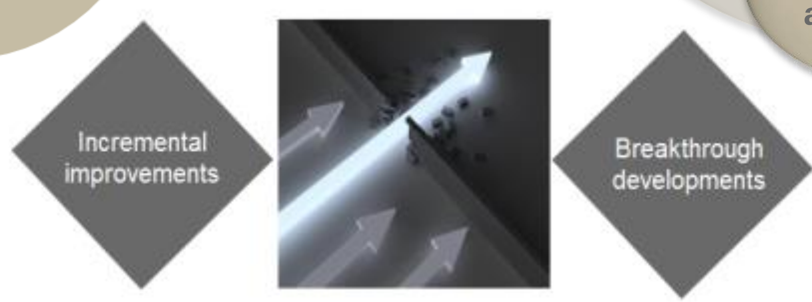
ArcelorMittal is the world's leading steel and mining company

Global R&D: Scope and Mission

- 1,300 full time researchers
- Broad, comprehensive portfolio and programs addressing business needs
- Worldwide network of laboratories: 12 labs in Europe and Americas
- Budget spending by focus area and range of activities:







R&D effort fully aligned with group strategy: geography, value chain, product differentiation

Customers' needs, examples

- **Automotive**: compromise between weight reduction, comfort, safety & durability
- **Packaging**: cost effectiveness, easy processing, weight reduction, innovative look, food compatibility, green products
- **Appliances**: cost reduction, antibacterial, aesthetics, environmental friendly…
- **Construction**: energy-efficiency, environmental issues, safe buildings, durability, fast erection, health & comfort, aesthetics,…
- **Metal Processing**: weight and cost saving, corrosion resistance, safety, reduced total cost of ownership, high temperature resistance
- **Electrical Engineering**: higher efficiency and power density machines through low loss, high permeability, high strength electrical steels
- **Energy pipes**: heavy gauge, high strength, corrosion resistance, improved welding






Wide market applications, large spectrum of performances

ArcelorMittal Automotive Worldwide

Automotive needs for new performance :
Design & Development of Next Generation Steels

Maximize Steel's Advantages

Address Steel's Limitations

Push UTS beyond 1500 MPa

Strength-Limited
- Rockers
- Cross Members
- Rail Extensions
- A-, B-Pillars

Energy -Limited
- Rails
- Lower B-Pillar
- Windshield Members

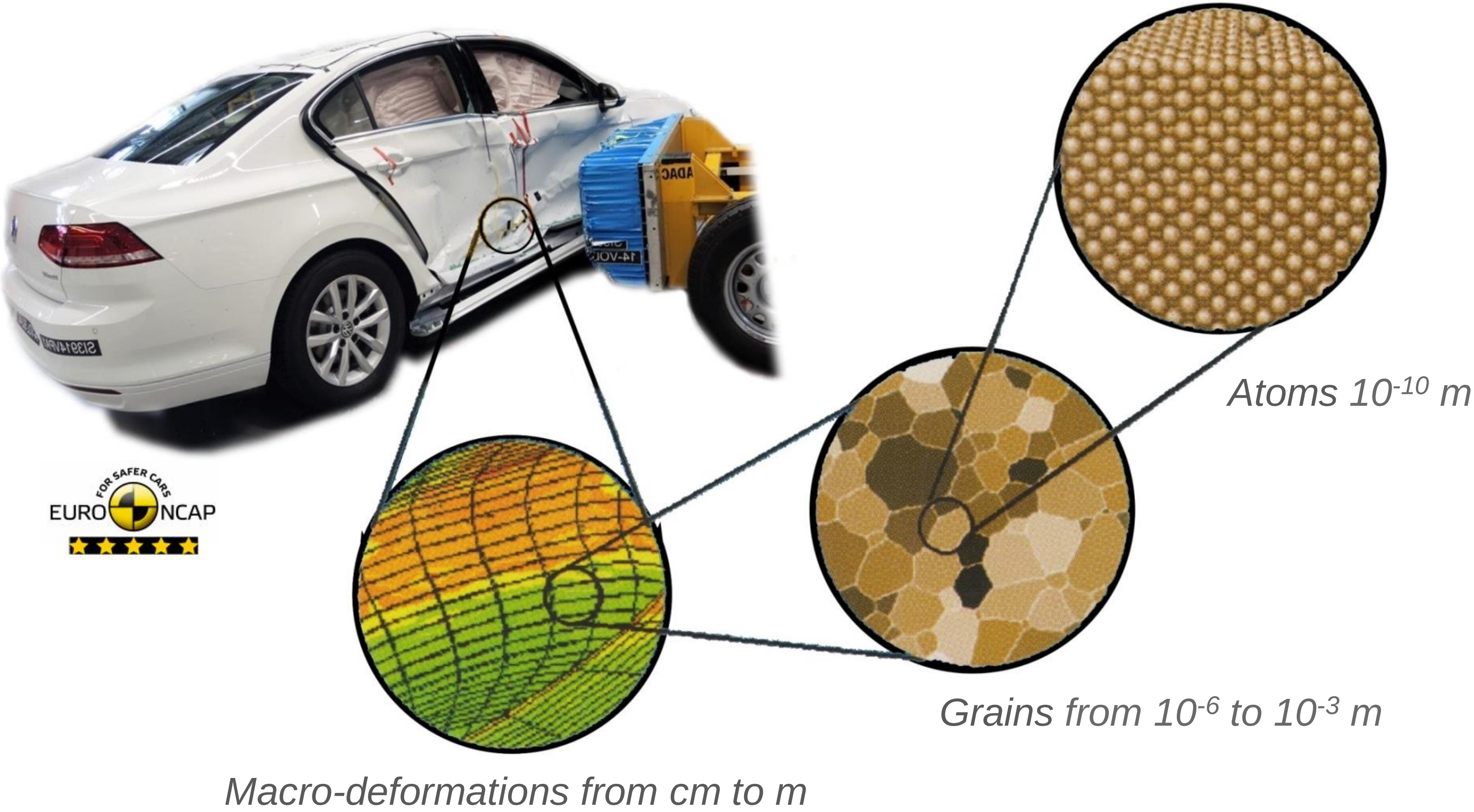
Develop High UTS plus High Elongation

Develop Low Density Steels

Stiffness-Limited
- C-Pillar Ring
- Closures
- Floor Pans
- Chassis

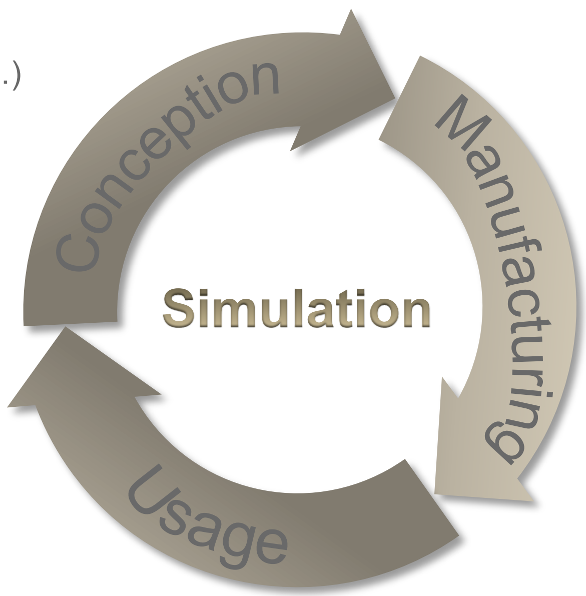
Develop High Modulus Steels

Microstructure engineering
Macro → Microstructure → Nanostructure



Playing with quasi-infinite possible solutions for steel design

- Part shape and thickness
- Steel properties
  - Large variety of constituents :
    - Austenite (CFC), Ferrite, Bainite, martensite (CC), Cementite (iron carbide), Pearlite (Lamellae ferrite/cementite)
    - With various fractions and spatial arrangements
  - and for each constituent
    - Size and shape (grain size, interlamellar spacing, …)
    - Solute elements : Mn, Ni, C …
    - Precipitates : AlN, TiN, Nb(C,N), ...
    - Crystallographic texture



→ Need simulation tools to describe, understand and define improved solutions

A large range of scales to be considered

Finite elements simulations

Analytical models

Cellular automats

Discrete Dislocations dynamics

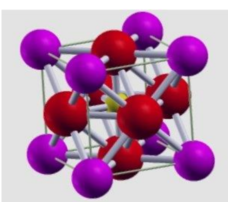
Mean field

Phase Field

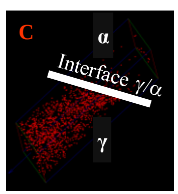
Monte Carlo

Ab initio | *Molecular Dynamics*

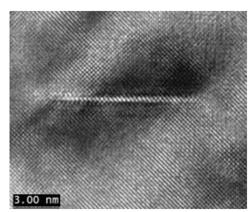
electron → Atom → Nanostructure → Microstructure → Macrostructure



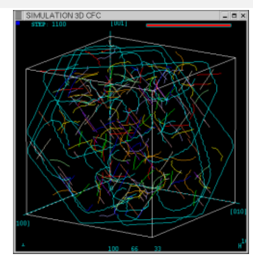
First principle calculations of FeAlC carbide



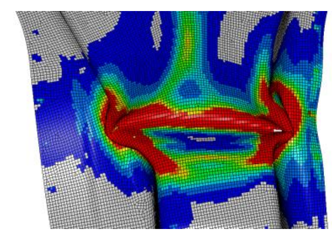
3D APT study of γ/α interface



First stages of NbN precipitation: monoatomic layer of pure Nb



DDD for grain size effect



FE for validation of crash resistance

→ Need to go from complex to more simple approaches
Let's go through few examples!

Starting from electronic interactions between atoms…

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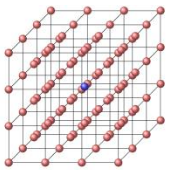
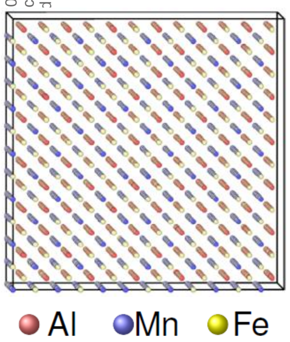
- … to determine the equilibrium states depending on the alloy composition and temperature

From J. Dequeker, A. Legris, UMET



Point defect in a 3 × 3 × 3 lattice.



Ab initio calculations (VASP software) using the Density Functional Theory (DFT)

↓

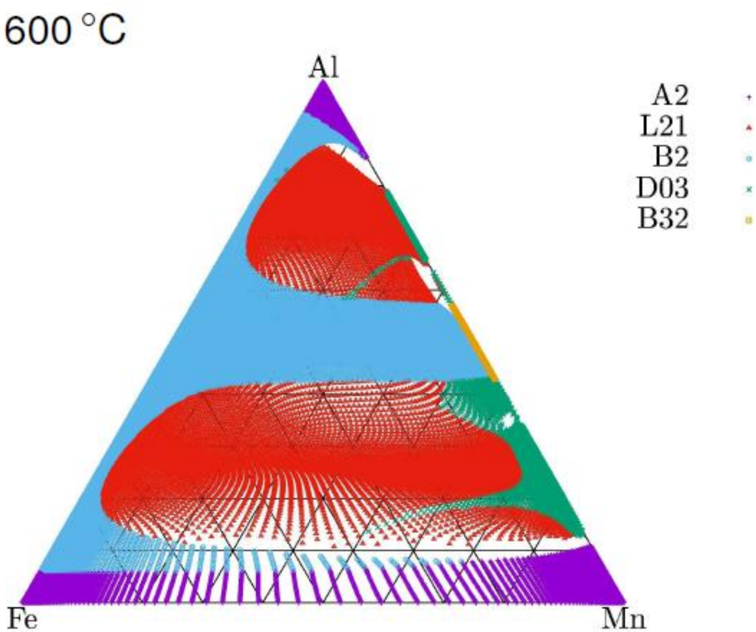
Ground state DFT energies
With different supercells for solid solutions

↓

Monte-Carlo simulations to evaluate the configurational part of free energy
Exact but time consuming

↓

Construction of phase diagrams



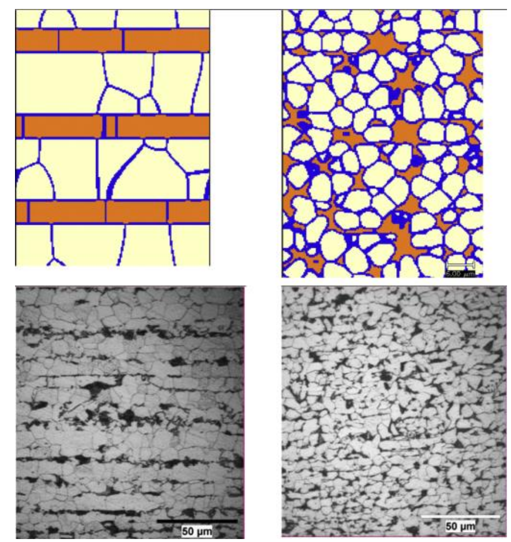
FCC phase still to be modelled

Predictive capacities of Ab initio simulations make it a true "computer experiment", capable of unambiguously identifying microscopic mechanisms underlying the phenomena or properties studied

… to predict the microstructure formation

- Mean-field approaches to describe the microstructure evolution, for instance the γ to α transformation in homogeneous microstructure
    - Based on simple spherical geometry
    - Simple carbon diffusion profile

- Full-field modelling might become necessary in some cases
    - Phase field model approach : Diffuse interface model coupled with the diffusion equations describing the redistribution of alloying elements

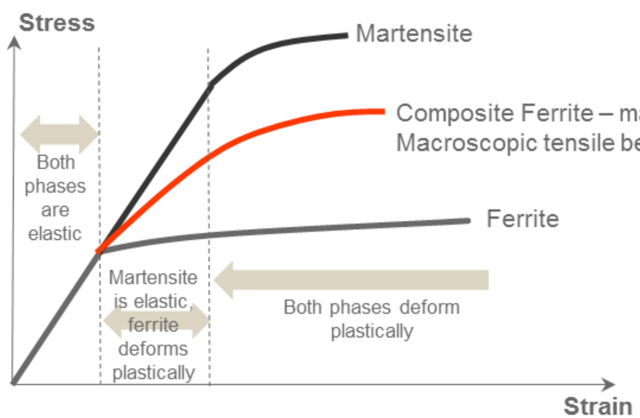


Prediction of banded structures linked with heterogeneous chemical compositions
Gouné et al. Mat. Sci. & Eng. R 92 (2015) 1–38

and the mechanical and damage properties

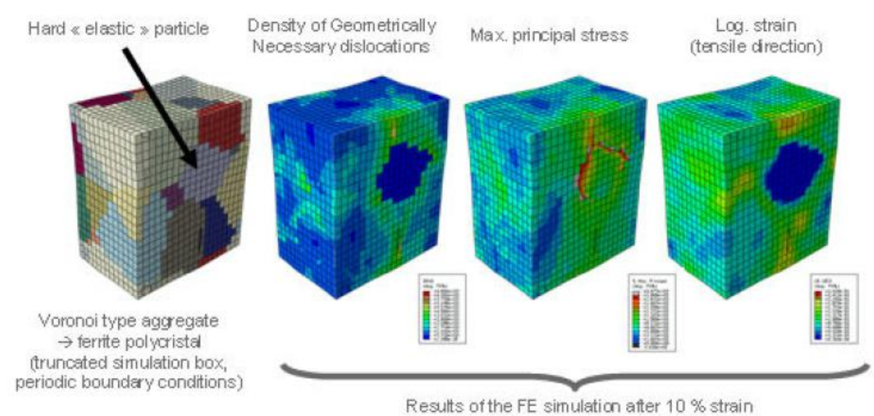
Prediction of basic mechanical properties

- can be done by physically based “mean field approaches” on the basis of very few microstructure inputs



Prediction of fracture and damage mechanisms

- requires the description of very local and rare events with a certain stochastic occurrence (weakest link theory)



- ➢ Which features are linked to the final performances?
- ➢ Which properties have to be controlled to ensure material quality?
- ➢ How to optimize and develop new materials to secure profitability?
- ➢ How to predict the risk of product failure?

From material properties to in-use properties of automotive parts and structures

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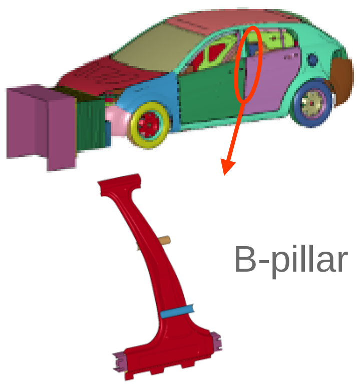
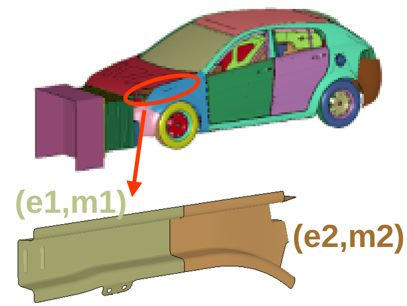
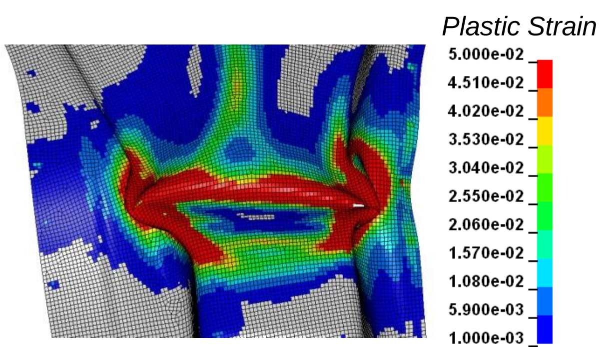




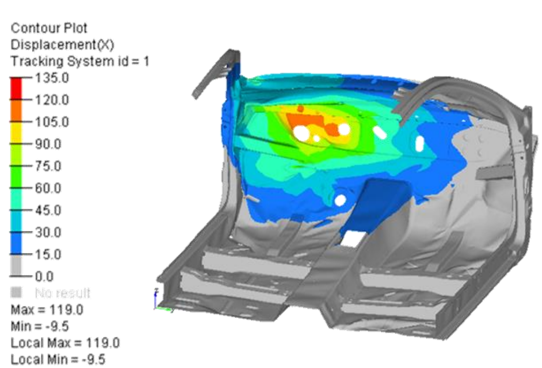
Front Side Member

Validation of crash resistance



Simulations of a on a B-Pillar in Usibor®1500 with LS-DYNA MAT224
Accurate failure prediction taking into account the deformation path

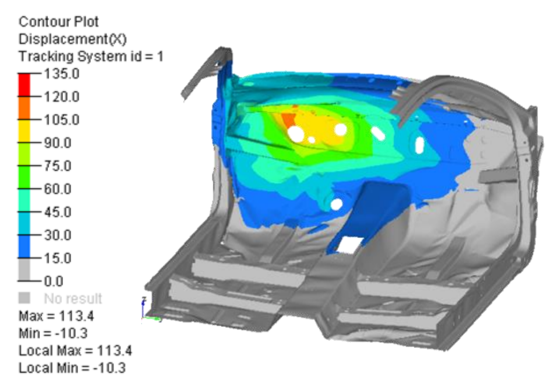
Evaluation of mass savings: -21.2%



Reference DP600

(e_1 = 1.7mm / e_2 =2.1mm)

Max intrusion on Dash: 119.0 mm



New 3rd generation steel

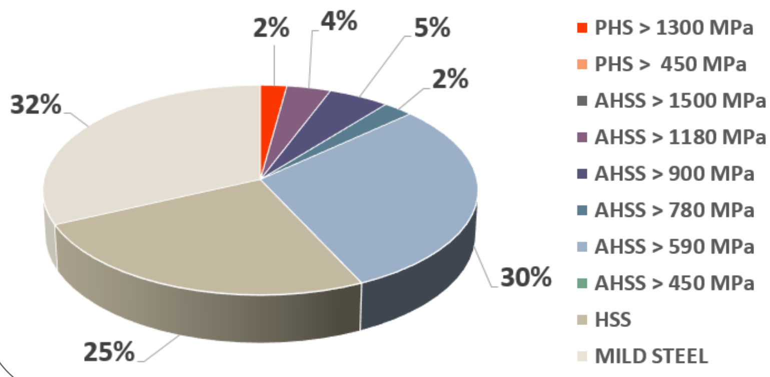
(e_1 = 1.3mm / e_2 = 1.7mm)

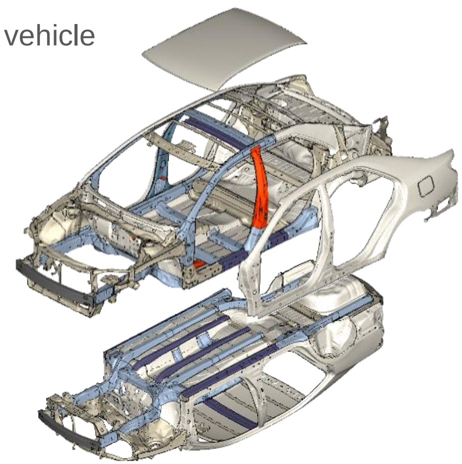
Max intrusion on Dash: 113.4 mm

From D. Hasenpouth, R&D Auto Applications

… To define optimum solutions for weight savings: S-in motion®

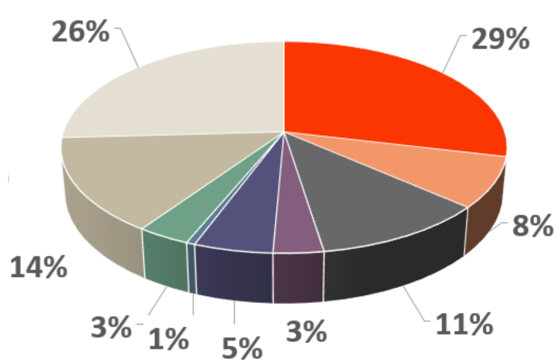
Baseline Representative of US Market. Midsize vehicle

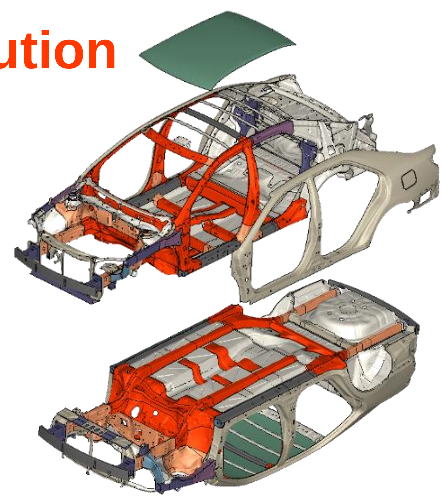




Component	Total Mass
Vehicle curb weight	1478.2kg
BIW	324.4 kg
Front Doors	16.5 kg (x2)
Rear Doors	13.9 kg (x2)
Total BIW + doors	385.2 kg

Near term grades Solution



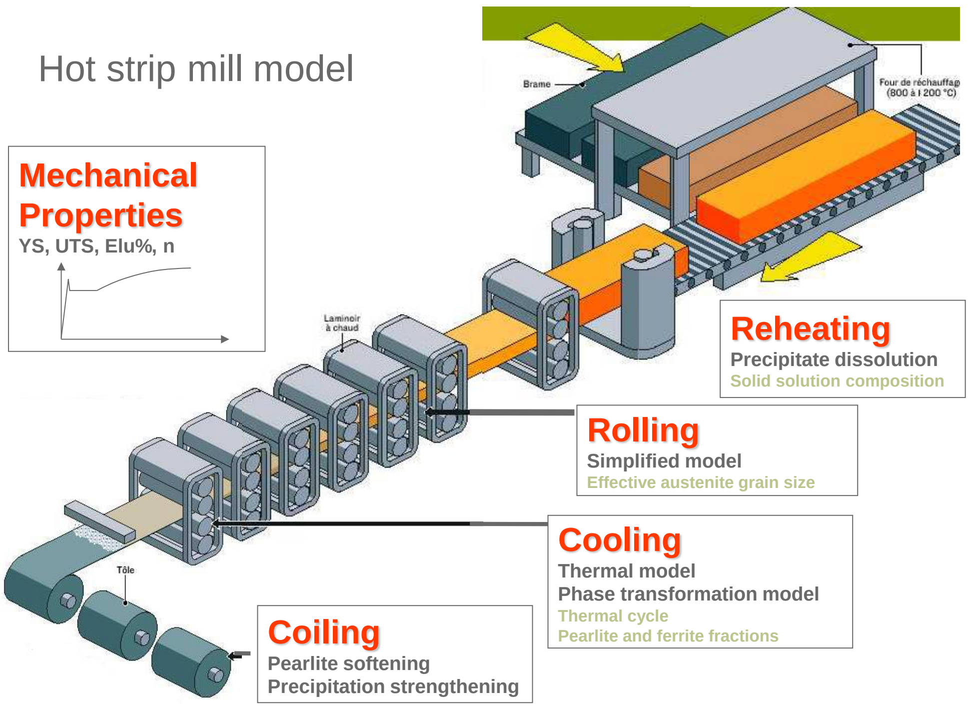


Component	Total Mass	Weight savings
Vehicle curb weight	1378.6kg	7%
BIW	235.0 kg	28%
Front Doors	14.1 kg (x2)	15%
Rear Doors	11.2 kg (x2)	19%
Total	285.6 kg	26%

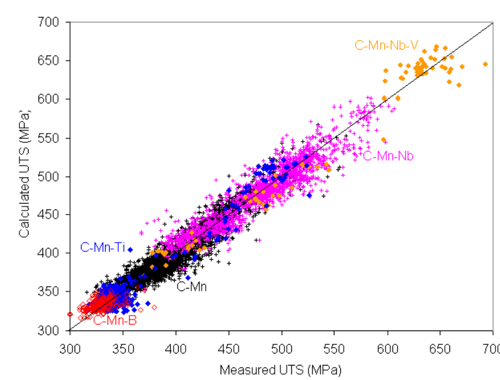
~ 100kg weight savings with near term steel grades

Product Manufacturability Mastering: « Industry 4.0 » which started more than 20 years ago

Hot strip mill model



- Start from physics
- Simplify
- Validate the chosen formalism on laboratory data
- Use massively data from plants to tune
- Constant back and forth between data from plants and details of the model



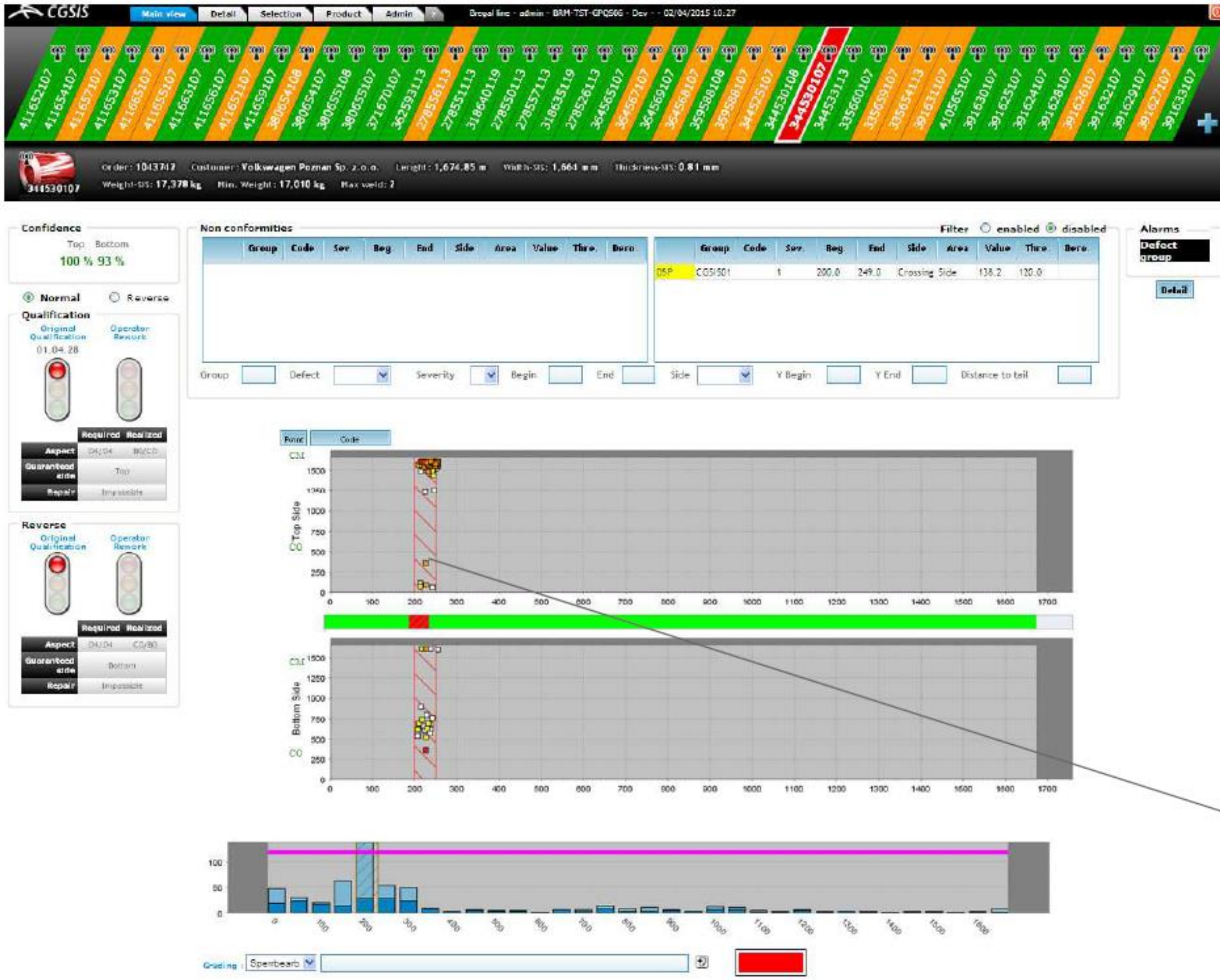
Product Manufacturability Mastering: « Industry 4.0 »
Some applications

- Preset and on-line control process: Dynamic run out table simulator
- Metallurgical design and constraint relief
- Automatic delivery

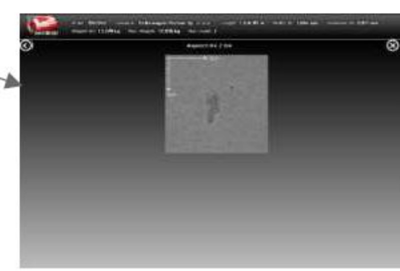
Progressively using ***new simulations technologies***:

- Quality control in the plant
  - ➢ The real time checking of the process allows to detect early any drift, far before any damageable consequence on the equipment or on the product
  - ➢ Accurate Automatic Surface Inspection Systems (ASIS) thanks to deep learning technics
- Support to plant investments, for instance by data-driven evaluation

« Industry 4.0 »: How to produce the right product?



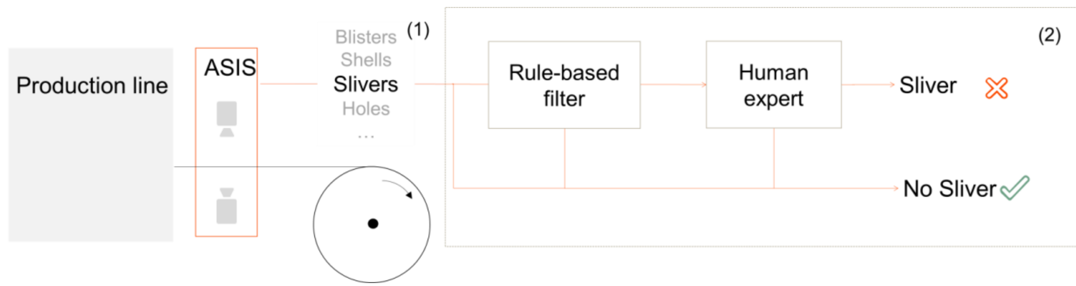
- Global Product Qualification System
- Data integration
- Data treatment
- Decision making



Deep Learning for radical quality control

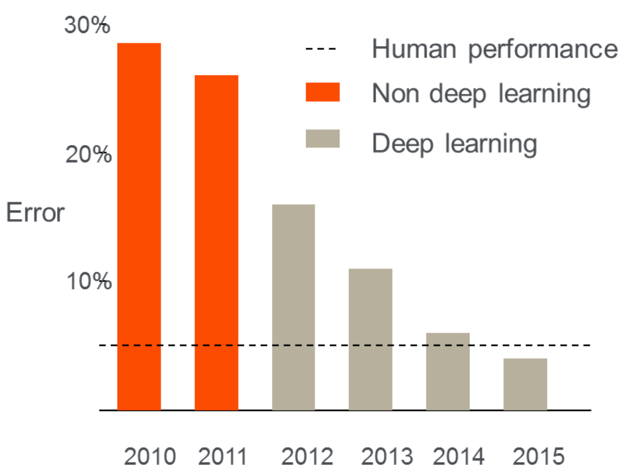
Slivers are still a production defect to be controlled

From Global R&D Asturias



- Data-driven approach based on well established model called neural networks
- Hierarchical Learning: Automatically discovers important patterns in data

Amazing results!



New Deep Learning techniques

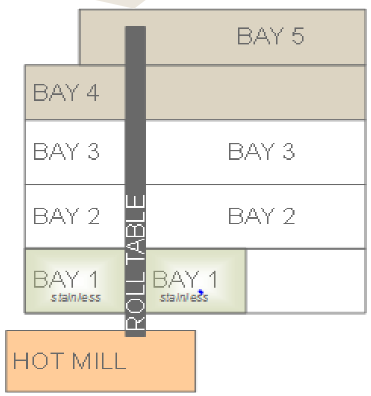
- Collaboration with nnaisense
- New Deep Learning techniques were applied on top of current ASIS, creating a model from a 100.000 images dataset
- Accuracy achieved is **similar to Traditional ASIS + rule-filtering + human inspection**
- Radical reduction of human inspection and model **can be rolled out**

An example of plant investment supported by innovative model

From Mónica Arias (Global R&D)

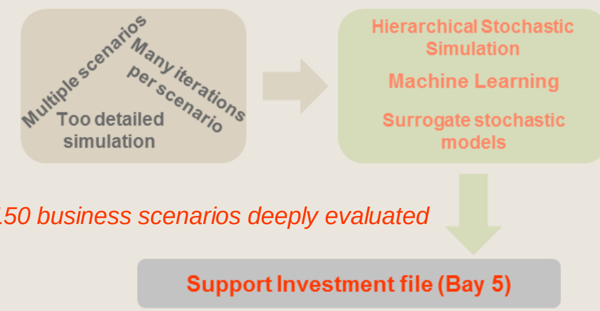
- **P**erformance and **R**isk **I**ntelligent **D**ata-Driven **E**valuation: Case of Slab Yard

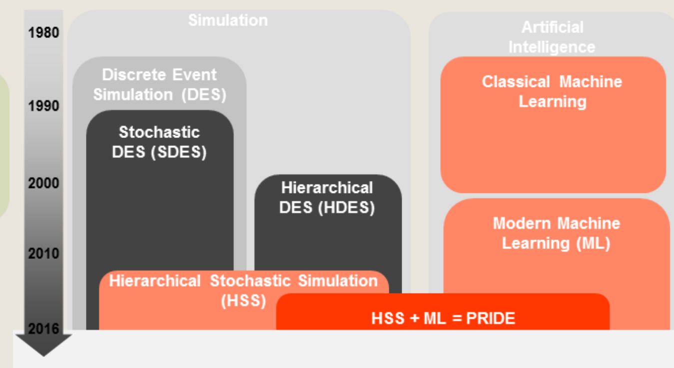
Bay 5 needed?



The problem: *Is a 4-Bay Slab Yard a feasible configuration to cope with the new context resulting from the production increase and the market changes (complexity increase in terms of number of slab articles)?*

The way



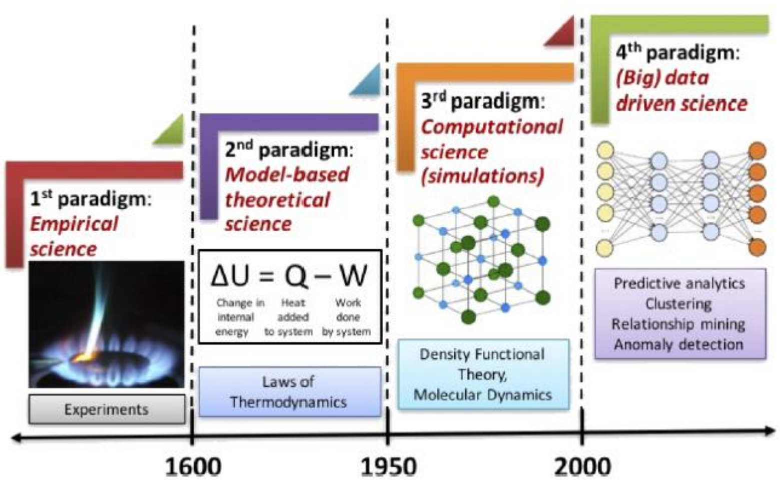


The mean: *The hardware used was key to perform the study in the limited time frame available; our **Cerebro** cluster consists of 38 heterogeneous Intel Xeon-based servers, totaling **1344 processing cores** across 666 processors with **12.7TB RAM**, and 90TB storage. This translates roughly in **25 trillion instructions per second** (25x10^6 MIPS).*

The result: *4-bay Slab Yard is not sufficient whatever the strategy.*

Concluding remarks

- Few examples of applications of simulations in the steel industry, especially in the framework of automotive steel development, have been presented:
  - Metallurgical modelling for improved knowledge and product design
  - S-in motion® to define best steel solutions at the customers
  - "Industry 4.0" for steel production support
- Objective is to develop a seamless simulation chain from conception to usage phase…
- … with various degrees of complexity depending on expectations and computer capacities
  - From more complex (Ab initio, full field simulations) → understanding purpose
  - To more simple (Mean field simulations for reduced computation time) → predicting purpose for off-line and on-line use
- … Progressively using new simulations technologies, mainly on the manufacturing side for the moment



From A. Agrawal, A. Choudhary, APL Mater. 4., 053208 (2016)

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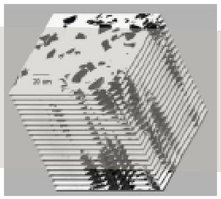
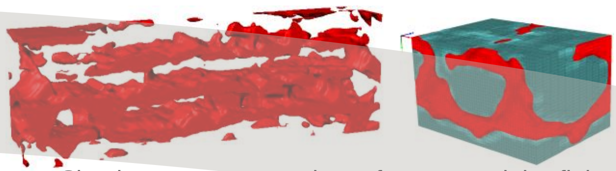
Back-up

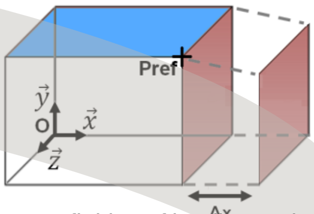
Simulation chain



Experimental data: Optical micrographs stake

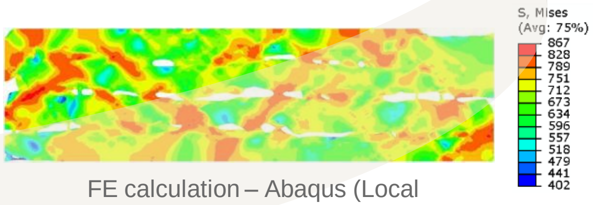


Simpleware reconstruction software permitting finite elements models in 3D

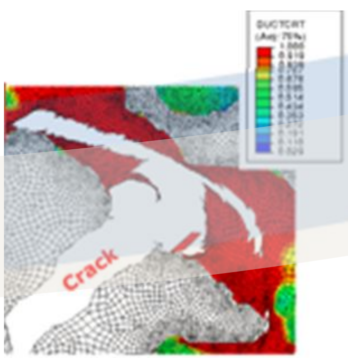


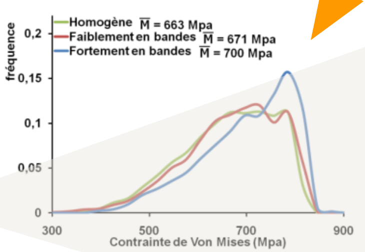
Definition of loading and boundary conditions

Possible substitutions in the simulation chain to find different CPU resources / simulation precision ratio



FE calculation – Abaqus (Local stress mapping)





Results analysis: comparison of microstructures based of fracture criterion

Statistical analysis of database

Reduced RVE

Different degrees of complexity having in mind the success criteria of industrial end-users (reliability but also pragmatic expectations, as computation time or lean preprocessing)