



**AGH** AGH UNIVERSITY OF SCIENCE  
AND TECHNOLOGY

**Design and implementation  
highly adaptive numerical code to  
creation of new simulation tools to  
support the design of new technologies**

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# AGENDA

1

The purpose of the presentation

2

Motivation

3

DEFFEM 3D software  
*(modules, design philosophy, modeling approach, solvers&postprocessor highlights)*

4

DEFFEM 3D software  
*(application examples)*

5

Conclusions & further work

**GOAL  
&  
MOTIVATION  
&  
DEFFEM 3D INTRODUCTION**



**Presentation of computing capabilities of in-house developed simulation software based on the Finite Element, Smoothed Particle Hydrodynamics and Monte Carlo methods.**

## MOTIVATION



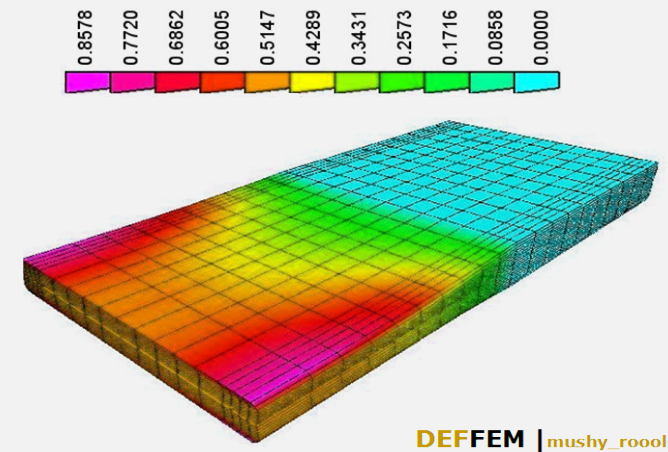
### Two important questions ?

..... the simulation systems developed will be effective and practical tools supporting the design of new technologies?

..... the alternatives, while maintaining the flexibility and adaptability possible solutions and methods developed into industrial practice?

### Problems & opportunities:

- verification in industrial conditions,
- thermo-mechanical data,
- high complexity of numerical models,
- simulation time,
- infrastructure,
- modern equipment (Gleeble, NANOTOM, GOM).



### Project:

*Development of software for the simulation of rolling steel in the semi-solid state*

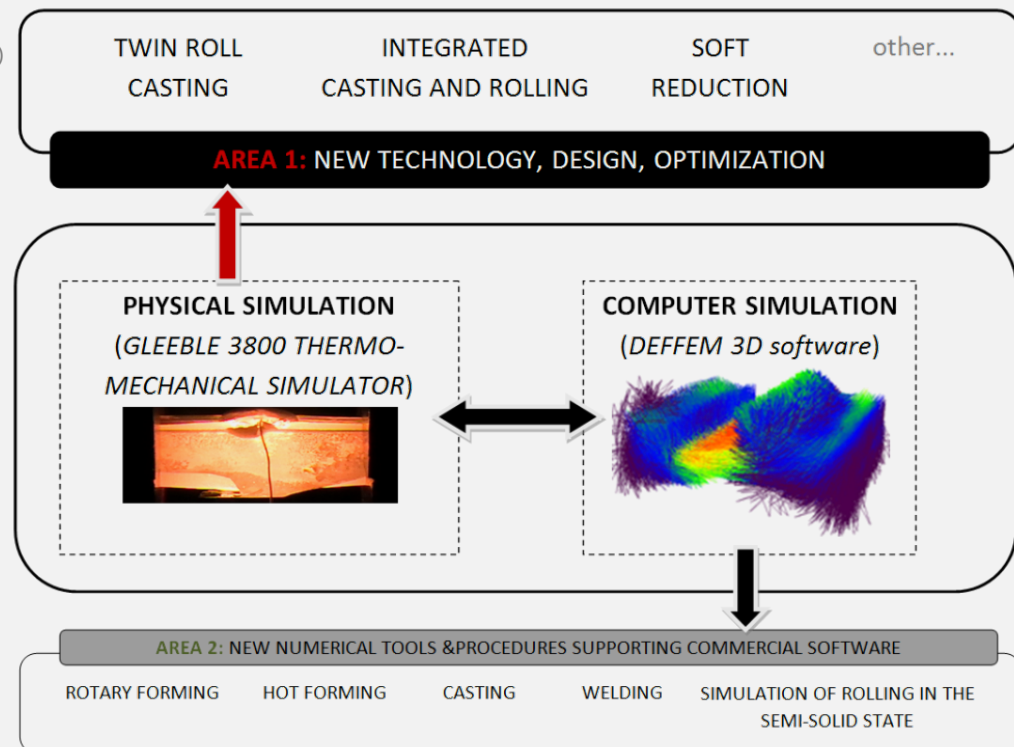
## MOTIVATION

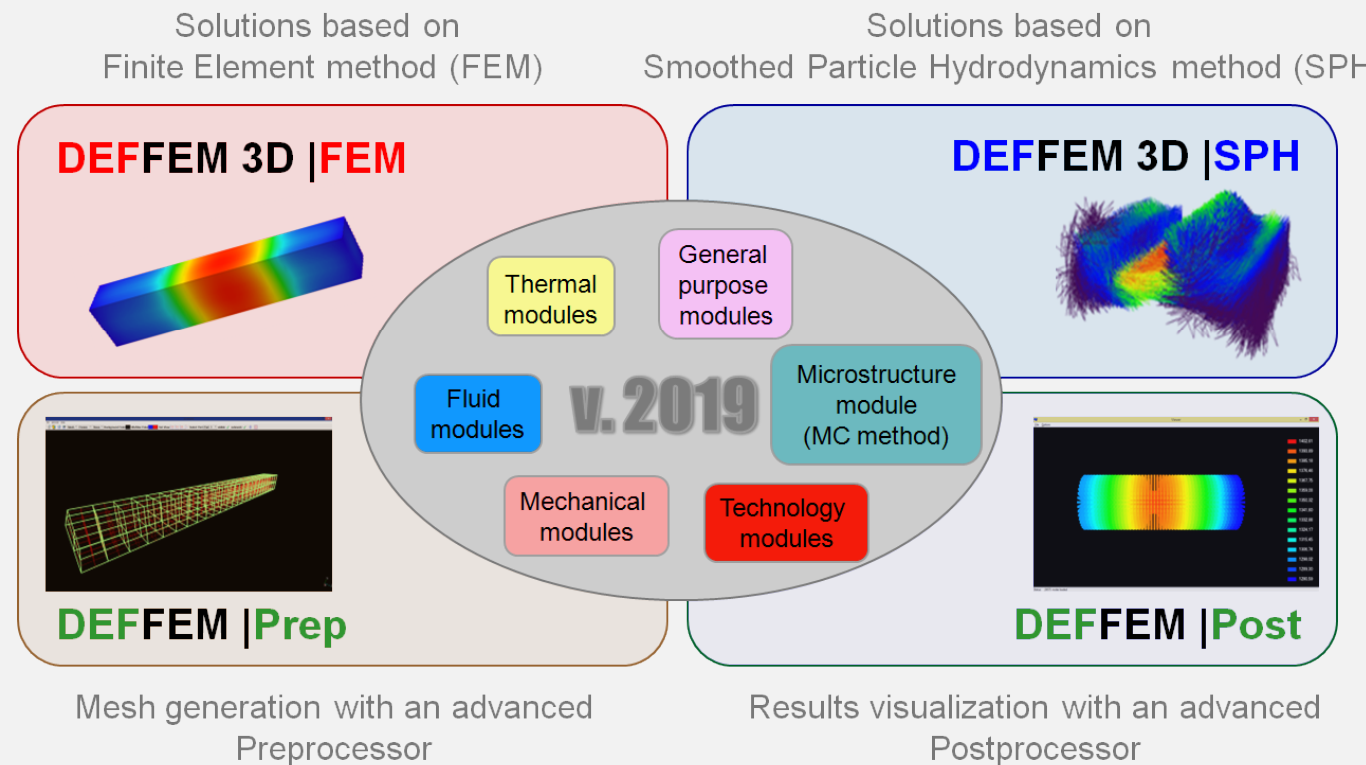
**1. CONCEPT** (integrated modeling methodology combining the advantages of physical and computer simulation)

**2. DESIGN** (from axial/2D to spatial solutions)

**3. IMPLEMENTATION** (scientific&industrial projects, 2009-till now)

highly adaptive numerical code  
=  
own codes, easy to use, easy to build a  
new dedicated simulation tools





- [illegible]

DEFFEM|Pre&Post Text editor

mest

control cards

Input deck

**KEYWORD STRUCTURE FOR SOLIDIFICATION SIMULATION (SPH 3D solver)**

```

*INCLUDE
61206 boundary.k
*INCLUDE
29791_particles.k
*SPH_PARTICLES
61206 29791 6930 30 1
*SPH_KERNEL
1 0.007
*SPH_EOS
1 0.05 0 7
*SPH_TIME
7 0.01
*SPH_TRANSFORM
0 0 0
0 0 0
*SPH_THERMAL_PROP
1412.42 1494.79 960.689 1264.274
303.585 0.68 0.811
*SPH_BOUNDARY_TEMP
20 1550
*SPH_MASS
0.001274385 0.000744386
*INITIAL_VELOCITY
0 0 0
0 0 0
*FUNCTION_INIT_ENTHALPY
0.811 51.756 3.686 -4245.206 0.68 0
0.811 51.756 3.686 -4245.206 0.68 0
*FUNCTION_INIT_DENSITY
-0.8048 8202.188 -4.0179 13053.13 -0.4657 8015.95
-0.8048 8202.188 -4.0179 13053.13 -0.4657 8015.95
*SPH_CONDUCTIVITY
-0.009 50.19
*SPH_FLAGS
0 0

```

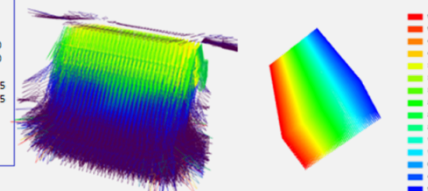
solver

**DEFEM|solver**

## results

DEFEM|Pre&Post

advanced visualization



```
Dr. Hojny Marcin  
Cell phone: +48 608 445 770  
email: mhojny@metal.agh.edu.pl
```

---

```
DEFFEM: A Program for Plastic Tests  
Analysis in the Gleeble 3800 equipment
```

Features enabled in this version:

- O: Fluid flow
- O: Thermal conductivity
- O: Solidification

---

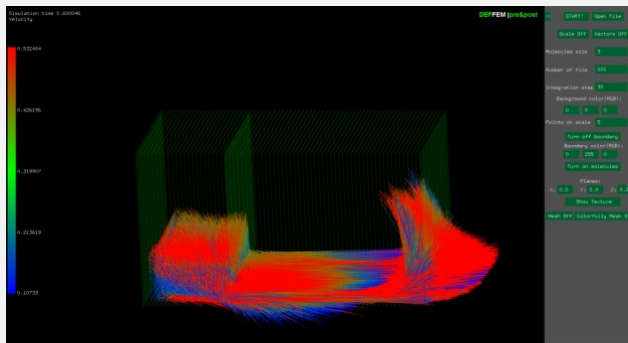
```
File main.k - opened  
Status keyword structure - OK!  
TOTAL SIMULATION TIME: 7.000000000000000000  
Boundary definition file - opened  
Status - OK!
```



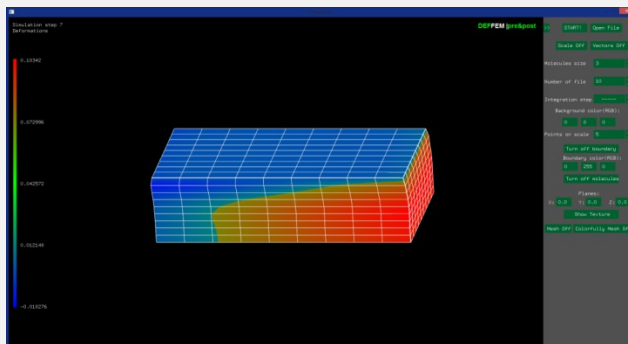
## DEFFEM 3D SOFTWARE



### HIGHLIGHTS (POSTPROCESSOR)



Fluid flow (vector velocity, *GLSL language*)



Forging (shading option, *OpenGL*)

- full vector visualization based on GLSL graphic pipeline programming language;



- isolines algorithms;

- stereoscopic algorithms (dedicated for BARCO Gemini system, microstructure 3D results analysis & mesoscale fluid flow);



- virtual reality GUI;



Virtual reality GUI (Gleeble 3800 simulator – full feedback with DEFFEM 3D)

### HIGHLIGHTS (SOLVERS)

01

#### MODIFIED RIGID-PLASTIC MODEL

A high accuracy in fulfilling the constant or controlled volume condition is required in the proposed solution. This approach arises from the fact, that errors caused by not fulfilling these conditions may be comparable with the volume changes caused by the variable metal density in the mushy zone. Also because of large differences in the yield stress for individual sub-areas of the deformation zone, which in the temperature range in question are caused by even slight temperature fluctuations, and related difficulties in meeting the non-compressibility condition, this condition was included in the analytical form, which makes the solution more complicated, but substantially improves its accuracy.

02

#### FUNCTIONAL MODEL OF RESISTANCE HEATING

The heat source efficiency in the model is a function of resistance, which in turn depends on temperature and special function which represents intensify of heating.

03

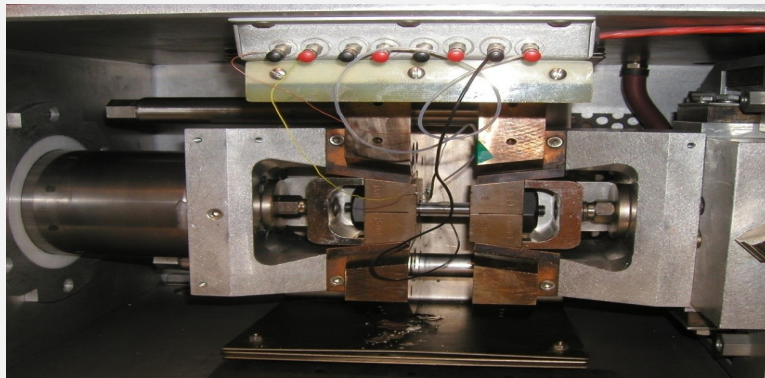
#### MICRO GRAIN-GROWTH MODEL

Considering the temperature gradient on the intensity of grain growth during **heating-melting-cooling (complex cycle)** process (scaling function).

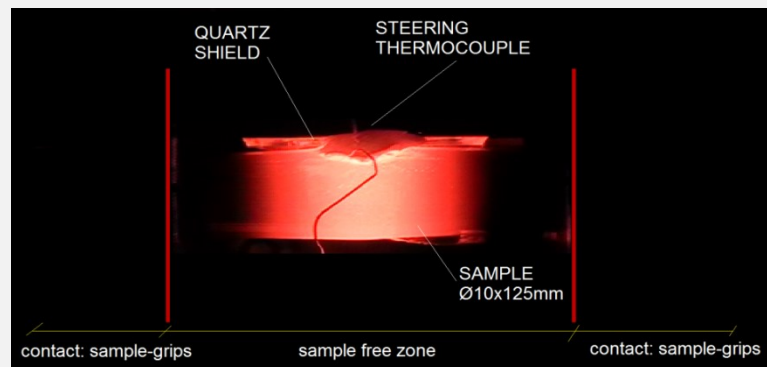
# APPLICATION EXAMPLES

## DEFFEM 3D SOFTWARE

### EXPERIMENT SUPPORT



*The experimental equipment of Gleeble 3800 simulator*



*Simulation of resistance heating (S355 grade steel)*

Materials testing and processes:

- mechanical properties (mushy-zone),
- melting and solidification,
- continuous casting,
- hot rolling,
- forging,
- extrusion,
- heat treatment,
- welding and so on....

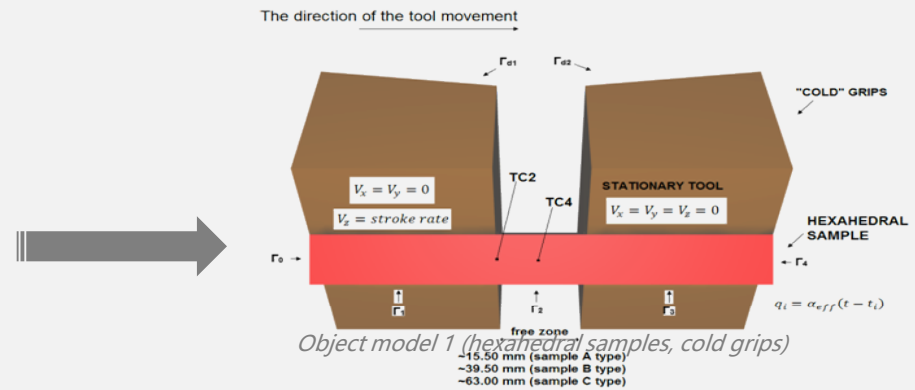
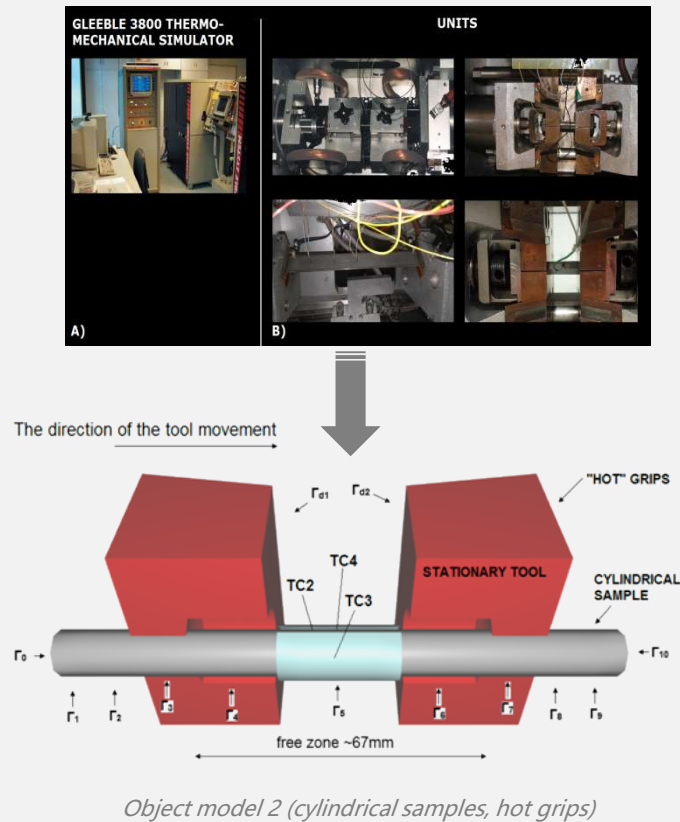
The essential aim of the simulation was the reconstruction (on a small sample) the changes of temperature and stress for material which was subjected deformation in conditions similar to industrial process.



In this case, the exact response of the material to the applied loads is precisely recorded, which is not possible directly during real production.

# DEFFEM 3D SOFTWARE

## EXPERIMENT SUPPORT



Object model includes:

- die/grips geometry&configuration (mesh),
- sample geometry (mesh),
- boundary conditions (thermal&mechanical),
- initial conditions,
- thermocouples locations (numerical sensors),
- steering parameters & functions.

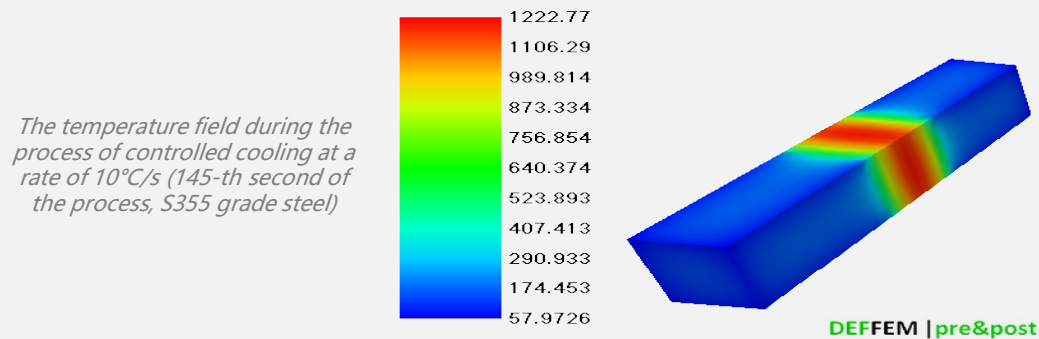
# DEFFEM 3D SOFTWARE



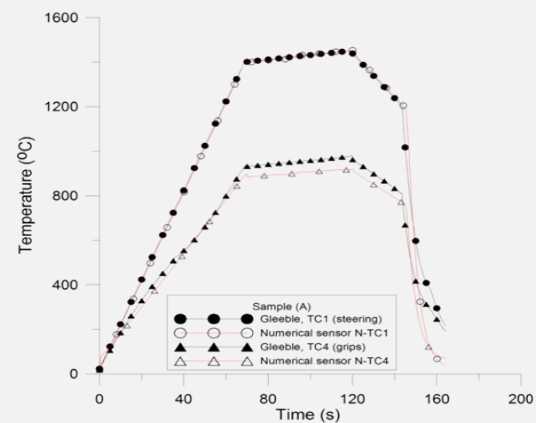
## 01: EXPERIMENT SUPPORT

### RESISTANCE HEATING

Heating-melting-cooling simulation process.



Changes in temperatures obtained by physical and numerical simulations according to the readings of thermocouples and numerical sensors



Heating velocity 5° C/s						
TC4, [° C]	100	300	500	800	1200	1440
TC3, [° C]	106.22	308.96	509.32	816.14	1226.81	1481.89
TC3-TC4, [° C]	6.22	8.96	9.32	16.14	26.81	41.89
Heating velocity 10° C/s						
TC4, [° C]	100	300	500	800	1200	1440
TC3, [° C]	104.15	308.15	508.75	815.07	1226.56	1482.45
TC3-TC4, [° C]	4.14	8.15	8.75	15.07	26.56	42.45
Heating velocity 20° C/s						
TC4, [° C]	100	300	500	800	1200	1440
TC3, [° C]	105.68	305.40	507.37	816.32	1226.22	1482.13
TC3-TC4, [° C]	5.68	5.40	7.37	16.32	26.22	42.13

Experiment (measured temperatures)

Heating velocity 5° C/s						
NTC4, [° C]	100	300	500	800	1200	1440
NTC3, [° C]	102.08	306.96	511.42	818.41	1227.52	1473.03
NTC3-NTC4, [° C]	2.08	6.96	11.42	18.41	27.52	33.03

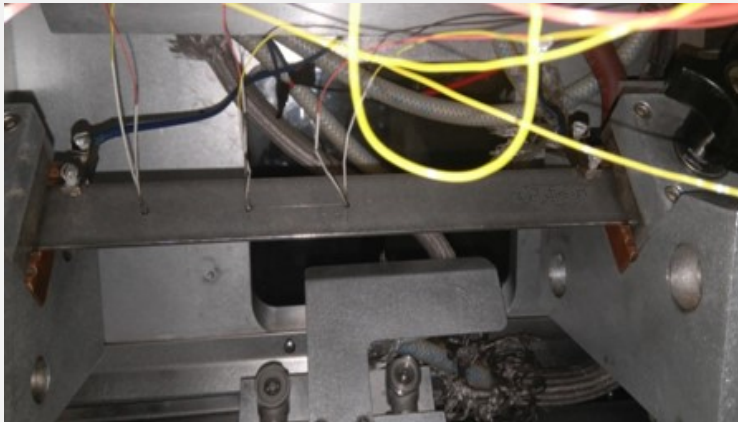
Simulation (calculated temperatures)

## DEFFEM 3D SOFTWARE

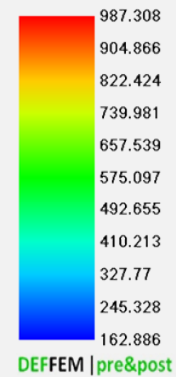
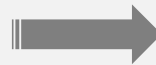
### 01: EXPERIMENT SUPPORT

#### RESISTANCE HEATING

Heating-melting-cooling simulation process.



*Resistance heating of the sheet in the simulator Gleeble equipment*



*Temperature distribution after resistance heating  
(Inconel 718, heating velocity 10°C/s)*

Temperature reached during experiment: **999°C**

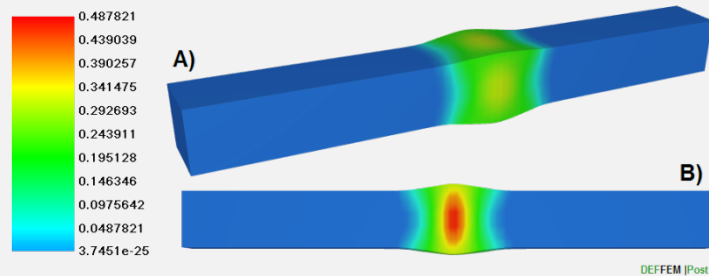
Calculated temperature: **987°C**

## DEFFEM 3D SOFTWARE

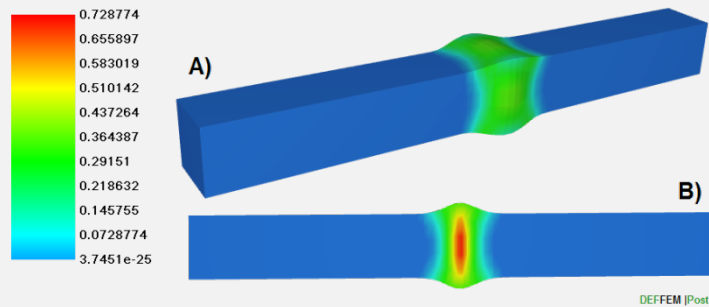
### 02: EXPERIMENT SUPPORT

#### DEFORMATION

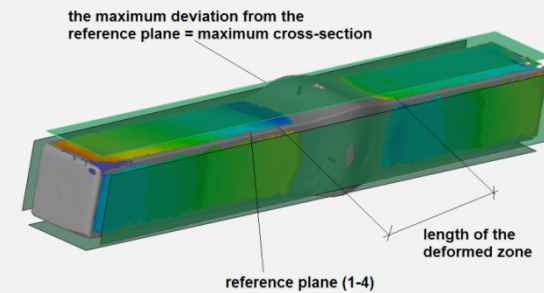
Deformation in the semi-solid state.



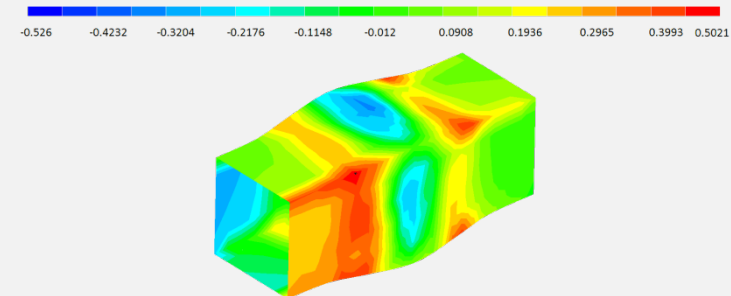
Strain intensity field distribution after deforming the sample at 1300°C  
(A/whole sample view, B/longitudinal section, S355 grade steel)



Strain intensity field distribution after deforming the sample at 1435°C  
(A/whole sample view, B/longitudinal section, S355 grade steel)



Methodology of measurement of the deformation zone executed  
with the ATOS Triple Scan photogrammetric system



Comparison of the 3D virtual geometry of the deformation zone received  
by numerical calculations and the experiment (T=1300°C)

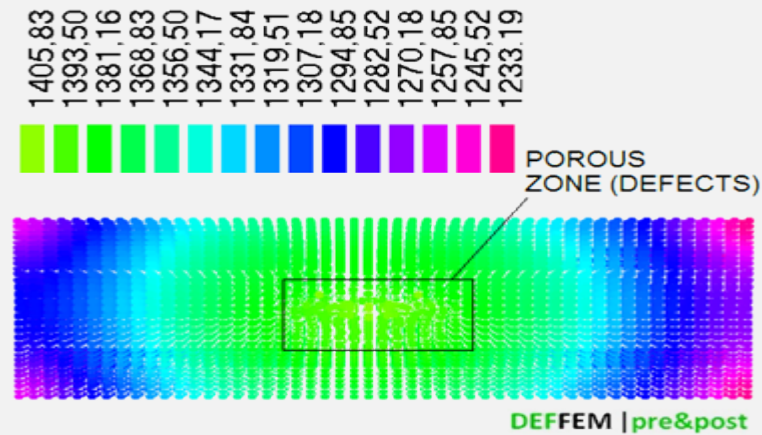


## DEFFEM 3D SOFTWARE

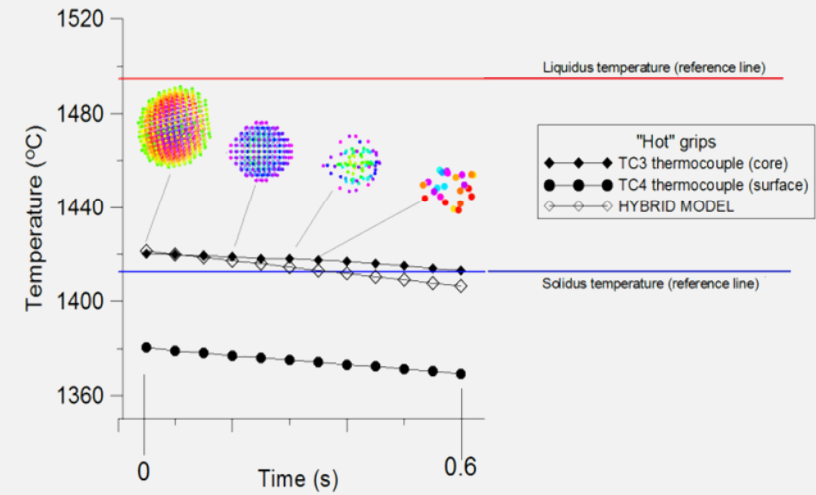
### 03: EXPERIMENT SUPPORT

#### SOLIDIFICATION

Hybrid solutions (FE+SPH). Heating-melting-cooling simulation process with local flow of liquid steel.



Particle temperature distribution in the longitudinal-section of the sample after completion of the solidification process with visible possible porous zone (defects) within the sample (C45 grade steel)

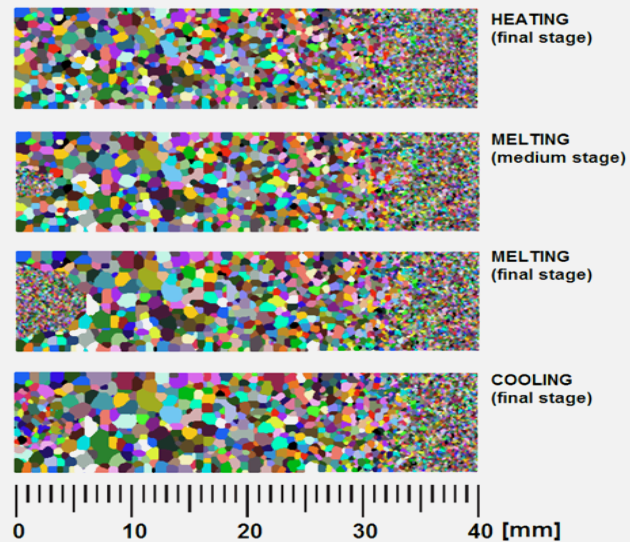


Temperature change vs. time (experiment and hybrid model, solidification stage)

### 04: EXPERIMENT SUPPORT

#### GRAIN GROWTH

Grain growth simulation with boundary mobility function. Resistance heating combined with the melting and controlled cooling of steel samples.



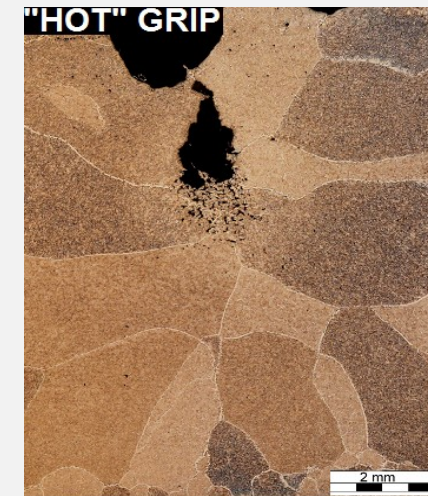
*Virtual macrostructure of the sample in the longitudinal section  
in the sample axis for the selected four process stages  
(second degree boundary mobility function, S355 grade steel)*

#### SIMULATION



*Macrostructure after heating the sample to the nominal test temperature of 1450°C  
and cooling at 1° C / s („hot” grips, S355 grade steel)*

#### EXPERIMENT



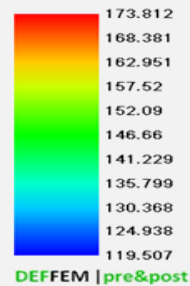
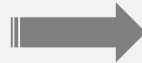
## DEFFEM 3D SOFTWARE



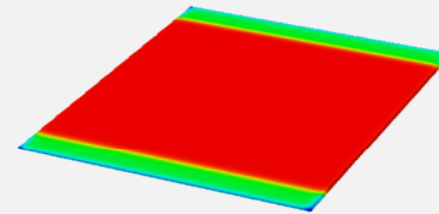
### 01: INDUSTRIAL IMPLEMENTATIONS

#### HOT FORMING (RESISTANCE HEATING OF THE BLANK)

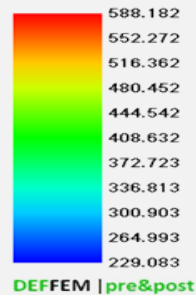
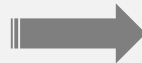
Support in the design of hot forming technology for the strengthening of the intermediate hull directing airflow in a jet engine.



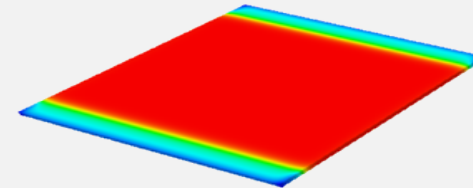
Temperature achieved during the industrial test: **181 °C**  
Calculated temperature: **173 °C**



Inconel 625



Temperature achieved during the industrial test: **603 °C**  
Calculated temperature: **588 °C**



Inconel 625

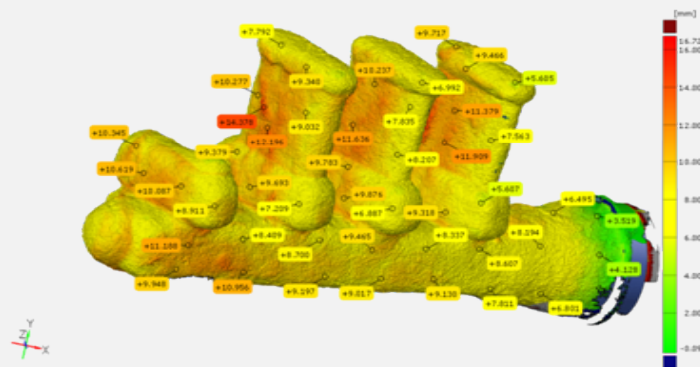
## DEFFEM 3D SOFTWARE

### 02: INDUSTRIAL IMPLEMENTATIONS

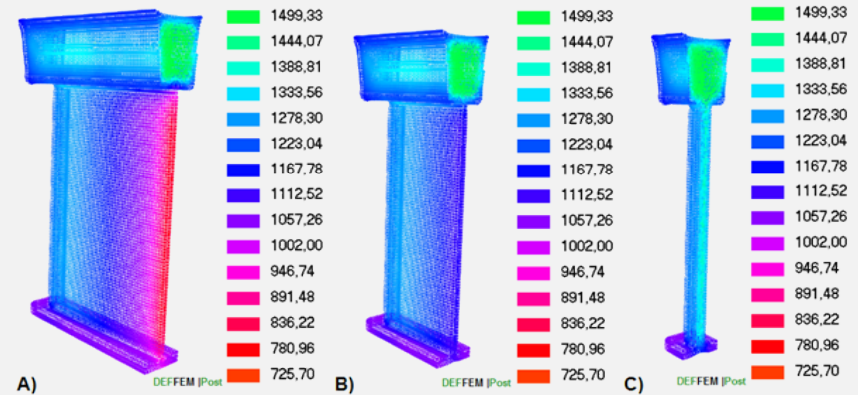
#### CASTING

Simulations of casting in ceramic molds obtained using the lost wax method.

Application of the DEFFEM 3D package in computer-aided design of casting critical parts of aircraft engines.



*The map of real thickness of the mould obtained in mapping the 3D scans of the ceramic mould and the wax system*



*The temperature field distribution in chosen cross-sections of the blade (section by the X plane)*

**An innovative feature of the solution is the coupling of the SPH solver based of the DEFFEM package with 3D scanning systems.** The proposed solution will allow the numerical calculations to take into account the actual geometry of the mold for variable thickness distribution on the cross-section of the ceramic mold wall.

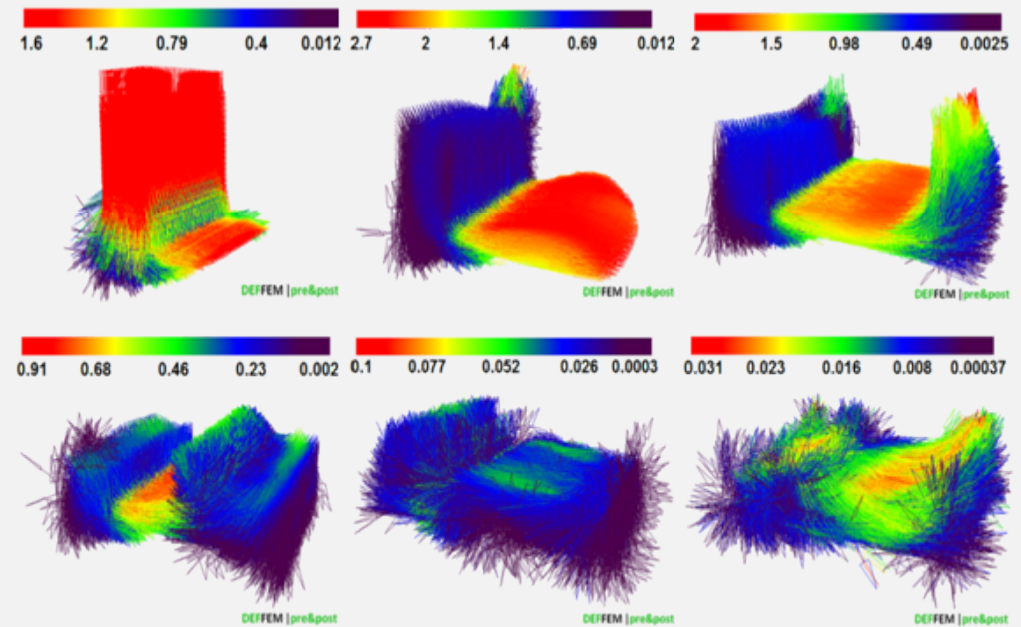
## DEFFEM 3D SOFTWARE

### 03: INDUSTRIAL IMPLEMENTATIONS

#### FLUID FLOW

Fluid flow simulation with optional thermal effect.

*brake fluid reservoir*



*Velocity distribution (selected stages of test simulation, one chamber)*

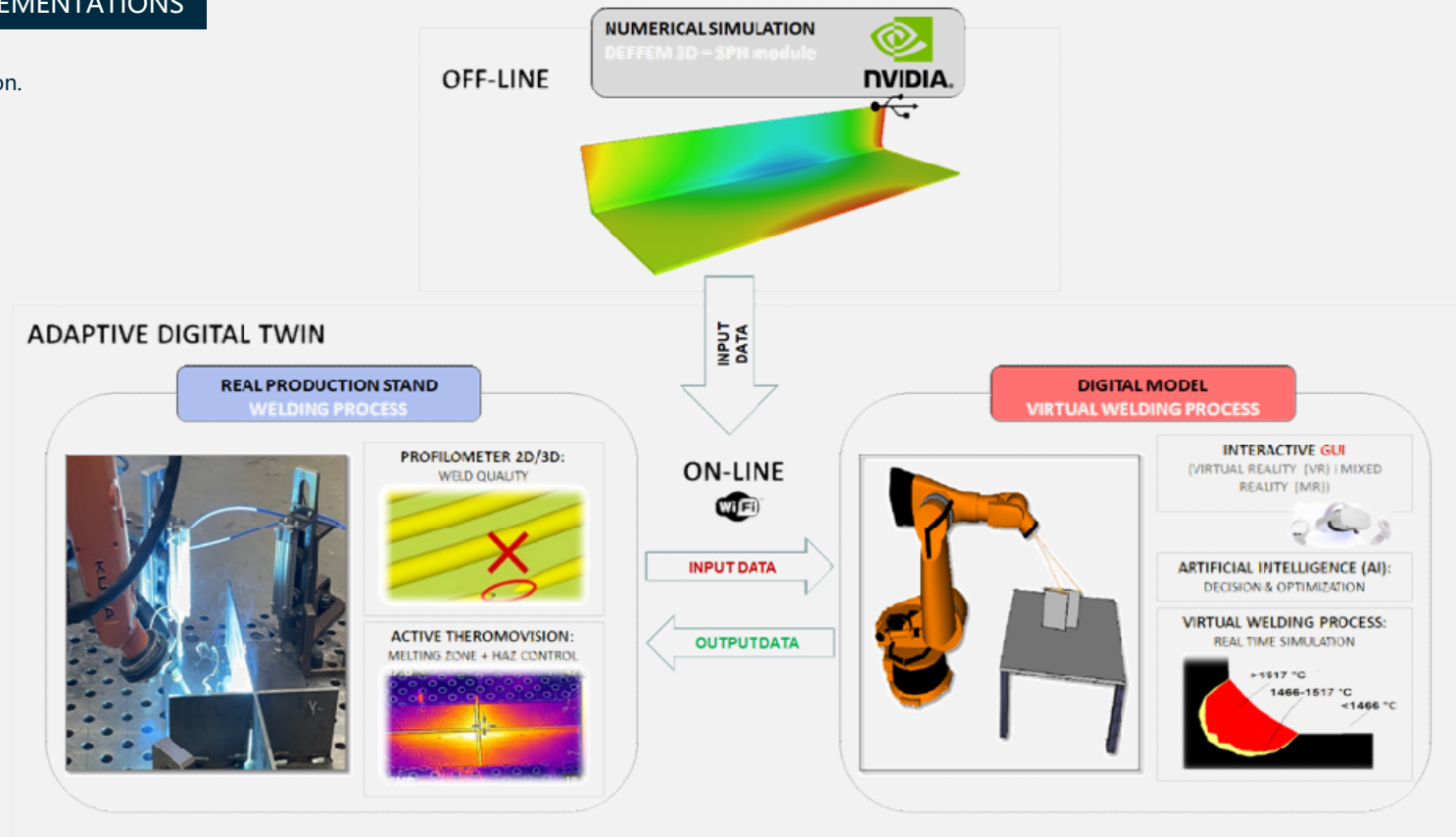


## DEFFEM 3D SOFTWARE

### 04: INDUSTRIAL IMPLEMENTATIONS

#### WELDING

Melting zone + HAZ prediction.



## CONCLUSIONS AND FURTHER WORK

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1. The developed methods and numerical tools, combined with the capabilities of modern thermo-mechanical simulators of the Gleeble series, allow theoretical support for the design of new technologies.
2. The modular structure of the source code allows the development of new solutions (quickly, easily).
3. Directions for further work in the area of software development (the most important):
  - *automatic 3D contact algorithm (3D solver based on FEM),*
  - *friction model (3D solver based on FEM),*
  - *grouping of particles, group flow during the solidification process (3D solver based on SPH),*
  - *source code adaptation (CUDA Fortran architecture).*





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