# Modelling microstructure and mechanical properties of cast iron

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# Outline

1. Introduction and main objectives
2. (Part of the) physics of the solidification
3. Simulation procedure (Courtesy of Fonderia Casati Spa, Italy)
4. Example 1: part cooled in the mould vs. part with mould shake out (Courtesy Caterpillar Inc., USA)
5. Example 2: graphitisation and porosity (courtesy of Furesa and Azterland, Spain)
6. What we have learned

# Introduction and main objectives

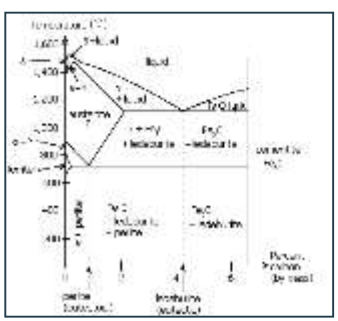
- Introduction
- Main objectives
  - To go through some aspects of the relations between alloy, microstructure and material properties
  - To present the modelling technique of the microstructure
  - To present examples of industrial applications

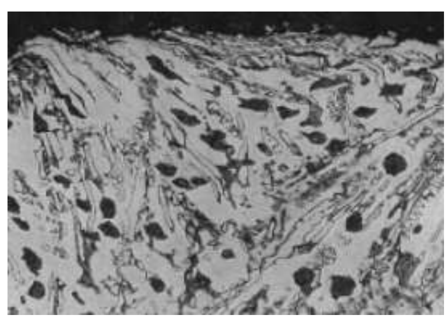
# Alloys, microstructure and material properties

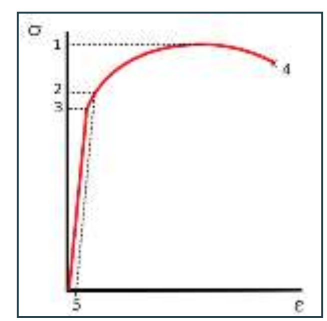
Process parameters: cooling rate, melt treatment

Volume fractions of the phases, grain size, grain shape

Alloy composition → Microstructure → Mechanical properties







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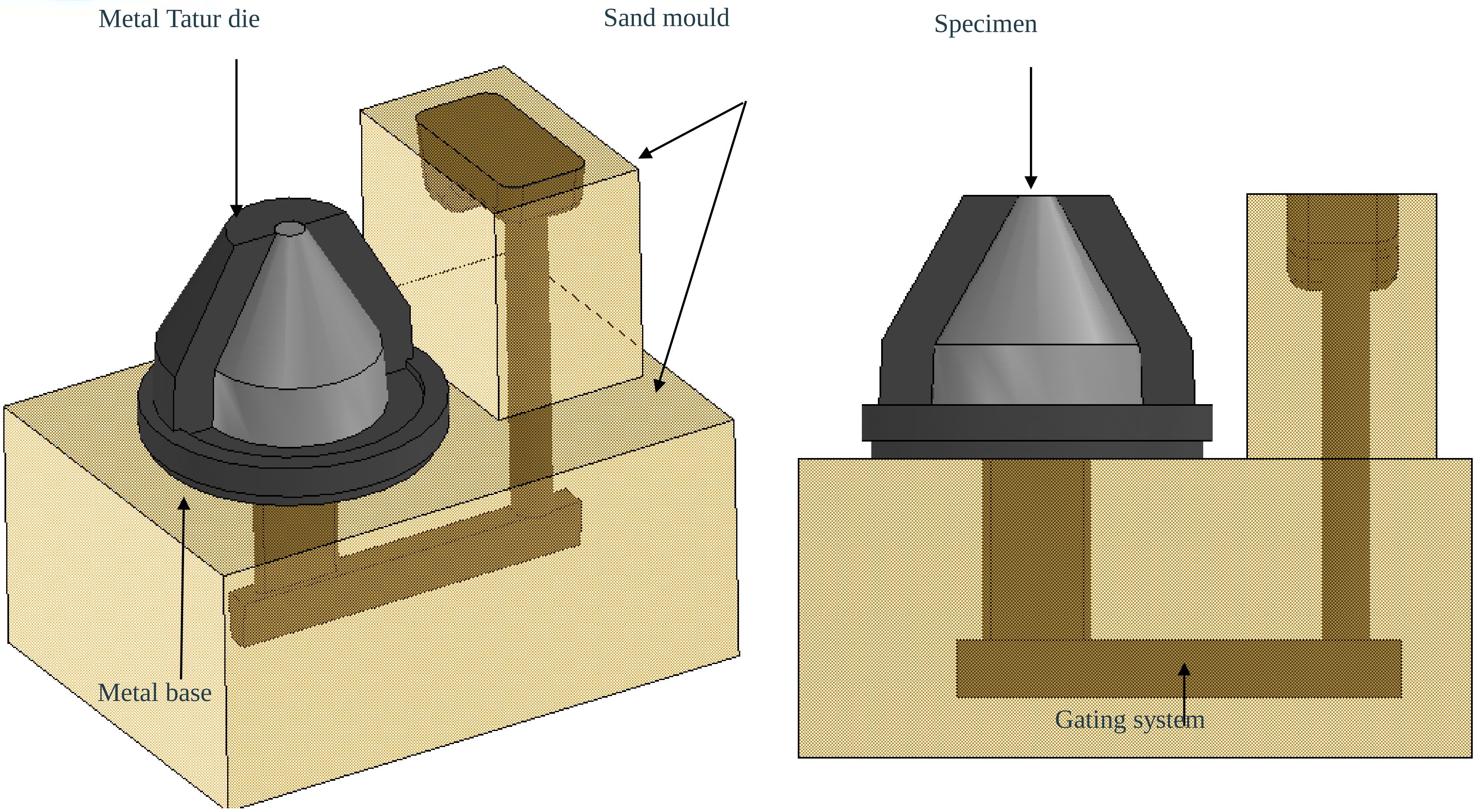
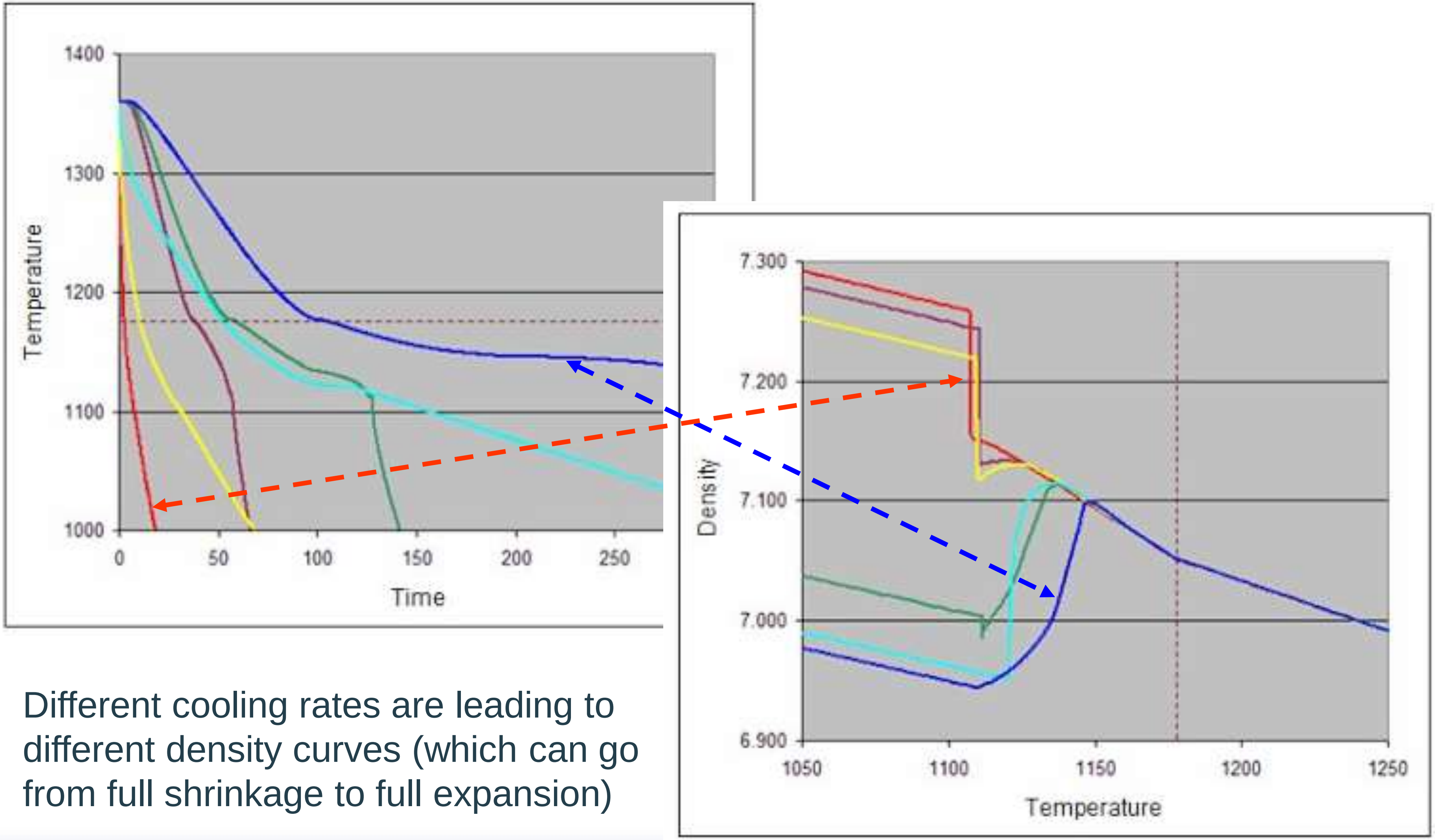
# Experimental device

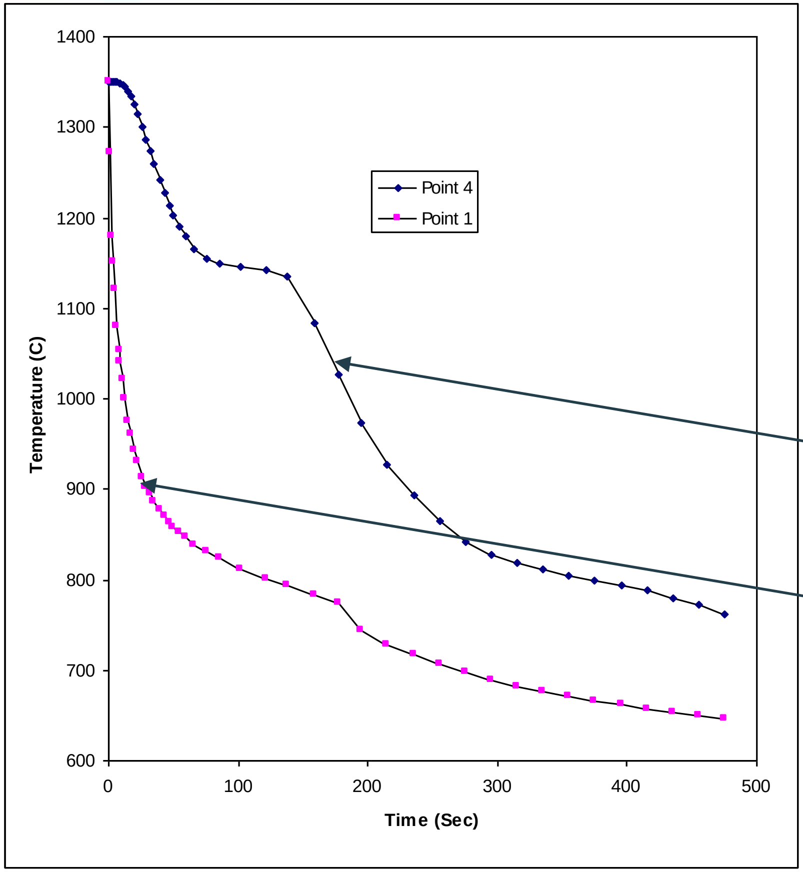


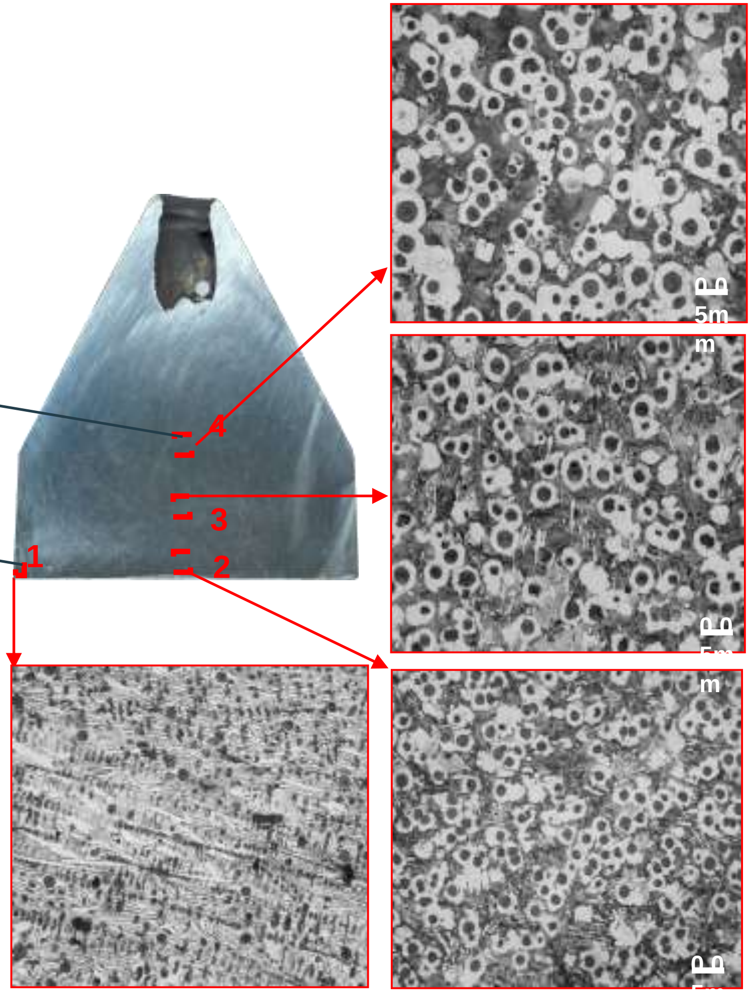
# Local cooling history




Different cooling rates are leading to different density curves (which can go from full shrinkage to full expansion)

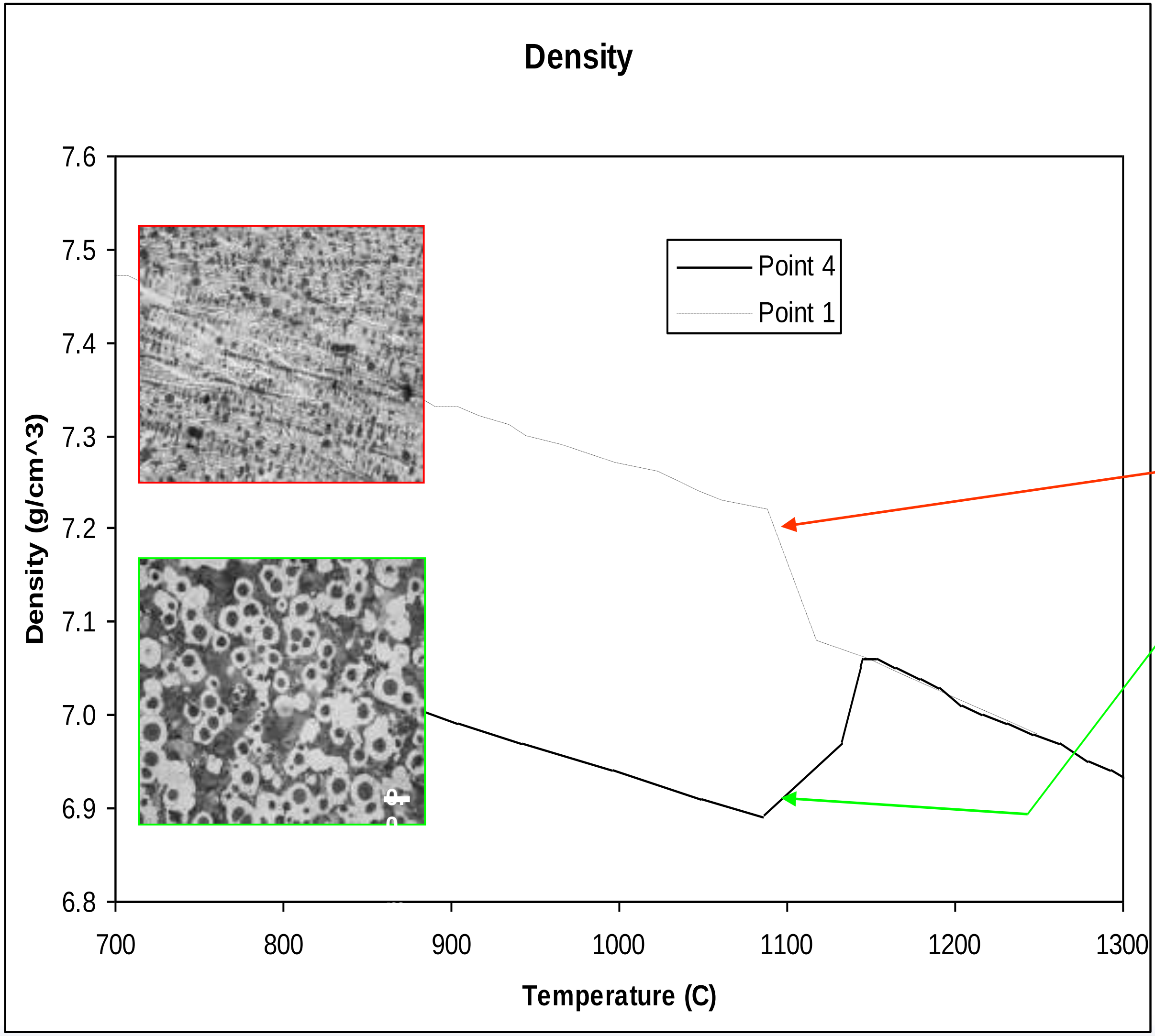
# Microstructure and local cooling rates

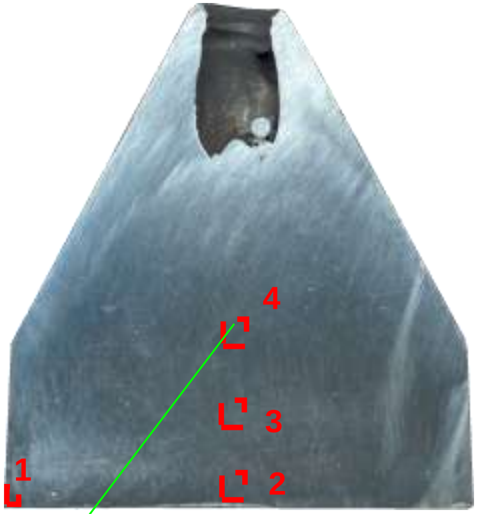



Cooling at point 1 is much faster than that at point 4. This is the reason why there are a lot of metastable phase formed at point 1.

# Microstructure and variations of density

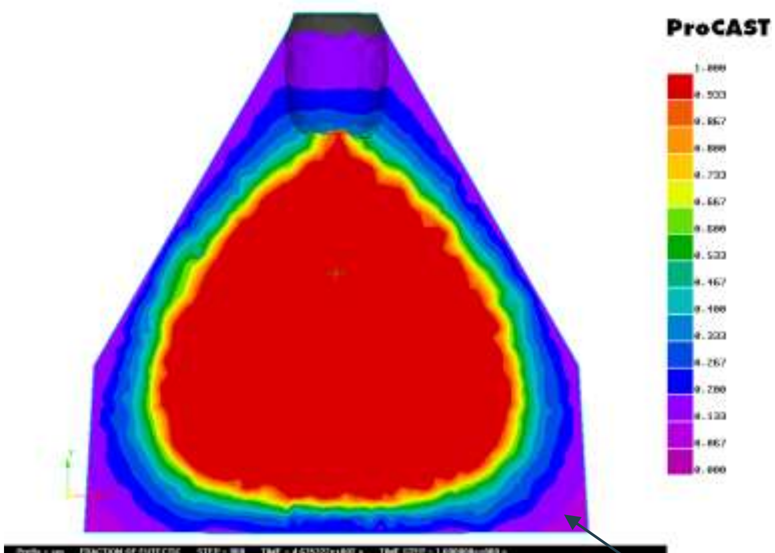


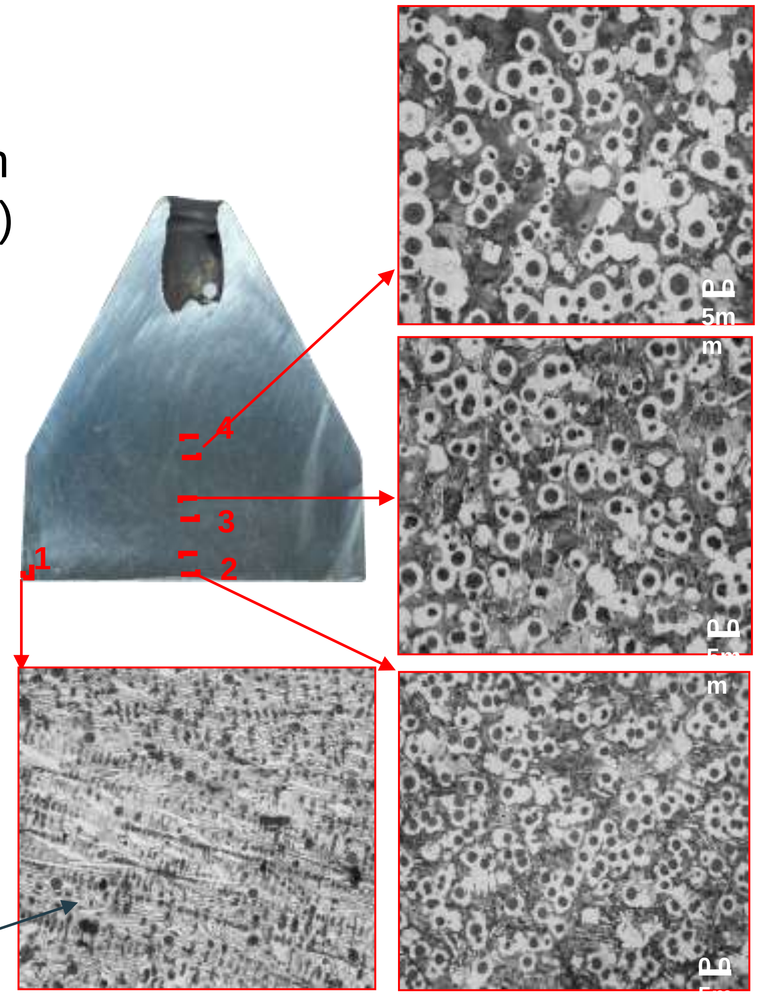

There is no expansion at the location where there are a lot of metastable phase (point 1)

# Microstructure

Because of the high cooling at the corner of the casting, there is big amount of metastable phase (Ledeburite) formed which has different density variation (no expansion)

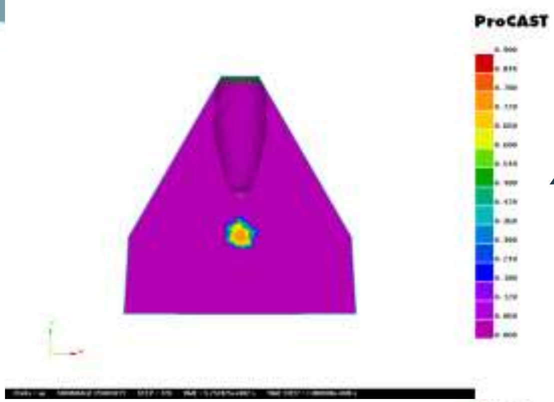



Fraction of stable phase

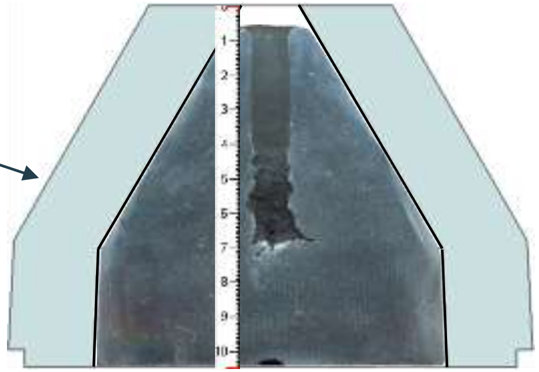



Ledeburite

# Piping

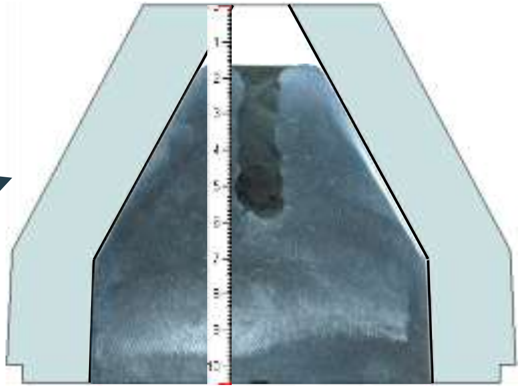


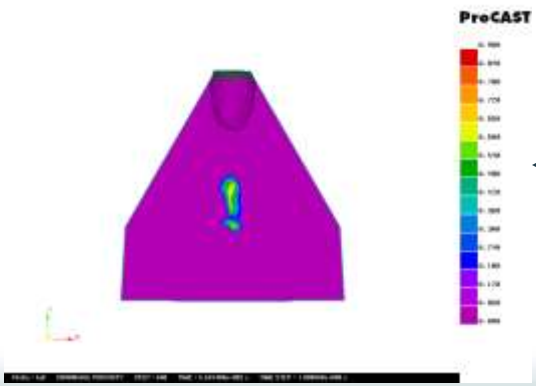

uninoculated

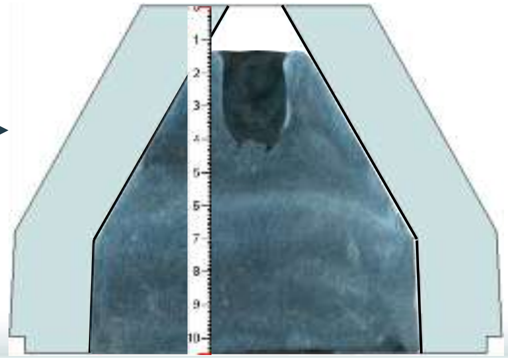
Without micro modeling

Inoculation – 0.15%






Inoculation – 0.4%



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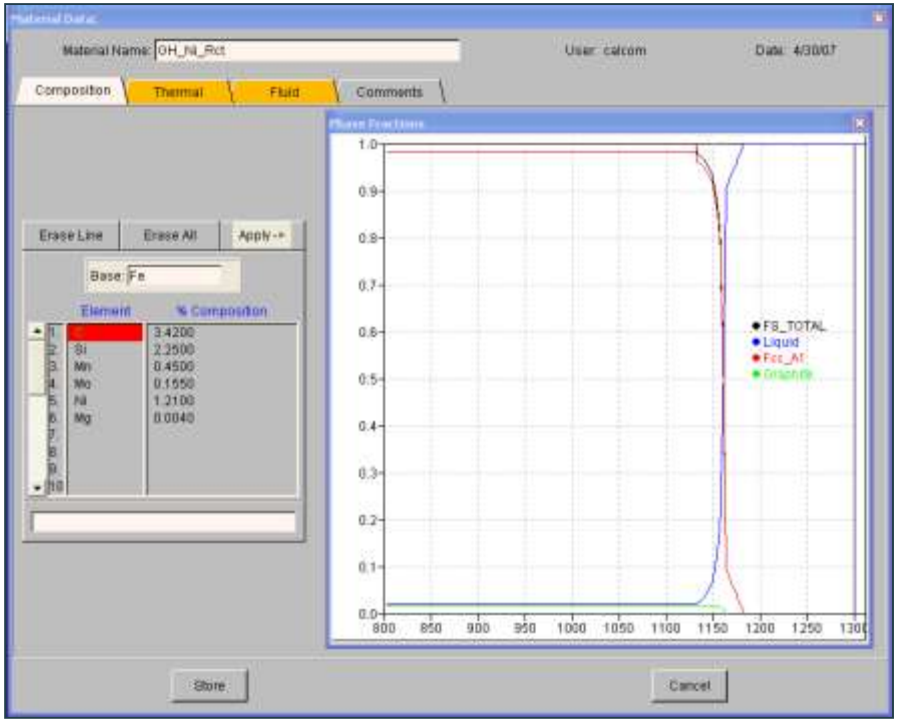
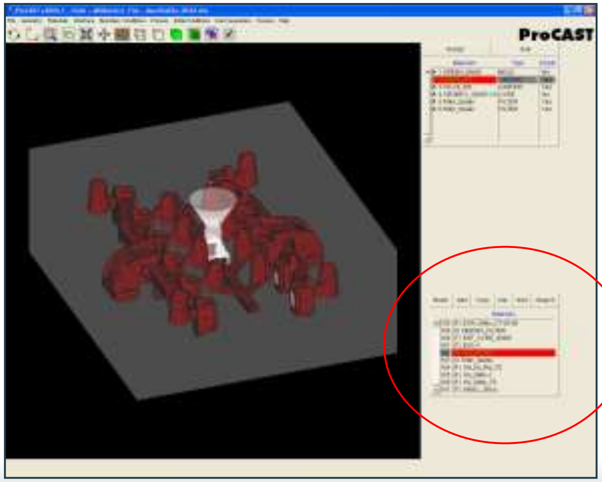
# Link with thermodynamic database

- Microstructure can be calculated on the base of the chemical composition of the alloy
- This can be achieved with the link of the module with thermodynamic databases

**Alloy composition and computation fractions of phases**

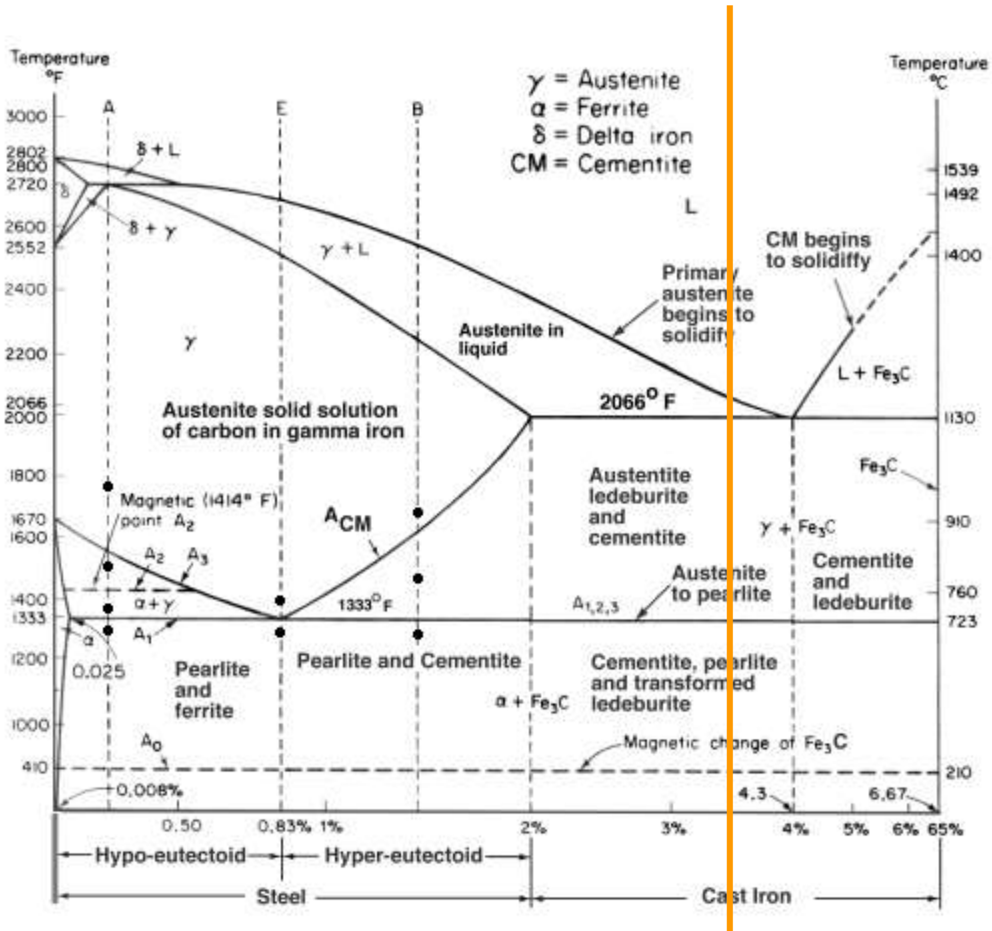



**Assignment of material properties with link to the material database**




Example of a model set-up for simulation with corresponding alloy composition, phases fractions vs. temperature

# Microstructure




Base: Fe

| | Element | % Composition |
|---|---|---|
| 1. | C | 3.4200 |
| 2. | Si | 2.2500 |
| 3. | Mn | 0.4500 |
| 4. | Mo | 0.1550 |
| 5. | Ni | 1.2100 |
| 6. | Mg | 0.0040 |

**CE= 4.1 (Hypo-eutectic alloy)**

**Automatically computed**

**MICRO Output**

- Primary Dendrite Radius
- Primary Solid Fraction
- Secondary Dendrite Arm Spacing
- Nodule Count
- Austenite Radius
- Graphite Radius
- Fraction of Eutectic
- Fraction of Metastable Phase
- Pearlite Spacing
- Tensile Strength
- Yield Strength
- Elongation
- Brinell Hardness
- Fraction of Ferrite
- Fraction of Pearlite
- Density

# Microstructure

***Dendritic primary phase and eutectic secondary phase***

- Primary Dendrite Radius
- Primary Solid Fraction
- Secondary Dendrite Arm Spacing
- Eutectic Grain Radius
- Fraction of Eutectic
- Eutectic Inter-lamellar Spacing

***Special case of Fe-C alloys - nodular cast iron (eutectic composition)***

- Nodule Count
- Austenite Radius
- Graphite Radius
- Fraction of Eutectic
- Pearlite Spacing
- Tensile Strength
- Yield Strength
- Elongation
- Brinell Hardness
- Fraction of Ferrite
- Fraction of Pearlite

***Special case of Fe-C alloys - grey iron (lamellar eutectic)***

- Primary Dendrite Radius
- Primary Solid Fraction
- Secondary Dendrite Arm Spacing
- Fraction of Eutectic
- Fraction of Metastable Eutectic
- Eutectic Grain Radius
- Metastable Eutectic Grain Radius
- Eutectic Inter Lamellar Spacing
- Pearlite Spacing
- Tensile Strength
- Yield Strength
- Brinell Hardness
- Fraction of Ferrite
- Fraction of Pearlite

***Special case of Fe-C alloys - nodular cast iron (hypo-eutectic composition)***

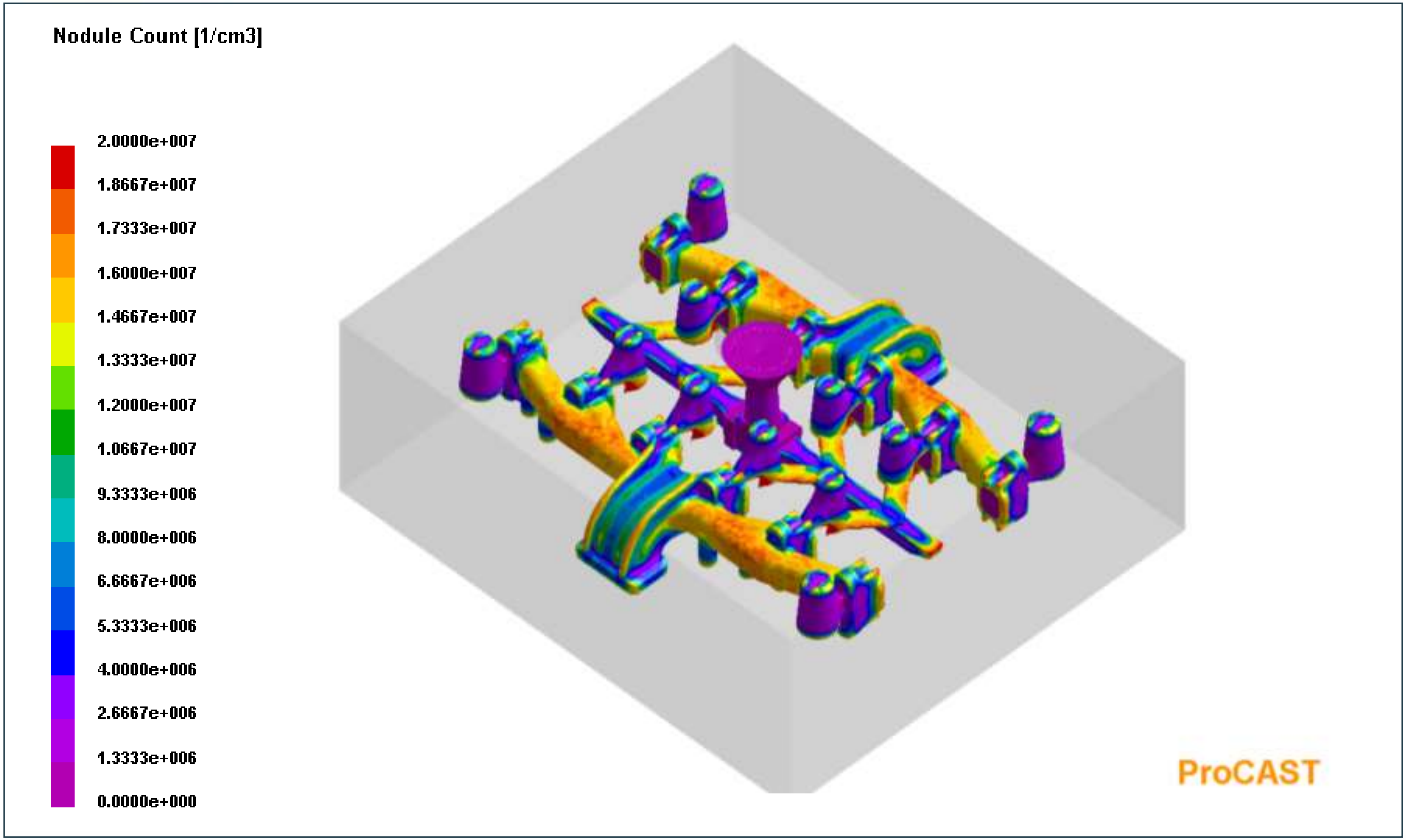
- Primary Dendrite Radius
- Primary Solid Fraction
- Secondary Dendrite Arm Spacing
- Nodule Count
- Austenite Radius
- Graphite Radius
- Fraction of Eutectic
- Pearlite Spacing
- Tensile Strength
- Yield Strength
- Elongation
- Brinell Hardness
- Fraction of Ferrite
- Fraction of Pearlite

***Special case of Fe-C alloys - steel***

- Primary Dendrite Radius
- Primary Solid Fraction
- Secondary Dendrite Arm Spacing
- Fraction of Peritectic
- Fraction of Eutectoid
- Fraction of Proeutectoid

Type of results is different depending on the alloy composition

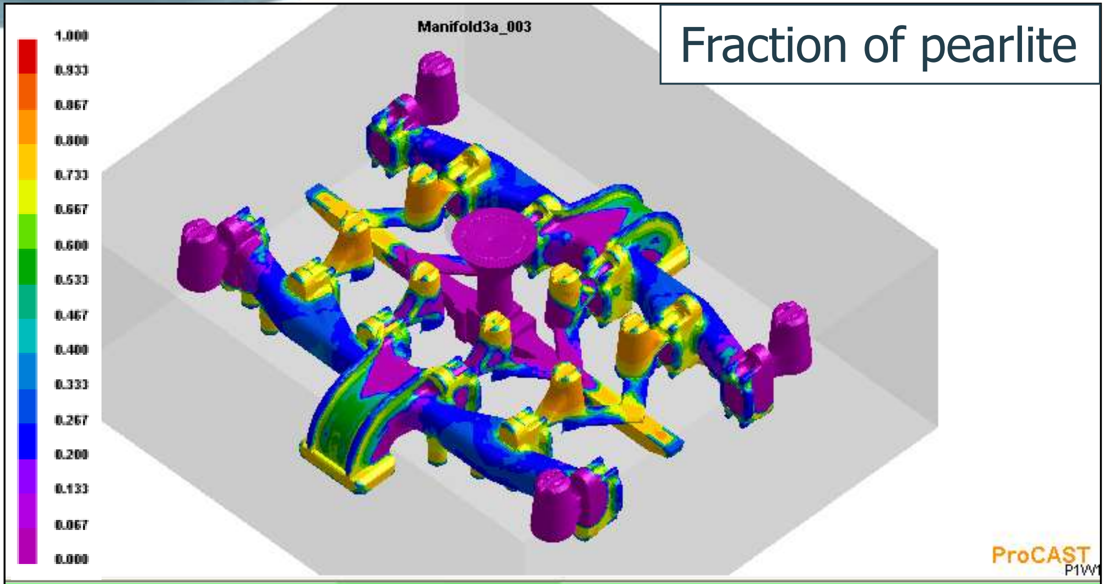
# Nodule count



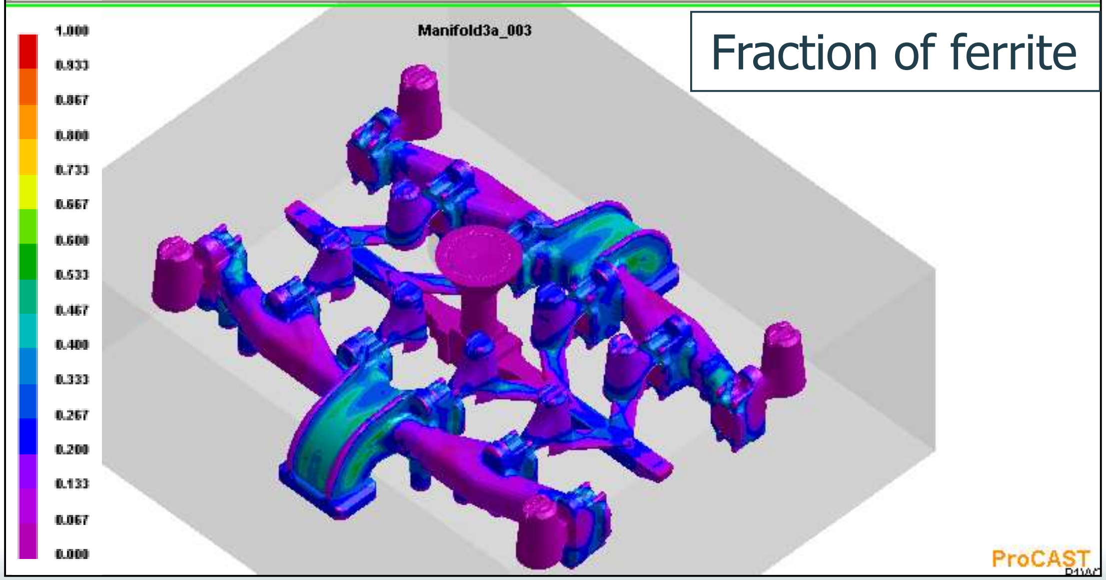



Courtesy of

# Instantaneous distributions of fractions of pearlite and ferrite
## with corresponding temperature distribution

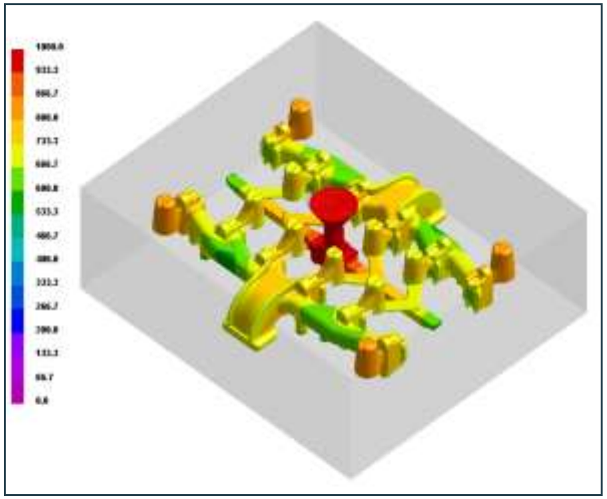



Fraction of pearlite




Fraction of ferrite

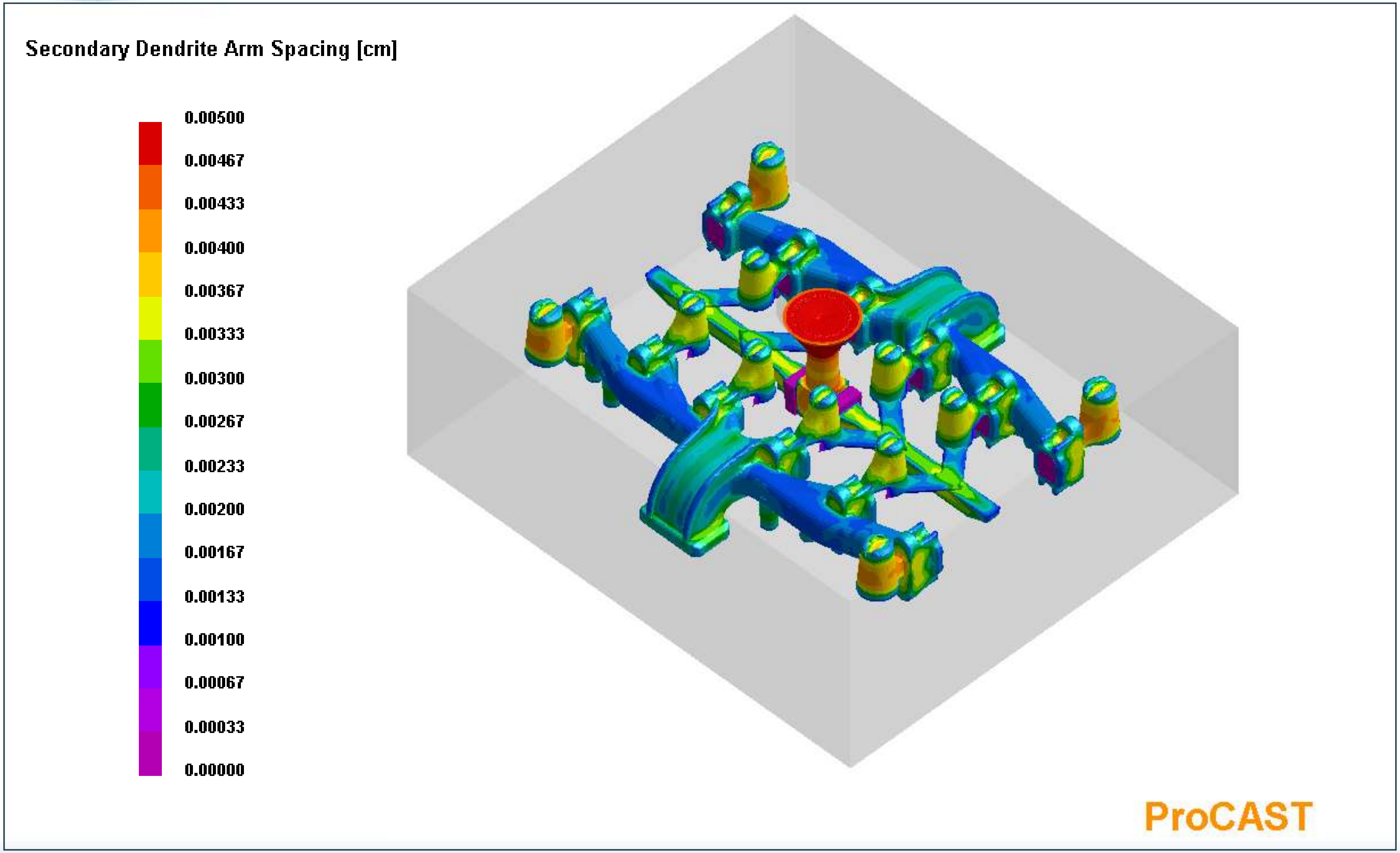
Temperature range is 500 – 700°C





Courtesy of

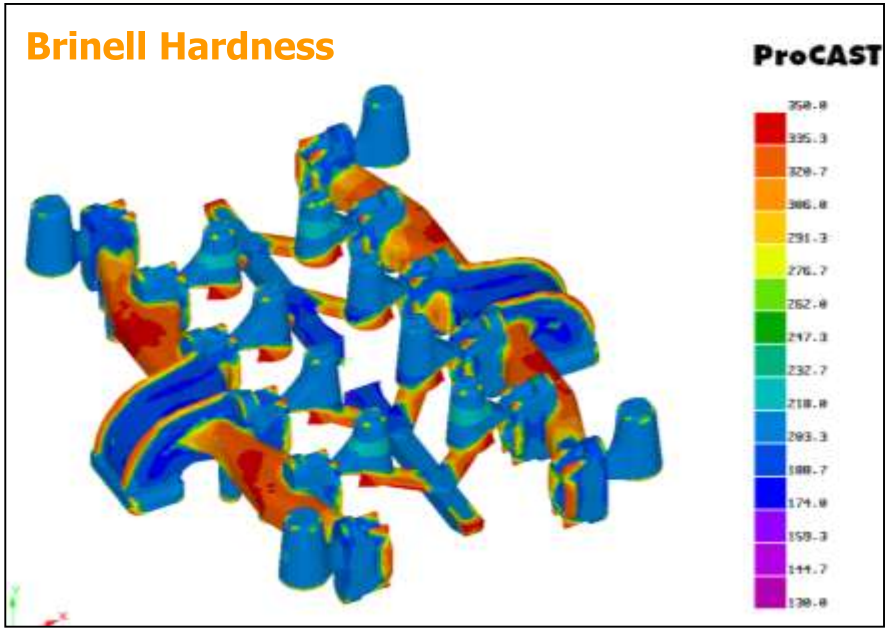
# Secondary dendrite arm spacing

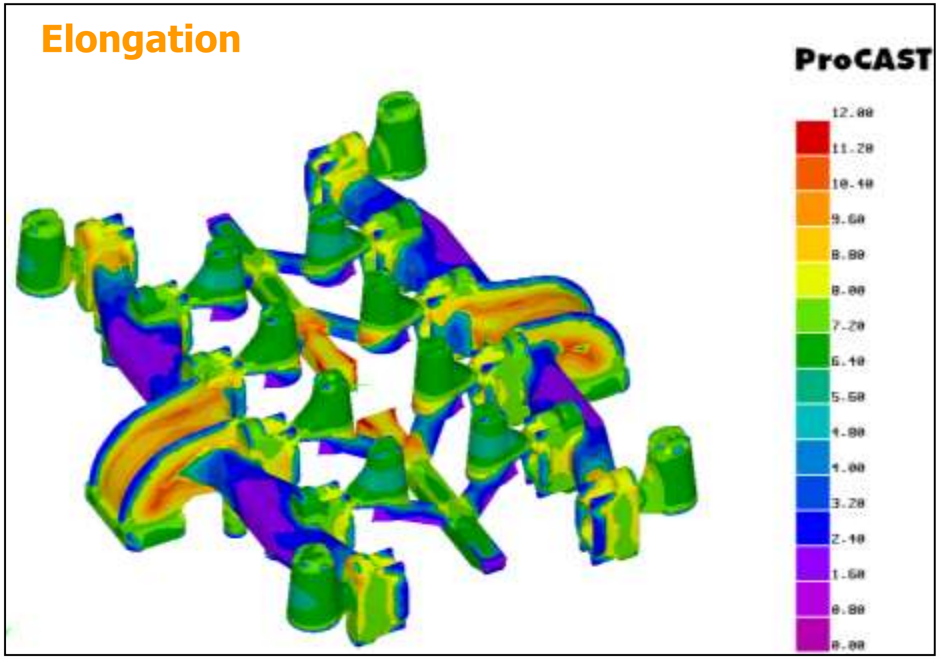





Courtesy of

# Microstructure → Mechanical Properties



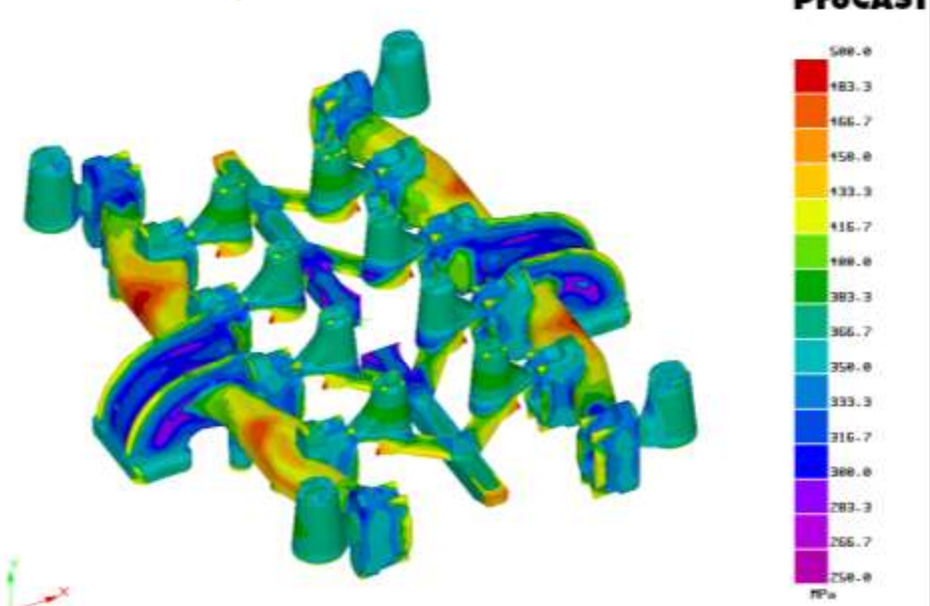

**Temperature in the range of 300°C and 500°C**



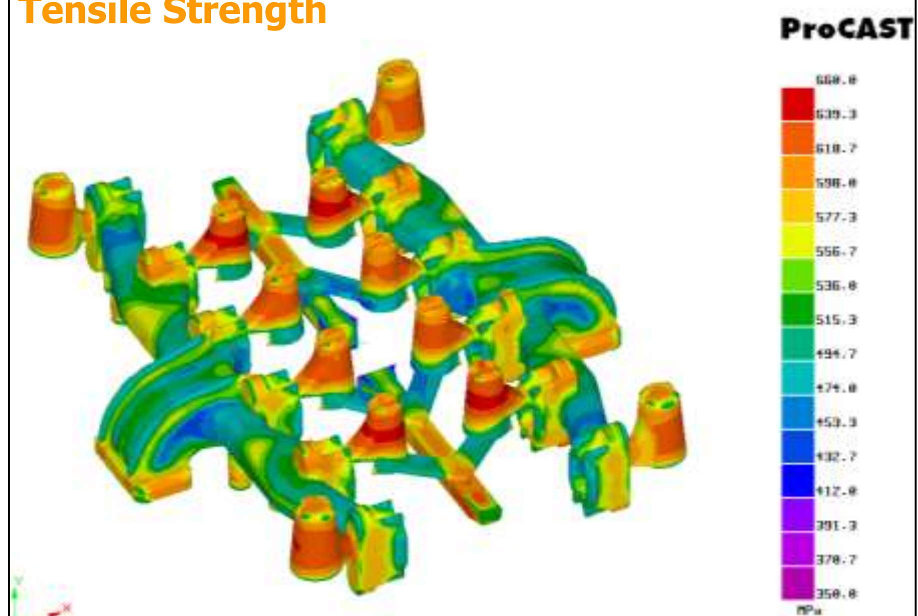
Courtesy of

# Microstructure → Mechanical Properties

## Yield Strength




## Tensile Strength




**Temperature in the range of 300°C and 500°C**

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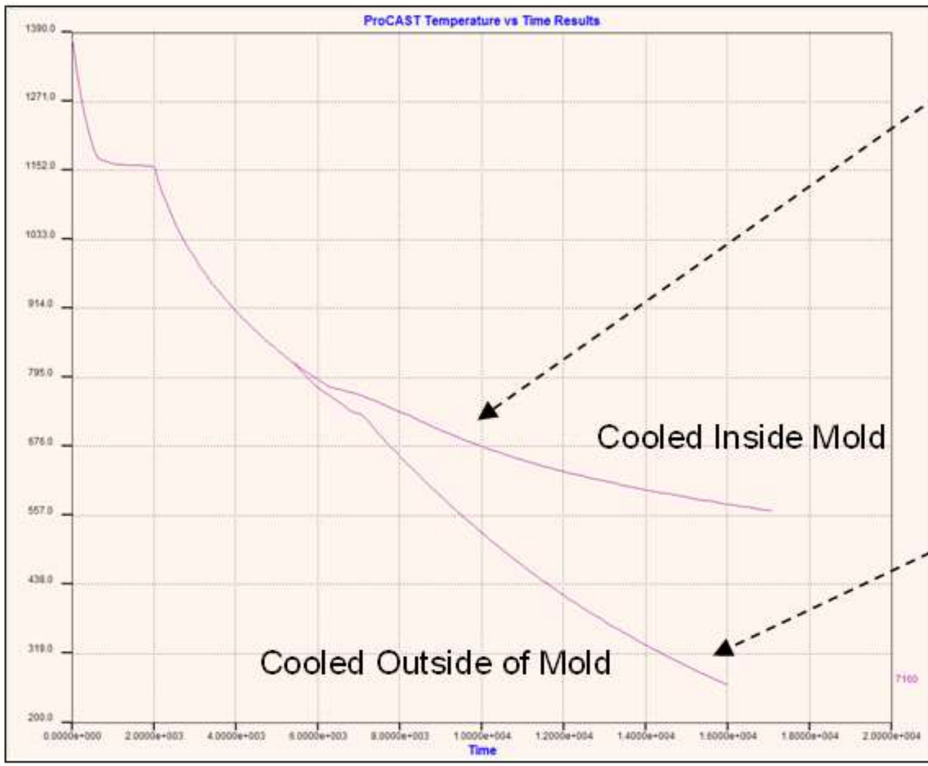
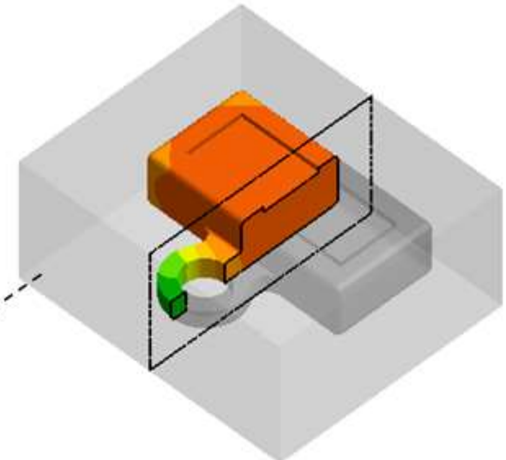
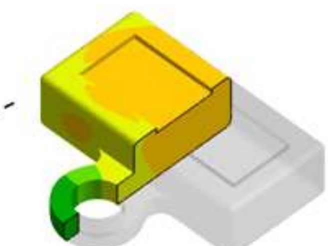
# Effect of cooling rates on mechanical properties



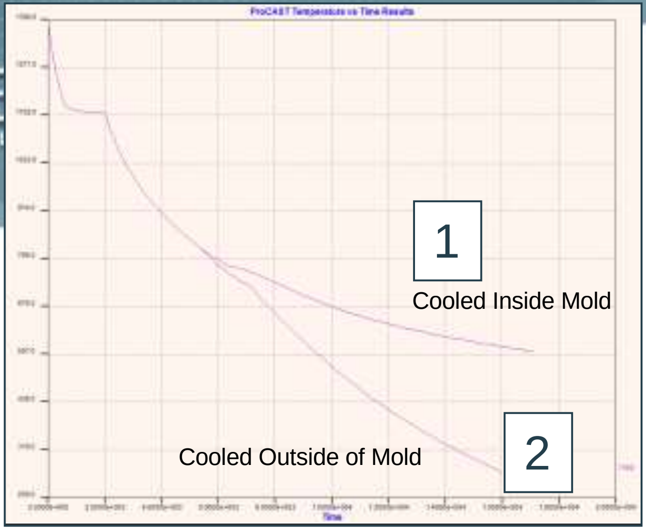



The part is shaken out after solid state temperature

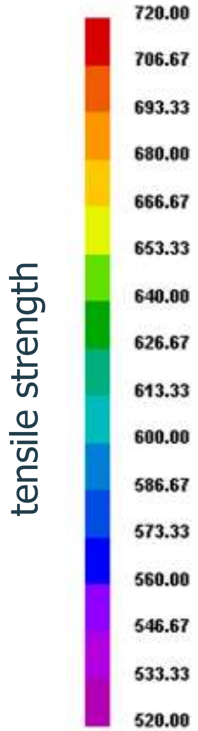


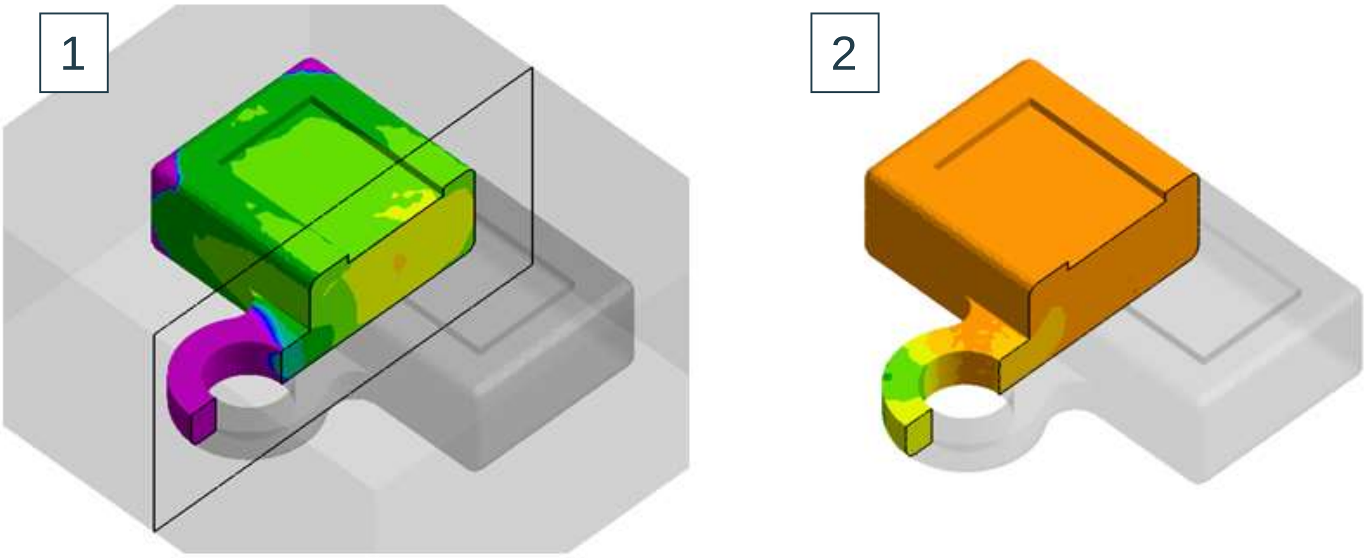
Shakeout occurring just after solidification, but before the solid state temperature was achieved

# Effect of cooling rates on mechanical properties




**Tensile Strength plots display material property differences between a part that is shaken out after (left) versus before (right) solid state temperature is reached (Courtesy of Caterpillar, Inc., USA).**




**The part is shaken out after solid state temperature**

**Shakeout occurring just after solidification, but before the solid state temperature was achieved**

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# Graphitization

- The amount of expansion depends upon the amount of “graphitization” (or graphite precipitation).
- The amount of graphitization that occurs in reality may depend upon the alloy, the processing procedure, etc…

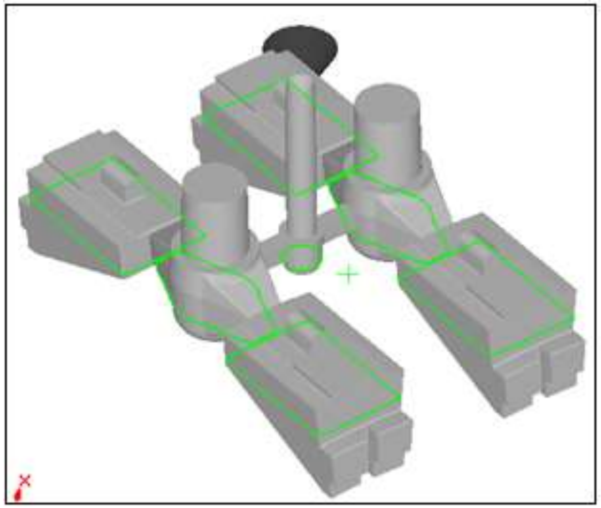
# Porosity in Cast Iron (expanding) Coupling with the Micro module

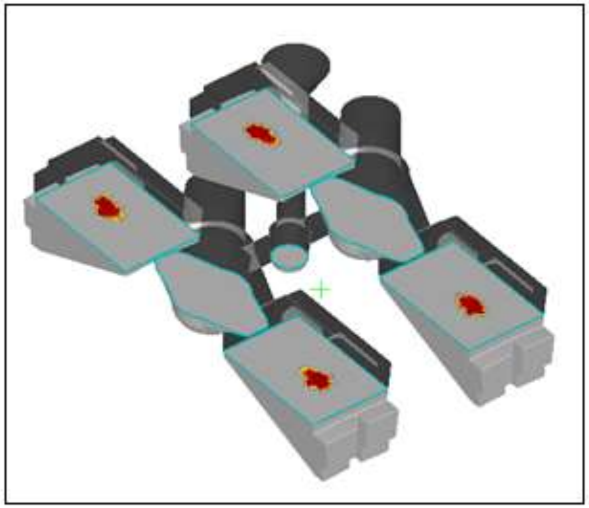
- In real Cast Iron castings, the amount of expansion is depending upon the microstructure.
  - This means that the density curve is not unique throughout the casting, but depends upon the location

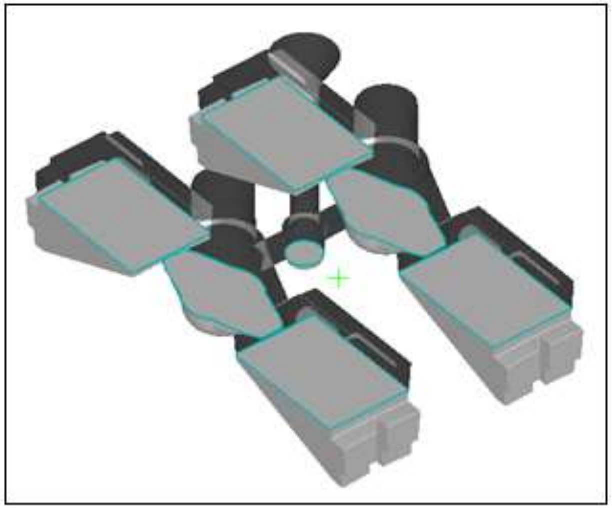
- The microstructure module is calculating the microstructure and thus the density (including the expansion) at each node and each timestep.

- As a consequence the porosity prediction is much more accurate in the case of cast iron when a coupled thermal-micro calculation is performed (only needed for cast iron, not for other alloys)

# Local compensation of porosity by graphite expansion







**On the left, picture shows the geometry of the casting with a green line indicating the cross-sectional cut of right pictures.**

**In the middle, picture shows cross-section contour plot of shrinkage porosity where yellow (red means empty) indicates macro pores when not considering the graphite expansion and considering the mould as soft, i.e. not helping for feeding.**

**On the right, shrinkage porosity prediction is shown when considering graphite expansion. We then see on this specific industrial case that graphite precipitation and thus expansion can compensate locally all the shrinkage of the liquid during solidification. The result is inline with the reality as the as-cast part is soundness.**

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# What we have learned

- Relation between alloy composition, microstructure and resulting mechanical properties
- The microstructure calculation takes into account the local density, including the graphite expansion effect
- Process conditions do also influence the microstructure. For example, the effect of cooling rates on mechanical properties have been simulated
- Good agreement with experimental results

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