LTU Casting Course 2025 & METACAST webinar

Introduction to solidification modelling

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Luleå, 28 Nov 2025

Solidification II - WEBINAR

Fundamentals and modelling
Industrial measurements and validation

Join us for an in-depth session on solidification fundamentals!

*We will explore key concepts including nucleation, heat and mass transfer, fluid flow principles, microstructure modelling, stress–strain analysis, and advanced characterization and validation techniques. As part of the discussion, two EU-funded RFCS projects—**Shell-Crack** and **SUNSHINE**—will be showcased as case studies, highlighting practical applications and research insights.*

Time	Topic
10:00-10:15	Welcome
10:15-11:30	Solidification Fundamentals
11:30-11:45	Q&A session
11:45-13:00	Lunch break
13:00-13:45	Introduction to solidification modelling
13:45-14:15	RFCS Shell-Crack
14:15-14:45	RFCS SUNSHINE
14:45-15:15	Industrial measurement techniques for model validation
15:15-15:30	Final Q&A session and End of seminar

Introduction to solidification modelling

(microstructure and stress modelling)

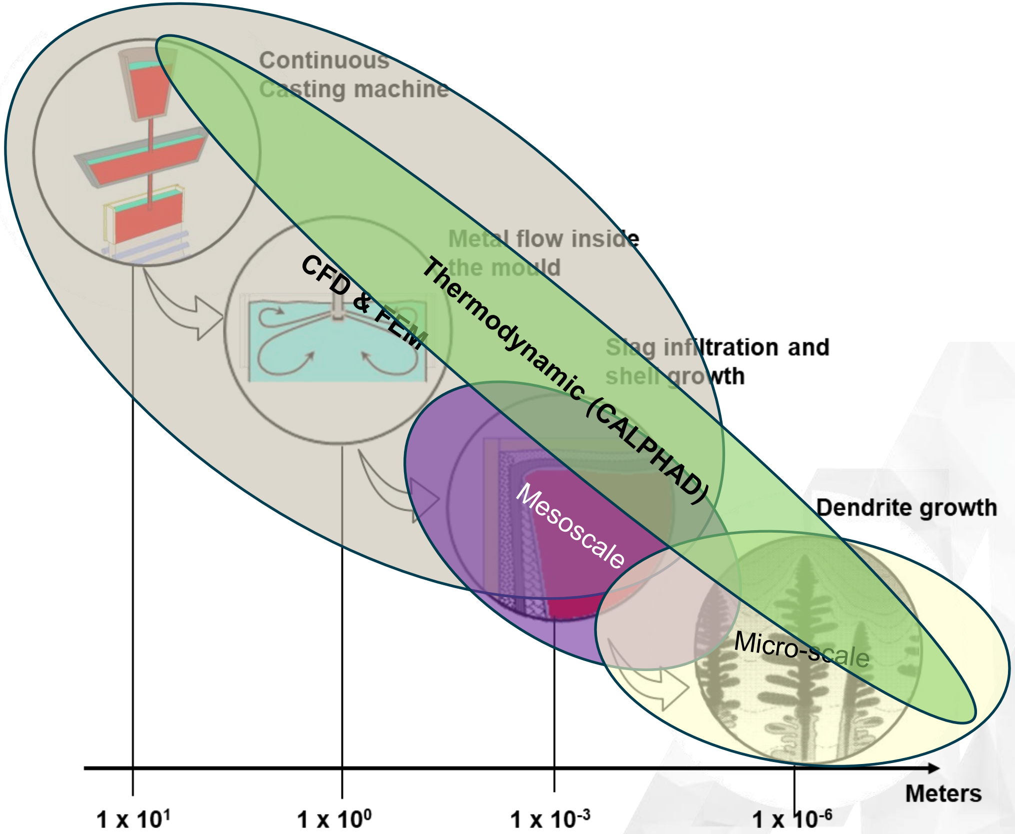
Multi-scale challenges

CC models should be capable of addressing…

Macro/Micro scale

+

Complex physical phenomena



There is no ”One model to rule them all…”

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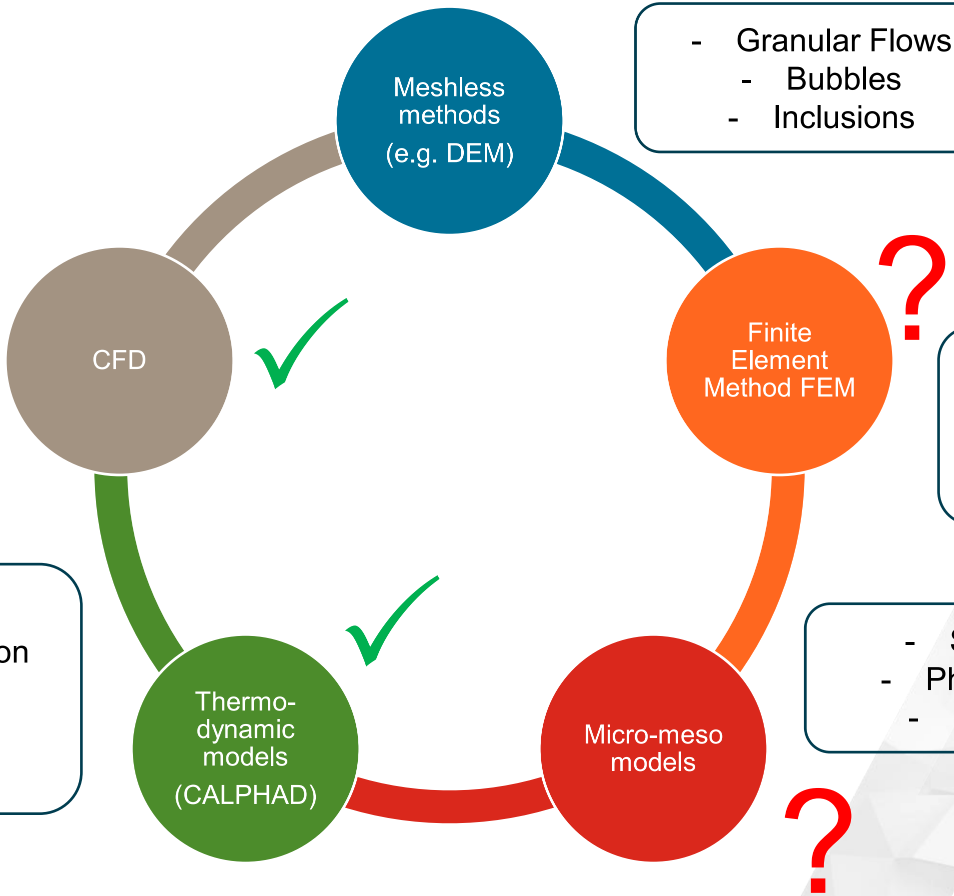

- Granular Flows
- Bubbles
- Inclusions

- Multiphase flows: (slag, steel, gas)
- Heat transfer
- Solidification
- Electro-magnetics

- Stress-strain
- Cracking
- Rolling
- Forging

- Mat props
- Phase evolution
- Slag/metal reactions
- Inclusions

- Solidification
- Phase evolution
- Segregation

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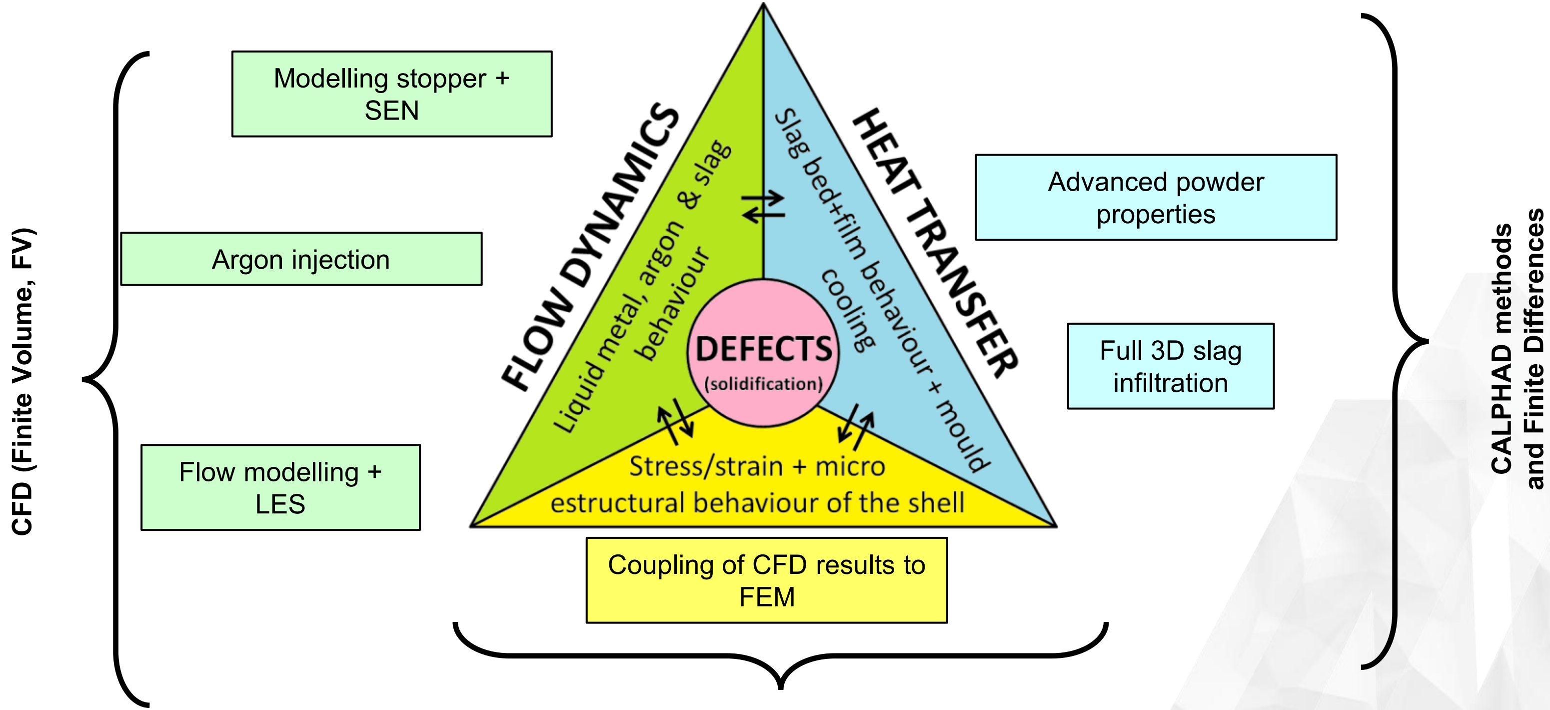
Modelling approaches



CFD (Finite Volume, FV)

Modelling stopper + SEN

Argon injection

Flow modelling + LES

FLOW DYNAMICS

Liquid metal, argon & slag behaviour

HEAT TRANSFER

Slag bed+film behaviour + mould cooling

DEFECTS
(solidification)

Stress/strain + micro estructural behaviour of the shell

Advanced powder properties

Full 3D slag infiltration

Coupling of CFD results to FEM

CALPHAD methods and Finite Differences

FEM (Finite Element) & Micro-models (Phase field, Cellular Automaton)

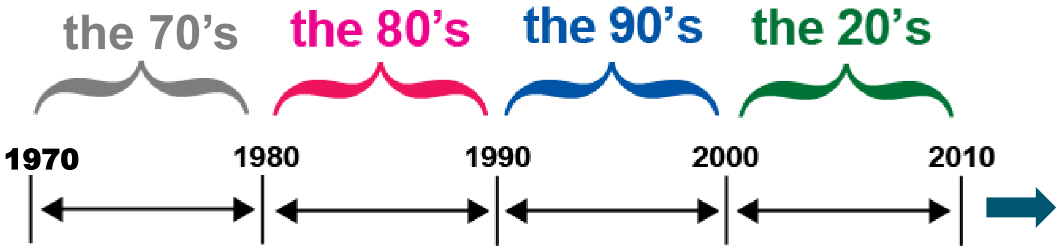
Quick modelling timeline…

Starting in the 70's and 80's with the advent of personal computers, the first generation of models managed to predict the overall behaviour of the caster based on empirical data. (see Brimacombe & Pritchard)

Models in the 90's saw the addition of Computational Fluid Dynamics (CFD) and solidification to casting simulations. (B.G. Thomas, Sekely, Hasan and Others)

Faster computers and improved codes allowed huge progress regarding multi-phase applications (e.g. bubbles and inclusions) combined with calculations of flow and solidification in the past decade. (Thomas, Ludwig, Louhenkilpi, etc)

Currently, a wide variety of commercial and in-house codes are available for CC such as PROCAST, COMSOL, TEMPSIMU, CON1D/2D, etc.



A recent trend is the development of thermo-mechanical models coupled to flow dynamics for solving the combined flow, solidification and stress-strain during casting.

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Microstructure modelling

Nucleation and growth are simulated to reproduce the formation of grains, dendrites, eutectics, solute segregation and micro-pores.

At present, the main numerical methods include:

- *Deterministic methods*
- *Stochastic methods*
- *Mesoscopic methods*

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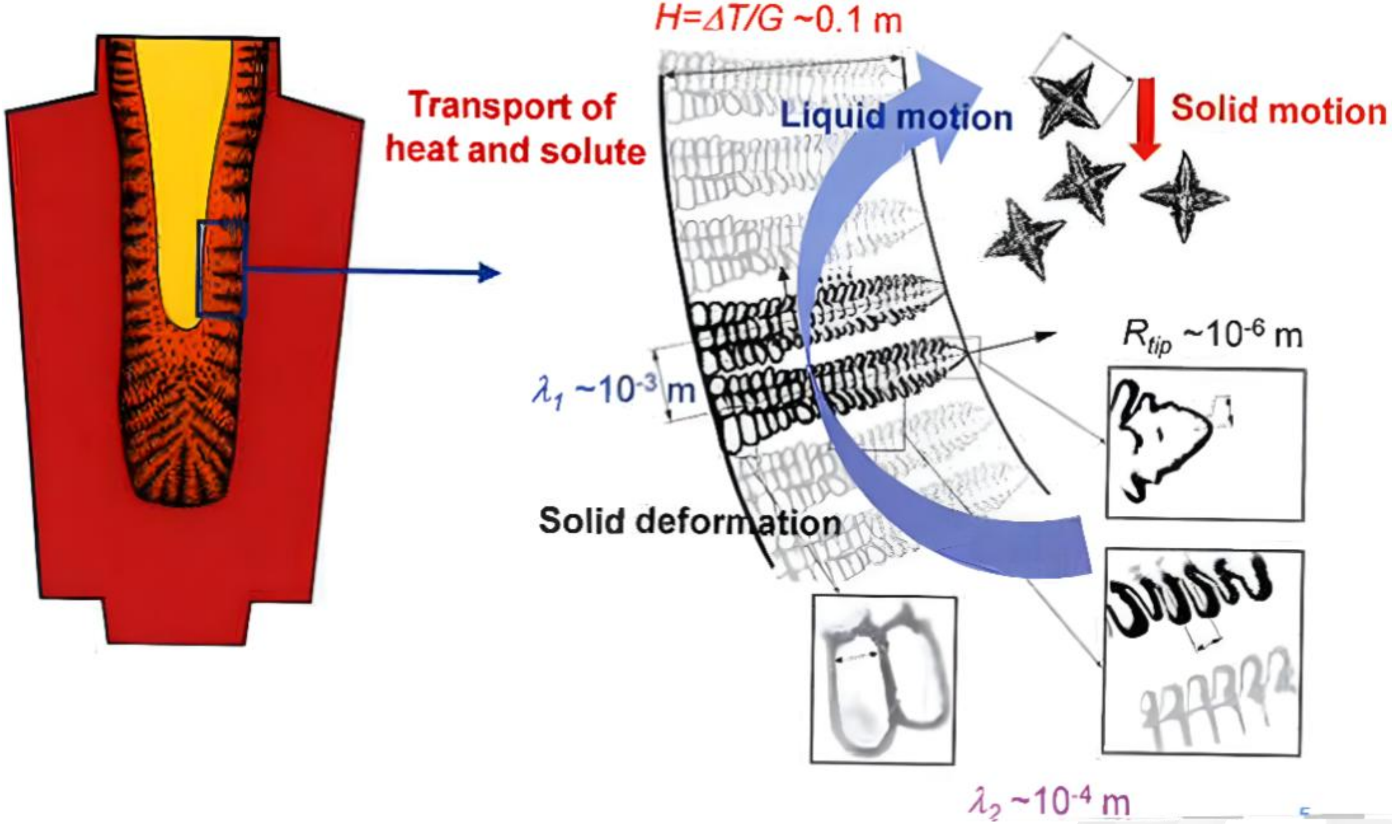
Ingot example



Deterministic modelling

The deterministic method is based on classical solidification kinetics and crystal growth characteristics.

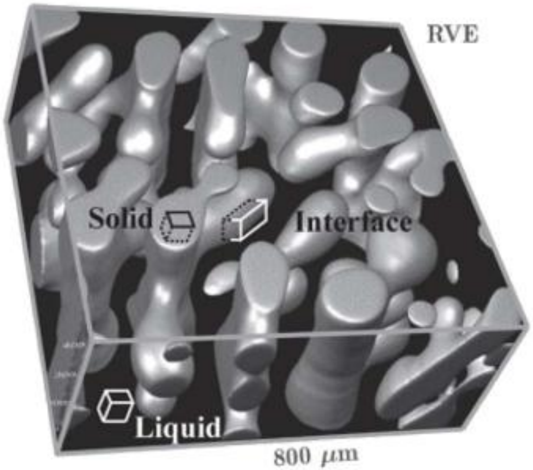
The deterministic functions of crystal nucleation, density and growth rate in the melt are derived, which can describe the changes of nucleation density, dendrite tip radius and growth rate with solidification conditions.

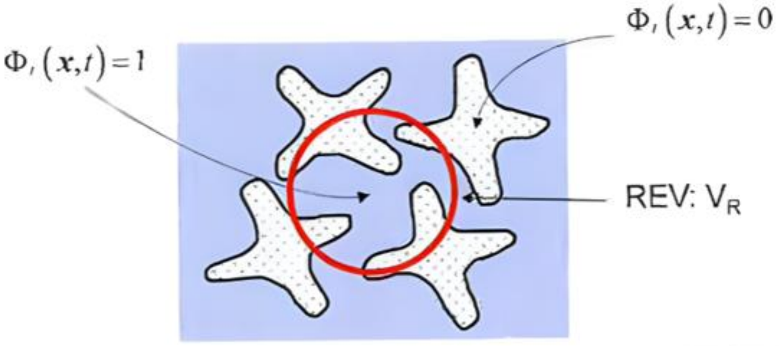
3 types of approaches are the most common

- *Mixture theory*
- *Volume averaging*
- *Ensemble averaging*

Representative Volume Element (RVE)

- Consider the volume element which is located in the mushy zone.
- The volume element is assumed to be sufficiently large to accurately represent the local structure at the mesoscopic length scale, yet small enough that important variations in temperature, enthalpy and volume fraction of the solid are resolved for the problem of interest.
- We refer to this volume as a 'Representative Volume Element' or RVE

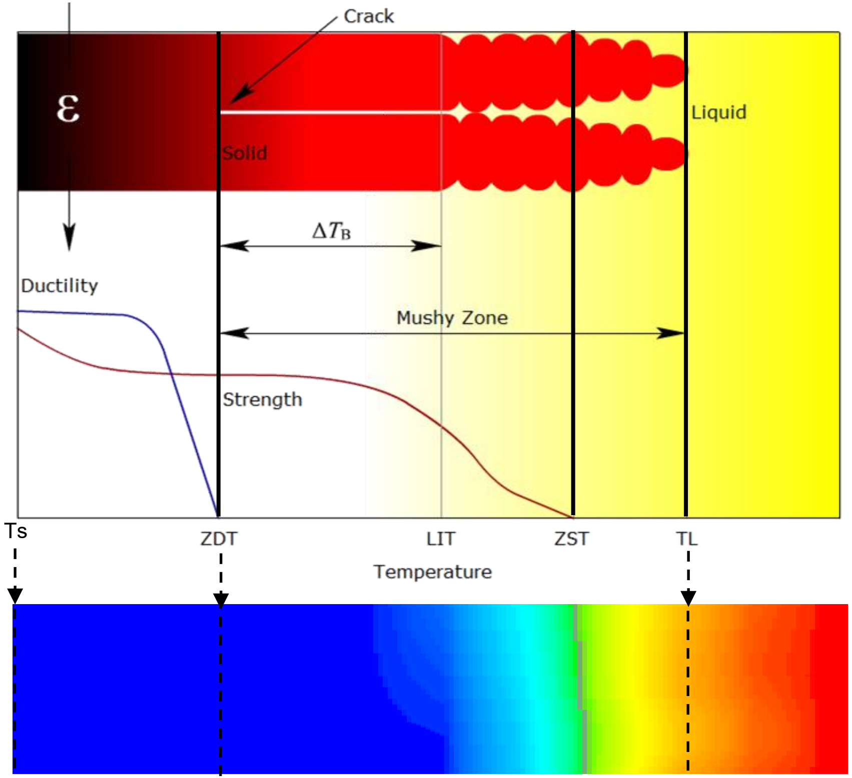




$$\phi_\alpha(x,t)=\begin{cases}1 \text{ in the } \alpha \text{ phase}\\ 0 \text{ in the other phase}\end{cases}$$

https://solidification.mechanical.illinois.edu/Book/pdf/Chap4-7page.pdf

Deterministic solidification model



$$S_s = \frac{(1-f_l)^2}{(0.001+f_l^2)} A_{mush}(\vec{v} - v_c)$$

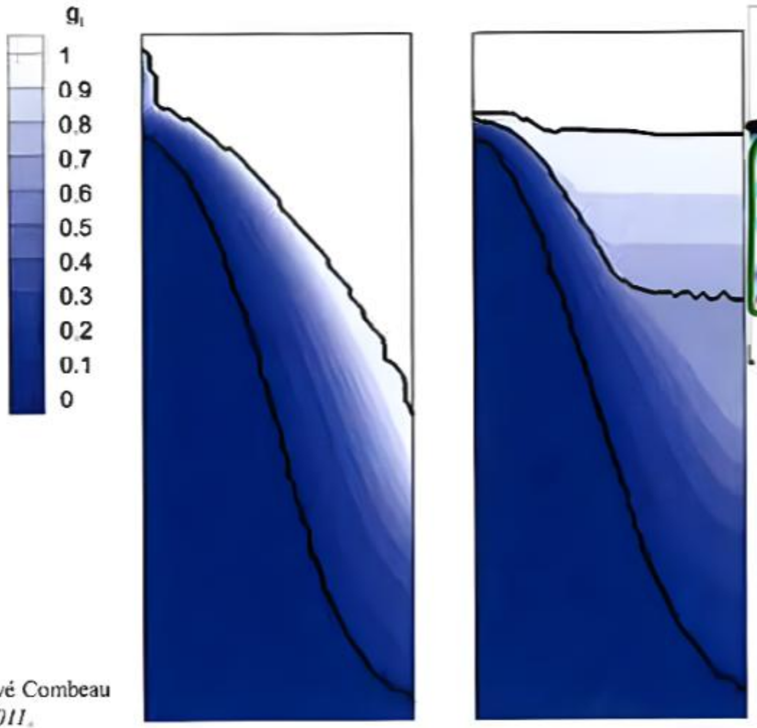
Real
solidification

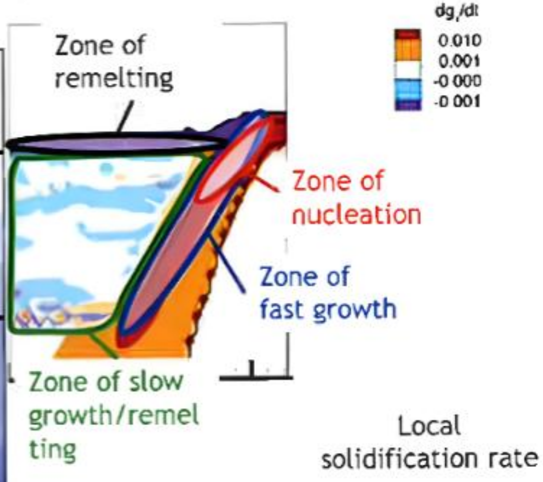
Deterministic
model
(CFD)

Limitations

Influence of grain motion on the liquid pool depth and the shape of the mushy zone.

DC-casting of a 7449 Al alloy





- Slab 350 x 2600 mm
- Alloy 7449
- Casting speed 75 mm/min
- Grain refiner Al-Ti-C (0,4 kg/t)

Miha Založnik, Arvind Kumar, Hervé Combeau Marie Bedel et al. in *Light metals 2011*.

Pro’s & Con’s of deterministic models

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Pro’s	Con’s
• Fast • Easy to code • Require relatively low computational time • Is ubiquitous (widespread)	Cannot consider some random phenomena in the solidification process: • Random nucleation distributions • Random crystal orientation • CET • Competitive elimination of dendrites • Fusing and bifurcation of dendrite arms, etc.

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Stochastic modelling

Stochastic methods divide the calculation element into N microelements on the grid, and the grain nucleation and growth on each node are calculated according to a probability model.

Often, these methods treat the grid element as a cell. The state values of the cell include physical parameters such as temperature, solubility, solid fraction, growth orientation and liquid phase flowrate.

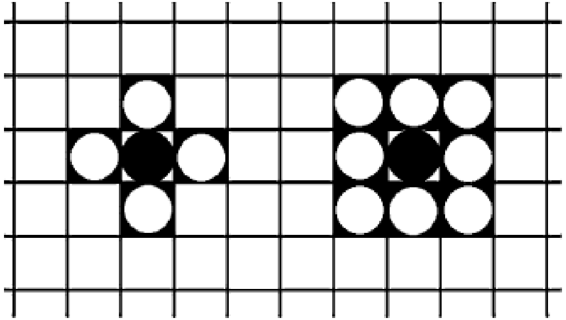
At each step, the state values of each cell and the transition of the interface are realized by solving control equations such as temperature and solute field, coupling dendrite growth and capture algorithm

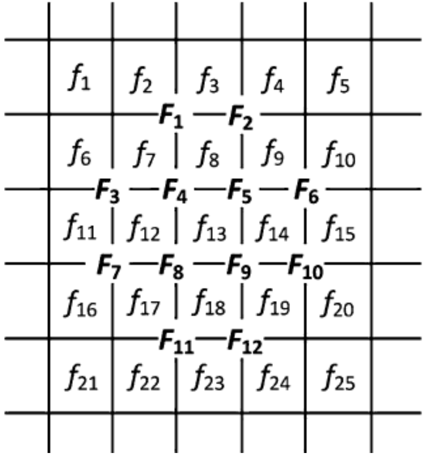
3 types of approaches are the most common:

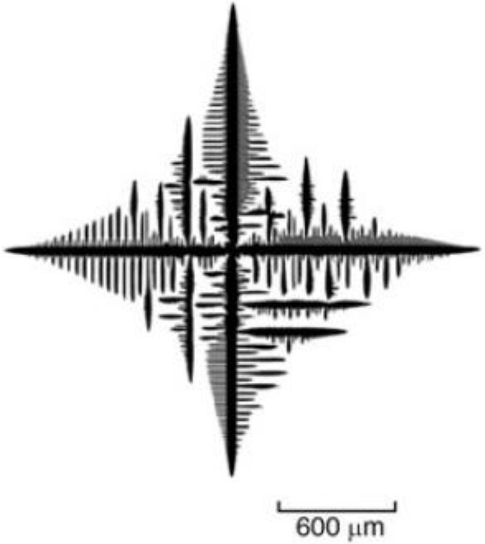
- Monte Carlo methods
- Cellular automaton (CA)
- Phase Field

Cellular Automaton

Cellular Automaton (CA) is a computational model that simulates the process of a liquid turning into a solid by dividing a material into a grid of discrete cells. The state of each cell (e.g., liquid, interface, or solid) is determined by simple, local rules that dictate how it changes over time based on its neighbors, mimicking physical processes like nucleation and crystal growth. This approach is computationally efficient because only the interface cells are actively processed, and it can accurately predict complex microstructures like dendrites and eutectic patterns.

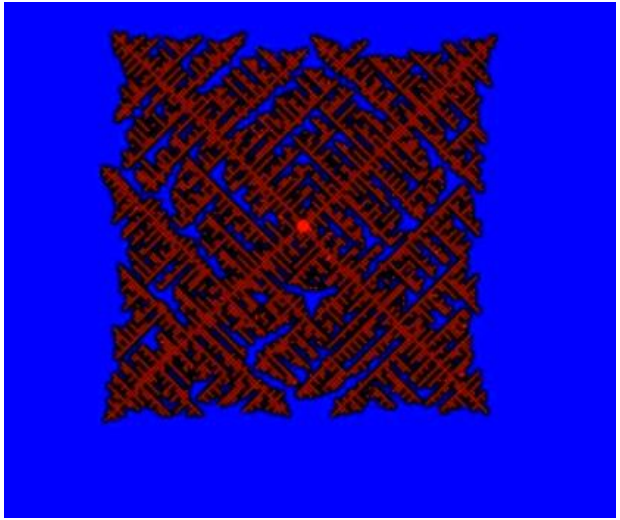






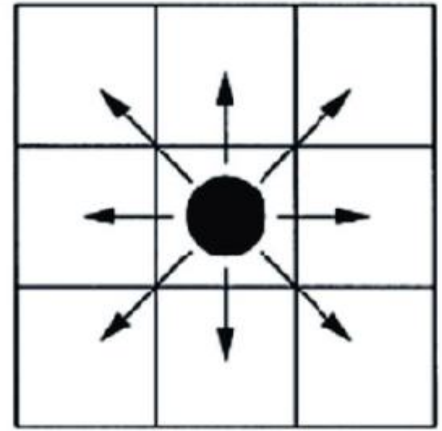
Wei, L., Lin, X., Wang, M. *et al.* A cellular automaton model for the solidification of a pure substance. *Appl. Phys. A* **103**, 123–133 (2011)

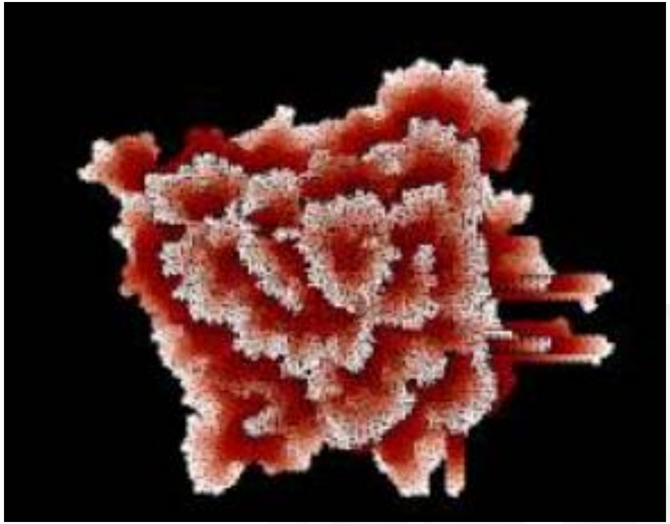
Cellular Automaton videos



https://www.youtube.com/shorts/GBSCnC9Yjc0

$M_{-1,-1}$	$M_{-1,0}$	$M_{-1,1}$
$M_{0,-1}$	$M_{0,0}$	$M_{0,1}$
$M_{1,-1}$	$M_{1,0}$	$M_{1,1}$





https://www.youtube.com/shorts/dJTACWSPEWg

Pro’s & Con’s of stochastic models

Pro’s	Con’s
Can consider complex phenomena in the solidification process: • Random nucleation distributions • Random crystal orientation • Transformation from columnar crystal to equiaxed • Competitive elimination of dendrites • Fusing and bifurcation of dendrite arms, etc.	• Computationally expensive • Requires user inputs for micro-structure • Slow • Only a limited size can be modelled (in the order of mm) • Requires coding experience • In-house codes • Commercial codes are rarely available and/or under development (e.g. MICRESS, SIGMA prime, etc)

Mesoscopic methods

A solidification envelope model is a mesoscopic modeling technique that simplifies a dendritic grain into a smooth, virtual surface called an envelope.

This envelope links the active dendrite branches, and its growth is calculated from the tip growth velocities of the dendrites, which are themselves determined by local liquid supersaturation.

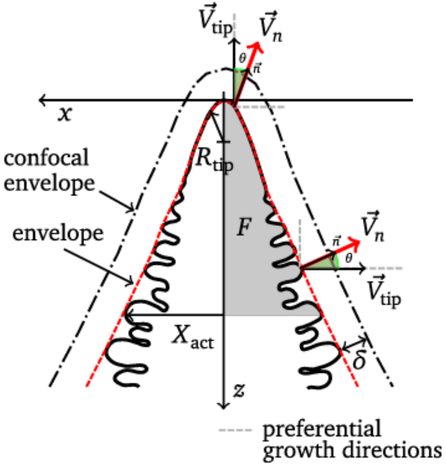
It is a multiscale model used to bridge the gap between microscopic and macroscopic approaches in studying dendritic solidification.

Mesoscopic models

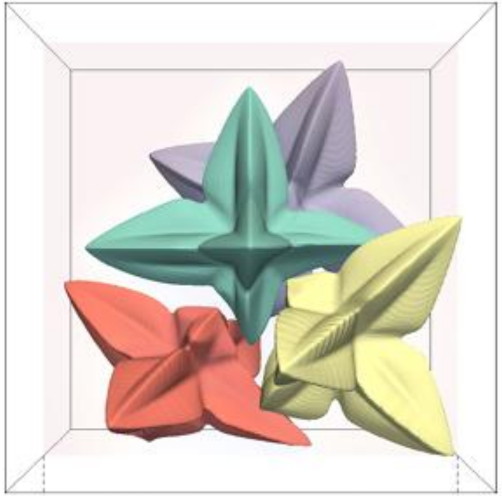
- Envelope models can accurately predict microstructural features like dendrite shapes and grain interactions.
- Offer faster simulation times compared to phase-field methods

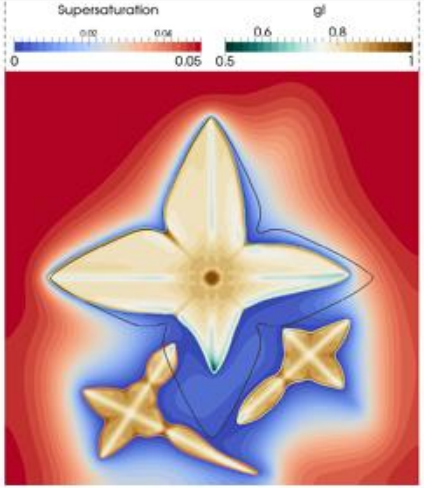
- Provide a bridge to upscale simulations to macroscopic models for large-scale applications.

- Possible to analyze complex phenomena such as hot tearing in welding or microstructure evolution in additive manufacturing with greater speed.



The envelope, the confocal envelope, and the stagnant film thickness, o. The envelope propagation velocity, Vn, is obtained by the projection of the tip velocity, Vtip, from the preferential growth direction forming the smallest angle 0 with the envelope normal, n.





Youssef Souhar, Valerio F. De Felice, Christoph Beckermann, Hervé Combeau, Miha Založnik, Three-dimensional mesoscopic modeling of equiaxed dendritic solidification of a binary alloy, Computational Materials Science, Volume 112, Part A, 2016, Pages 304-317, ISSN 0927-0256

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Finite Element Methods

Despite all the progress, the actual simulation of cracking during casting has remained elusive from modelling efforts.

This is partly due to the Multiphysics nature of the problem (e.g. dependent on heat transfer, solidification and stress-strain) as well as the high temperatures at which the process occurs (which limits possible measurements and data acquisition).

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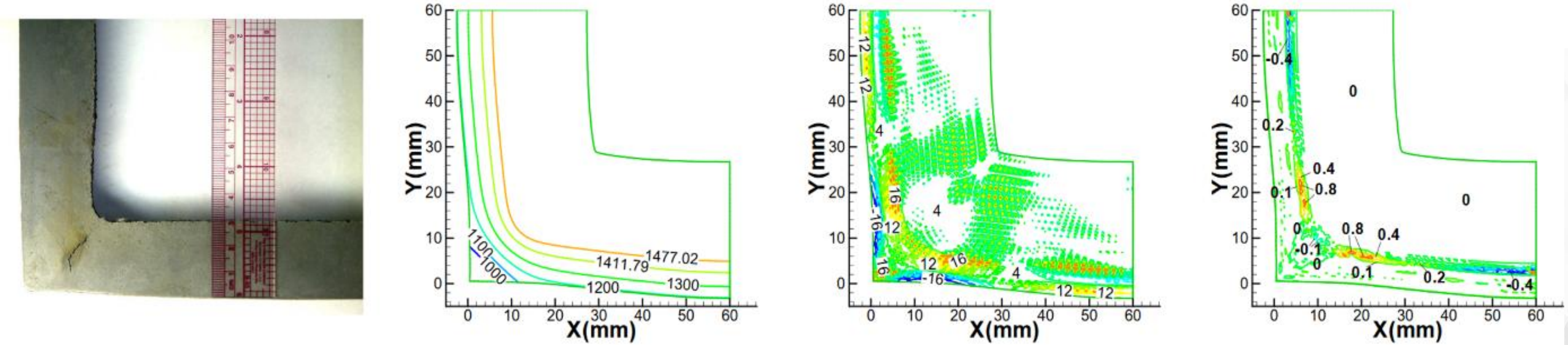
Cracking modelling

Process models are typically based on macro-scale FEM methods that aim at predicting the total strain and stress coming from the elastic, thermal and plastic strains by means of thermo-mechanical models



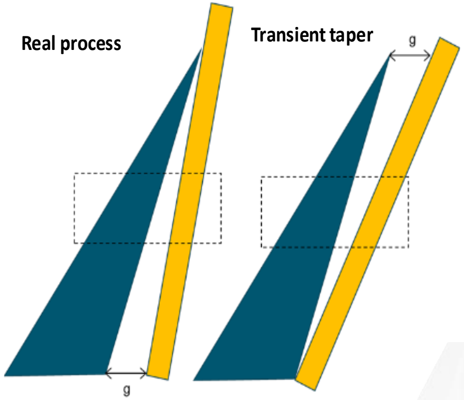
(a) Temperature (b) Hoop stress (c) Hot-tear strain

Fig: Sub surface Corner cracking in CC (extreme left) and thermo-mechanical modelling by Bellet & Thomas [1]

[1] Brian G. Thomas, Michel Bellet. Modeling of Stress, Distortion, and Hot Tearing. Edited by S. Viswanathan and E. DeGuire. ASM Handbook, Volume 15: Casting, ASM International, pp.Pages 449-461, 2008, ASM Handbooks, 978-0-87170-711-6. <hal-00509529>*]*

FEM model example

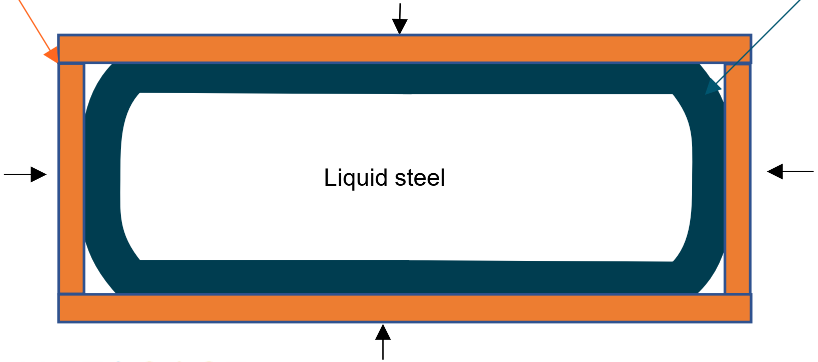
- Assuming that the process of shrinkage from cooling is reversible
- Assuming that a shell with properties of near molten steel is similar to the molten steel in real process
- Heating by setting inner edge to steel solidification temperature



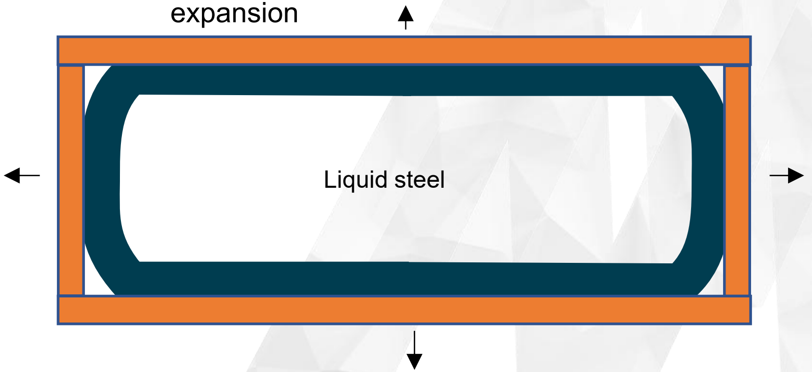
Mould walls

Movement of mould wall in caster due to cooling and shrinkage

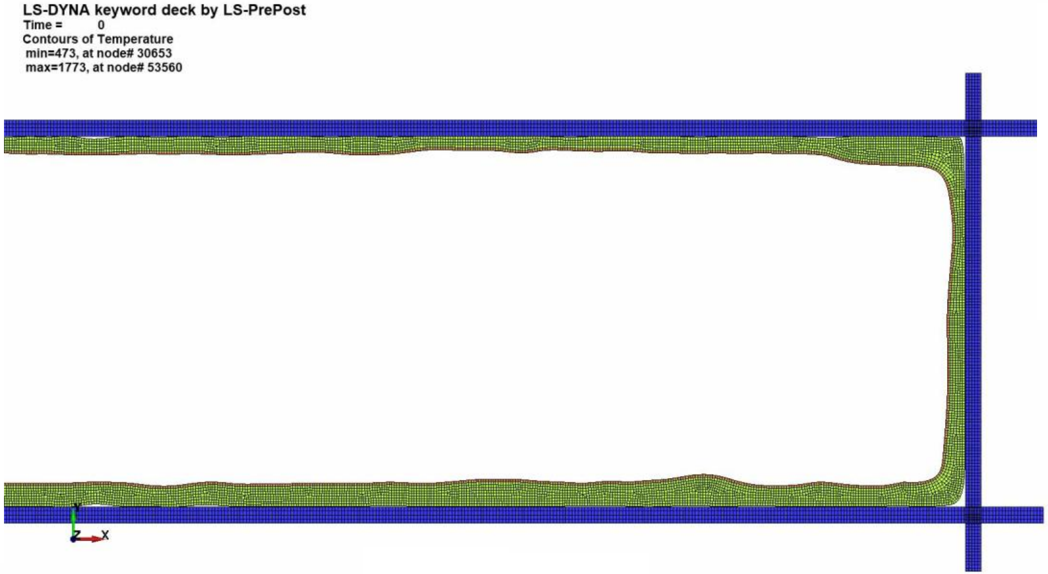
Solidified shell



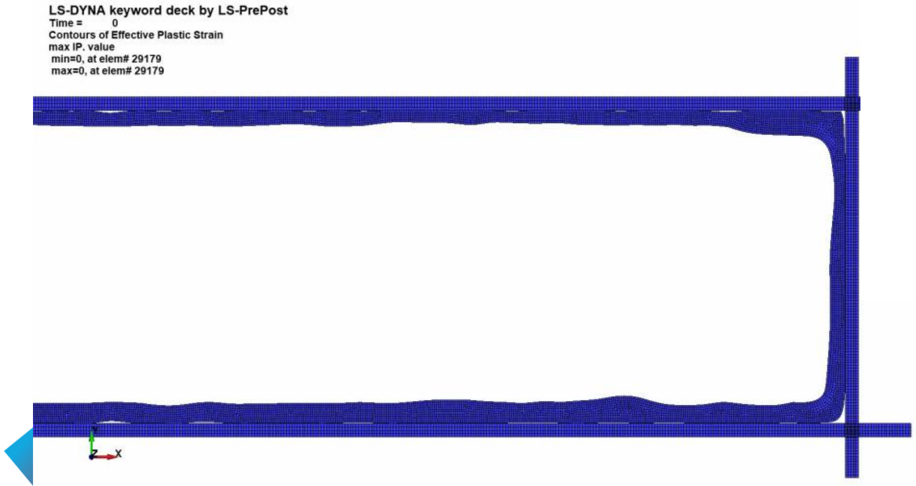
Movement of mould wall in simulation due to heating and expansion



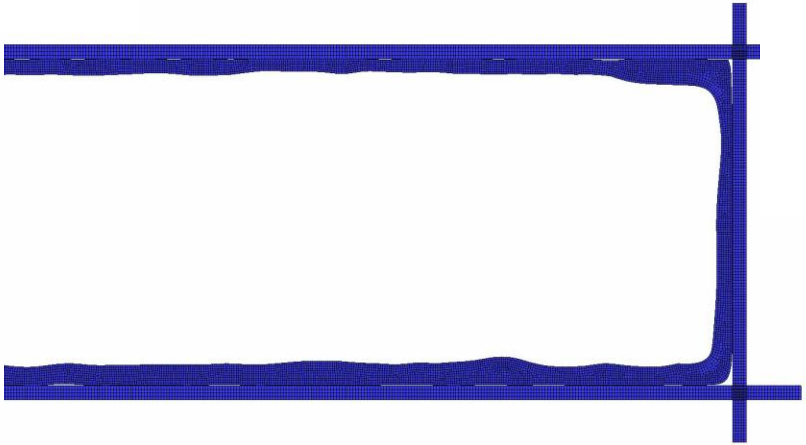
Strain



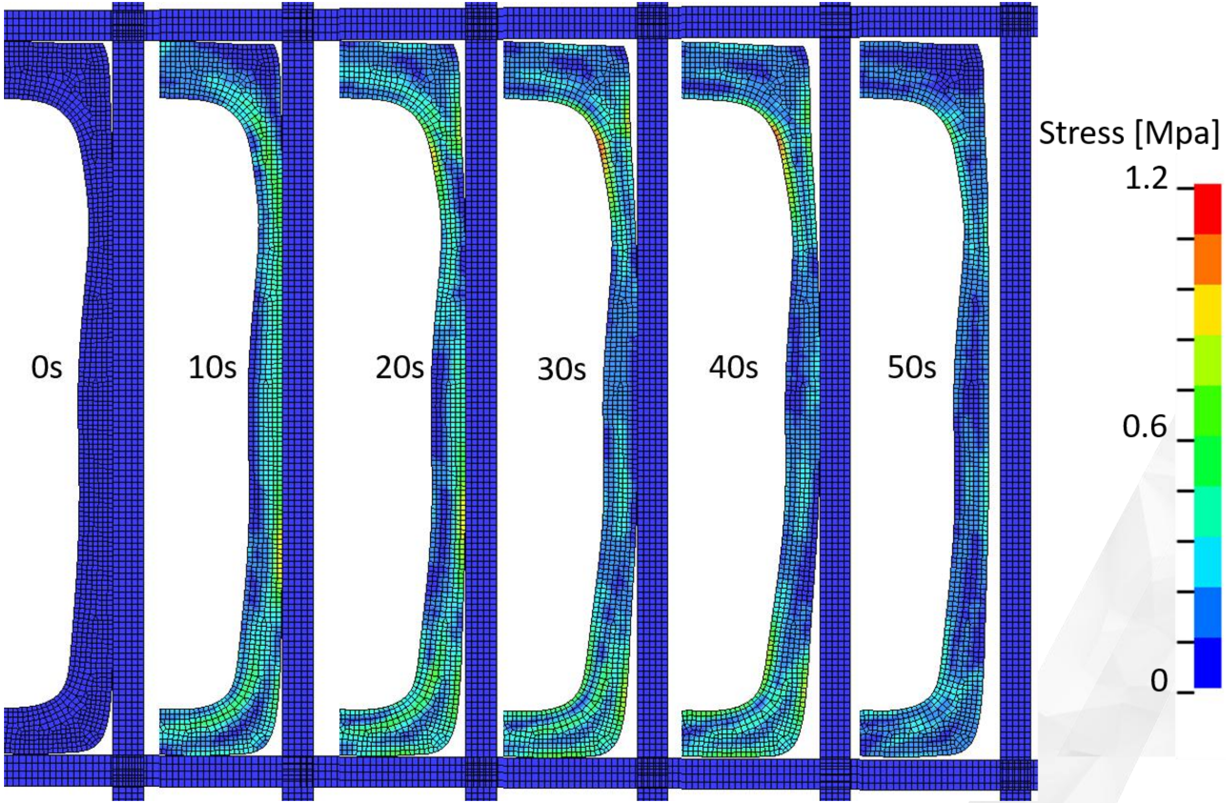
LS-DYNA keyword deck by LS-PrePost
Time = 0
Contours of Temperature
min=473, at node# 30653
max=1773, at node# 53560



LS-DYNA keyword deck by LS-PrePost
Time = 0
Contours of Effective Plastic Strain
max IP. value
min=0, at elem# 29179
max=0, at elem# 29179



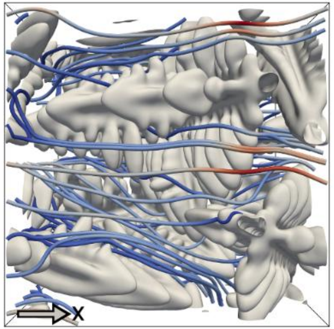
Stress



Summary

Engineering Applications

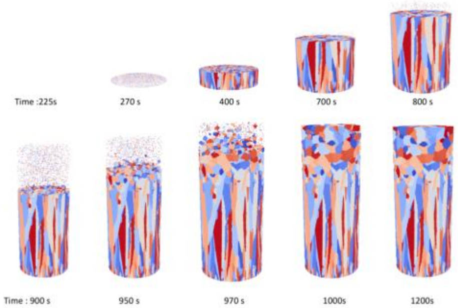
Microstructure



Phase-field & cellular automaton models: MICRESS and CAFE models.

- High resolution in prediction of microstructures formed during solidification.
- Coupled with thermodynamic databases e.g. Thermo-Calc or JMatPro.
- Small computational domain.
- High computational cost.

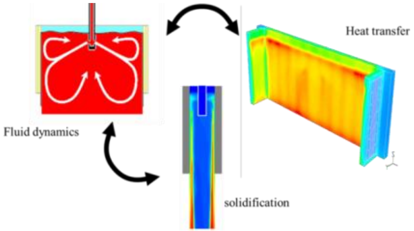
Meso-Scale Models



Coupled macro scale models with e.g. direct grains envelopes tracking technique:

- Prediction of fluid flow as well as solidification including a simplified microstructure & segregation model.
- Potential to be applied to industrial scale problems.
- Moderate computational cost.
- The model lacks the microstructure features from MICRESS and CAFE models.

Macroscale



Macroscale computational codes based on CFD, FEM, etc numerical methods: ANSYS, THERCAST and ABAQUS.

- Applicable to 2D-3D industrial scale problems.
- Lower computational cost.
- Coupled multiphase approach (steel-slag-argon gas)
- Possible coupling of slag-metal reactions through thermodynamic data bases.
- Coupled multiphysics e.g. EMS and EMBr applications.
- The model lacks prediction of microstructure and segregation.

µm mm cm m

Length Scale

Before pressing any button !!!...

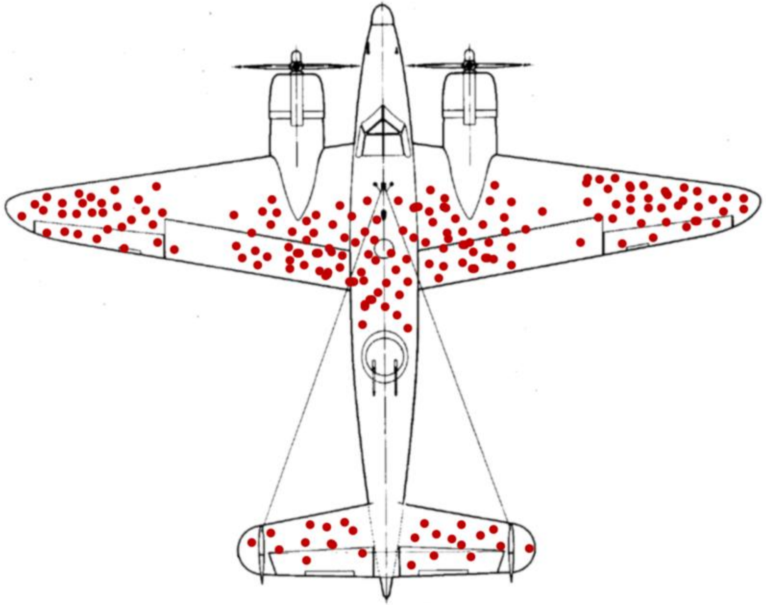
It is necessary to define the outreach, needs and expected outcomes from the analysis, since modelling often demands significant resources (e.g. hardware, software and manpower).

Some general questions must be answered:

- Why is the simulation required?

- What are the problem boundaries, size and geometrical constraints?

- What is the possible behaviour of the problem?



https://en.wikipedia.org/wiki/Survivorship_bias

Operations research

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