AM Module training course

Day 1 23-24 April'2025

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Schedule for training course

Day 1

09:00	Course overview
09:05	Introduction to PBF-LB process and AM Module
09:40	Theoretical background: Scheil-Gulliver model
09:50	Setting up an AM simulation
10:15	Q & A (with a short break)
10:30	Theoretical background: FE Solver, Enthalpy equations
10:50	Steady-state and transient simulations with example
11:50	Q & A + Home assignment



Schedule for training course

Day 2

09:00	Discussion: Home assignment
09:10	Theoretical background: Keyhole, fluid flow and absorptivity model
10:00	Printability maps with example
10:30	Q & A (short break)
10:45	Advanced setup: AM \rightarrow DICTRA and AM \rightarrow CET models, Calibration of heat source
11:45	Q & A
12:00	Closing of course



Introduction

Thermo-Calc Software's mission is to develop computational tools that allow engineers to generate the materials data they need in their daily decision making to drive innovation and improve product performance.

Software: Thermo-Calc with add-on Modules. (Kinetic, Application). Software development kits (SDKs)

Databases: Thermodynamic, Kinetic, Thermophysical properties

Property Model development framework









Course overview

What the course is about and what to expect?

- The Additive Manufacturing Module (AM Module) is used for better understanding of the powder bed fusion-laser beam (PBF-LB) process by predicting the temperature distribution and melt pool geometry as a function of process parameters
- It uses material properties (thermodynamic and thermophysical) calculated from Thermo-Calc databases
- This course will cover a short background into metal additive manufacturing (AM) process, effect of rapid solidification on microstructure development, defect generation during AM processing and coupling of AM process to our other modules such as Diffusion module (DICTRA) and Precipitation Module (TC-PRISMA)
- The graphical user interface and functionality will be showcased with some application examples



Introduction to metal AM and PBF-LB process



Introduction to metal AM and PBF-LB process

Metal additive manufacturing (AM)

- It is a layer-by-layer deposition process that produces near net shape components
- Starting raw material can be in powder or wire form and source of heat could be beam-based (laser/ electron beam), binder based or even light sources/ diffusion bonding methods
- Due to additive nature of process, most of the raw material is reused (~95%) thus leading to savings in material wastage





Raw material reusable after printing



Fresh out of print



After powder removal





Introduction to PBF-LB process



2D schematic for an EOS M290 PBF-LB system

Remelting and reheating phenomenon

Introduction to AM module



Introduction to AM module

Background/motivation

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- Thermophysical property were introduced in our databases around 2020
- This initiated an increased request from customers to export data to FEM simulations
 - Specific Heat, Density and Thermal Conductivity are important for Peak Temperature prediction
 - +Surface Tension and Viscosity important for melt pool predictions
 - +Thermal Conductivity, Specific Heat important for heat distribution in the build
- While the treatment of heat and fluid flow was state-of-theart in current FEM simulations, material properties were treated in a highly simplfied manner. This gave us the unique possibility to address the solidification problem during AM with the focus on a unified treatment of both process parameters and alloy dependent thermophysical properties



Ma, Li, et al. "Using design of experiments in finite element modeling to identify critical variables for laser powder bed fusion." *2015*

Introduction to AM module

Background/motivation

An integrated CALPHAD-based FEM tool designed for rapid predictions of melt pool dimensions, printability, thermal fields and solidification rate in the additive manufacturing of multicomponent alloys without need of user input materials property data.

This module leverages highly accurate composition and temperature-sensitive thermochemical and thermophysical properties through a seamlessly coupling with Thermo-Calc and provides unparalleled insights and optimization capabilities for complex additive manufacturing processes.

The resulting temperature profile can be used as inputs for microstructure simulation using DICTRA or TC-PRISMA



Transient AM simulation on beta-TiAl alloy





Unified Treatment of Material Properties and Process Parameters



Define alloy system, retrieve Thermodynamic and Thermophysical data Extraction of materials properties from evaporation down to RT including solidification segregation.

Obtain enthalpy, heat capacity, density, thermal conductivity, viscosity, surface tension, volume, molar mass of Gas and driving force for evaporation Simulate AM with parameters such as: Laser power, Scanning speed and Strategy Layer thickness, Base plate temperature.

Takes into account: Thermal conduction and Fluid flow, Powder density, and heat losses due to radiation and convection and evaporation Visualize in 3D, over a selected line or at a chosen point over time.

Plottable quantities: Temperature, Flow velocity, Surface tension,Thermal conductivity, Dynamic viscosity and Melt Pool dimension. Export time-temperature profile, melt pool dimension and/or temperature distribution in space to other Thermo-Calc modules like DICTRA or PRISMA, or to other external computational softwares.

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Unified Treatment of Material Properties and Process Parameters



System Define

Extended Scheil Calculation

M Module

Post processing

Export results

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Theoretical background: Scheil-Gulliver simulations



Scheil-Gulliver simulations: Introduction

As per [Gulliver, 1913] and [Scheil, 1942], the Scheil-Gulliver model assumes

- Diffusion in the liquid phase is assumed to be infinitely fast whereas it is zero in solid phase
- Solid/Liquid interface is in thermodynamic equilibrium

In Scheil, temperature is reduced step-by-step (default = 1 $^{\circ}$ C). When going below T_L(liquidus), equilibrium amount and composition of solid/liquid phase is calculated.

Solid phase is removed from the system and only the remaining liquid is considered for next calculation step. Procedure is repeated till last liquid disappears (default = 0.01μ -fraction of liquid)

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Scheil-Gulliver simulations: Introduction

- Comparing equilibrium and non-equilibrium (Scheil) solidification, we can see difference in T-f_s curve
- Classic Scheil does not consider cooling rates into account, only a step-wise treatment
- Scheil solves for non-equilibrium microstructures (true for most engineering materials)

2.



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1. Scheil, E. (1942). Bemerkungen zur schichtkristallbildung

Gulliver, G. H. (1913). The quantitative effect of rapid cooling upon the constitution of binary alloys. J. Inst. Met.

Scheil-Gulliver model: new models

Scheil with fast diffusers

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• Classical Scheil assuming elements are infinite diffusion in solid (interstitials)

Scheil with back diffusion in primary phase

- Takes into account back-diffusion of elements in primary solid phase, requires MOB + TC database
- Cooling rate (CR) dependence to back diffusion (CR $\frac{1}{\alpha}$ Back diffusion)
- Domain size considered (back calculated from CR and constants c, n from secondary dendrite arm spacing equation (SDAS = c. CR⁻ⁿ)

Scheil with solute trapping [Aziz/ Hillert model]

Deviation from assumption of thermodynamic equilibrium at solid-liquid interface.

- Only one primary solid phase forms dendrite
- Solute trapping in primary solid phase only, other solid phases have equilibrium compositions
- Dynamic liquidus for primary solid phases is dependent on solute trapping and solidifation speed
- Amount of solid phases dependent on solute trapping and solidification



1. Scheil, E. (1942). Bemerkungen zur schichtkristallbildung

M. J. Aziz, Model for solute redistribution during rapid solidification. J. Appl. Phys. 53, 1158–1168 (1982)

3. M. Hillert, Solute drag, solute trapping and diffusional dissipation of Gibbs energy, Acta Mater., 47(18)4481-45-5(1999)

Extended Scheil model for AM module

Inclusion of gas phase & temperature below solidus

- Standard scheil calculates from ~2500 K → solidus. Scheil for AM goes from 5000 K (to include evaporation) → RT (below solidus)
- This enables calculation of temperature dependent thermophysical properties of the system which is then used as input to AM simulation
- Accurate assessment of solidifying phases + accurate modelling of thermophysical properties is critical here





Temperature dependent properties from Scheil (5000 K \rightarrow RT)



Calculations conducted on AlSi10Mg alloys using TCAL9 databases in Thermo-Calc 2025a

Extended Scheil model for AM module

Phase-interface scattering

- Adjustment factor in thermophysical properties due to micro-segregation during solidification and grain boundary formation
- The electrical resistivity due to phase interface scattering is evaluated as the scattering constant times sum of the interaction between the volume fraction of phases
- The contribution to thermal conductivity is related to electrical resistivity, following the Wiedemann-Franz law
- This setting is available when the "account for phase interface scattering" checkbox is selected. The Phase interface scattering constant default value is $4.0e-8 \Omega$ -m.

Figure: AlSi10Mg eutectic Al-Si network for (L) As-cast microstructure and (R) As-printed microstructure

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1. Lefebvre, W., Rose, G., Delroisse, P., Baustert, E., Cuvilly, F., & Simar, A. (2021). Nanoscale periodic gradients generated by laser powder bed fusion of an AlSi10Mg alloy. Materials & Design, 197, 109264. https://doi.org/10.1016/j.matdes.2020.109264

Setting up a AM simulation

Setup of extended Scheil calculation in AM module

- 5000K RT : extraction of properties
- Phase interface constant : Important for GB scattering
- THCD averaging over AM simulation



Questions?

Short break for 15 minutes \odot



Unified Treatment of Material Properties and Process Parameters



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Different approaches to simulate AM process



Different approaches to simulate AM process

Finite element method

Division of entire volume into mesh (elements)

Mesh elements solved by partial differential equations Based on conservation laws: flux, momentum, energy etc. representing physical phenomenon

Historically used for structural simulations

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Computationally efficient and lower file sizes



Finite volume method

Division of entire volume into cells

Historically used for computational fluid dynamics (CFD) Computationally expensive and larger file sizes



https://www.machinedesign.com/additive-3d-printing/fea-and-simulation/article/21832072/whats-the-difference-between-fem-fdm-and-fvm

MOOSE : Our FE solver

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- Multiphysics Object Oriented Simulation Environment (MOOSE) is an open-source, parallel finite element framework initially developed by national laboratories in the US (mainly Idaho National Laboratory by Gaston et al.,2009)
- MOOSE is based on Jacobian-Free-Newton-Kryklov (JFNK) mathematical principle, wherein physics expressions are modularized as "kernels"
- One of the abilities is to create multiple nonlinear systems on the same mesh while solving two different equations independently. It can do thus multiphysics simulations in fraction of time
- In AM module, we create adaptive meshes with finer mesh around the beam for a better description of interaction close to the beam
- Hexahedral mesh defined for simulation. Tetragonal mesh for keyhole (discussed later)

Adaptive mesh in FEM solver

https://mooseframework.inl.gov/index.html

- https://en.wikipedia.org/wiki/MOOSE_(software)
- Gaston, D., Newman, C., Hansen, G., & Lebrun-Grandié, D. (2009). MOOSE: A parallel computational framework for coupled systems of nonlinear equations. Nuclear Engineering and Design, 239(10), 1768–1778. <u>https://doi.org/10.1016/j.nucengdes.2009.05.021</u>





Theoretical background

• Scheil-Gulliver simulations (Scheil module) \succ A

Already discussed

Models used in AM module

- Energy equation and formalisms
- Heat sources
- Keyhole model
- Absorptivity model
- Fluid flow

- To be discussed tomorrow



Energy equation and formalisms



Energy Equation: The Enthalpy Formulation

The temperature evolution in the AM module is predicted by using enthalpy method and is given by Eqn. 1:

where \dot{H}_m is the time derivative of the enthalpy (Eqn. 2), V_m is the molar volume (Eqn. 3), J_Q is the heat flux given by Fourier's law (Eqn. 4) and \dot{Q} is a source term and represents the heat added from the outside at a certain point. *div* is the divergence operator

The time derivative of the enthalpy \dot{H}_m is given by:

$$\dot{H}_m = \dot{f}^L \Delta H_m + c_p \dot{T} \qquad ----- (2)$$

where \dot{f}^L is the fraction of phases, ΔH_m is the latent heat, c_p is the molar heat capacity and \dot{T} is the time derivative of the temperature.

The molar volume V_m is given by:

where is the molar volume of a phase (say β), f^L is the liquid fraction and ΔV_m is the change in molar volume The heat flux J_Q is given by:

 $J_Q = -\kappa \operatorname{grad}(T) \qquad \qquad \operatorname{-----} (4)$

where κ is the thermal conductivity, grad is the gradient operator and T is the temperature.

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The Equivalent Heat Capacity Method

If it is further assumed that f^L is a unique fraction of temperature; $\dot{f}^L = \frac{df^L}{dT}\dot{T}$ ----- (5)

Then Eqn. 1,2 and 4 are combined to $\frac{c_p^{eff}}{V_m}\dot{T} = div(\kappa \ grad(T)) + \dot{Q} \quad ---- \quad (6)$

Where the effective heat capacity c_p^{eff} is given by: $c_p^{eff} = (\frac{df^L}{dT}\Delta H_m + c_P) \quad ---- \quad (7)$

This c_p^{eff} is then calculated using Scheil simulations; as shown for 316L stainless steel. Note that formation of ~0.1 vol% MS_B1 phase (MnS) effects the c_p^{eff} significantly which we can capture well.

Capturing these phenomenon are crucial to simulate AM calculations



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The Enthalpy Method and Steady-state Formulation

If we consider Eqn. 1 again

$$\frac{\dot{H}_m}{V_m} = -div(J_Q) + \dot{Q}$$

As per Rappaz(1989), there is no mathematical difference between enthalpy method or heat capacity method. We thus use enthalpy as it is calculated by Thermo-Calc as function of temperature. This equation solves the evolution of temperature during PBF-LB process for given material properties and process parameters

An important approximation is when one can solve the stationary heat-flow equation for a volume element moving with the heating source. In that case, we neglect the left-hand side of Eqn.8 and add a translation term

 $div(\kappa grad(T)) + \dot{Q} = \frac{v_b}{V_m}grad(H_m)$

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Where, v_b is the velocity of the heat source. We assume that as the scanning speed of laser used during processing.



Boundary condition for energy loss during AM

Four boundary conditions are imposed for capituring heat loss

1. Energy loss due to convection and radiation to gas

$$Q_L = h(T - T_{ambient}) + \varepsilon \sigma (T^4 - T_{ambient}^4)$$

Where h = convective heat transfer coefficient, $\varepsilon = \text{surface radition emissivity}$, $\sigma = \text{Stefan-Boltzmann constant}$ (5.669 x 10⁻⁸ W/m²K⁴). $T_{ambient}$ is the temperature of surrounding gas in build chamber (ambient temperature)

2. Energy loss due to heat lost through the vertical walls of the domain

 $Q_N = 0$

(adiabatic boundary condition)

3. Temperature of baseplate

 $T = T_{baseplate}$ (assumed as constant temperature input by user)

4. Heat loss due to evaporation of the material

 $Q_E = 0.82 J_E \Delta H_E$

Where J_E is the evaporation flux and ΔH_E is the evaporation enthalpy. For a multicompoent system, the evaporation flux is calculated with:

 $J_E = \frac{1}{\sqrt{2\pi MRT}} \left(P_0 \exp\left(\frac{-\Delta G_v}{RT}\right) - P \right)$

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Where ΔG_{ν} is the driving force for evaporation, *M* is molar mass of gas, *P* is the gas pressure inside the chamber, *P*₀ is the atmospheric pressure and *R* is the universal gas constant.

Even though we account for evaporation energy losses, we do not follow composition change with evaporation. To be implemented in coming releases©

101 **Evaporation** loss 10⁹ 🗕 q_dot q dot diffussionlesss Liq to gas — Gas to liq Zerc Radiation loss 100W 100um 300W 100um Convection h=20 Radiation e=0.8 Convection loss 105 1000 1500 2000 2500 3000 3500 4000 Temperature K

Different heat losses: Convection, Radiation and Evaporation. Evaporation losses at 100 W and 300 W laser power. Calculated on Ti-64 alloy with laser of ~100µm spot radius





Heat sources

Gaussian heat source

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The Gaussian heat source is modelled based on the <u>surface</u> heat source model initially proposed by Pavelec (1969) and is given by:

$$Q = \frac{2\varepsilon P}{\pi r^2} \exp\left(-2\frac{\left(x-X_p\right)^2 + \left(y-Y_p\right)^2}{r^2}\right)$$

where Q is the Power density deposited on the top surface (W/m²), $\varepsilon =$ Absorptivity of laser beam, P = Laser Power (W), r = Laser spot radius, x, y = coordinates of the computational domain and $X_p, Y_p =$ coordinates of the heat source.

Surface model means that power input from the heat source is only defined on the <u>top surface</u> of the workpiece and then heat energy diffuses into the workpiece depending on thermal diffusivity of the selected material.



Relationship between power intensity and size of gaussian beam ~100 µm diameter. **Beam diameter measured at 1/e² diameter** (86% radius in EOS)



Gaussian heat source

Heat sources

Double Ellipsoidal (Goldak) Heat Source (volumetric HS)

Model proposed by Goldak et al. (1984) and is used in welding/ AM simulations. The power input is defined on the surface and inside the powder bed, along the depth of powder bed. Heat distribution is given by two ellipsoids; one in front and other in rear quadrant

$$Q_{f} = f_{f} \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_{f} bc} \exp\left[-2\frac{\left(x-X_{p}\right)^{2}}{a_{f}^{2}} + \frac{\left(y-Y_{p}\right)^{2}}{b^{2}} + \frac{\left(z-Z_{p}\right)^{2}}{c^{2}}\right] \quad \text{---- For front quadrant}$$
$$Q_{r} = f_{r} \frac{6\sqrt{3}\varepsilon P}{\pi^{\frac{3}{2}} a_{r} bc} \exp\left[-2\frac{\left(x-X_{p}\right)^{2}}{a_{r}^{2}} + \frac{\left(y-Y_{p}\right)^{2}}{b^{2}} + \frac{\left(z-Z_{p}\right)^{2}}{c^{2}}\right] \quad \text{---- For rear quadrant}$$

 a_f , a_r are semi-axes of the front & rear ellipsoids. b, c are the semi-axes along the width and depth of the melt pool. f_f and f_r are proportional coefficients for front and rear ellipsoids, with the condition that $f_f + f_r = 2f_f$ is then written as $f_f = \frac{2a_f}{a_f + a_r}$

Conical Heat source (volumetric HS)

Gaussian heat distribution at top and conical distribution along the depth of the powder bed. This type of heat source is used more commonly in welding literature

$$Q = \frac{6\varepsilon P}{\pi H(r_e^2 + r_e r_i + r_i^2)} exp\left[-2\frac{(x - X_p)^2 + (y - Y_p)^2}{r_o^2}\right]$$

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With $r_o = r_e + (z - ZP) \frac{(r_e - r_i)}{H}$, where r_e and r_i are the cone radii at the top and bottom, while H is the height of the cone.



Axis definition of double ellipsoidal (Goldak) heat source



Axis definition of conical heat source

J. Goldak, A. Chakravarti, M. Bibby, A new finite element model for welding heat sources. Metall. Trans. B. 15, 299–305 (1984)

Power densities (W/m^3)

Steady-state and transient calculations



Steady-state

- Steady-state simulations are modelled as a "snapshot" for that parameter. It is true for AM simulations when you are certain melt pool has reached steady state and no perturbations are disturbing the process
- Scheil runs as normal to compute temperature dependent properties and then FE solver runs for one time to solve temperature field due to HS applied for that instant
- Useful for computing printability maps, knowing G vs v ratios etc.



Steady-state experiment setup IN625 Heat source: Gaussian



Transient Calculations

- Full-scale transient simulations in a 3D build part. User can define scanning strategy comprising multiple tracks and multiple layers
- The height, width, and length of the build or a representative segment of the build is specified. A scanning strategy with scan rotation either for a single track or for multiple tracks can be provided



Transient bidirectional setup with 67 scan rotation between layers Width: 4 mm, length: 5 mm and hatch: 0.165 mm



Transient single track experiment setup IN738 Heat source: double ellipsoidal with two probes placed in center, edge of melt pool



1. Grange, D., Queva, A., Guillemot, G., Bellet, M., Bartout, J. D., & Colin, C. (2021). Effect of processing parameters during the laser beam melting of Inconel 738: Comparison between simulated and experimental melt pool shape. Journal of Materials Processing Technology, 289. <u>https://doi.org/10.1016/j.jmatprotec.2020.116897</u>

Transient with steady-state

- Fully-transient calculations are computationally expensive but lead to better results both in terms of temperature distribution and melt pool dimensions
- Recommended if single tracks conducted or simple setup involved. It can <u>not</u> simulate with keyhole model yet
- For a more multi-layer and multi-track approach, Transient with heat source from Steady-state is recommended. It assumes that temperature distribution and fluid flow inside melt pool instantly reaches steady state. The solver calculates for energy equation, fluid flow and considers keyhole for given parameter in Steady-state
- Once the solution is reached, the melt pool is mapped as a heat source in transient simulations, instead of time resolved Navier-Stokes solution. This significantly reduces simulation time without compromising on accuracy of solution



Steady-state and transient calculations : example

- Different calculation types
- Setup:
 - Steady state calculation (Gaussian HS) : IN625
 - Transient calculation (double ellipsoidal HS) : IN738
- Discussion



Microstructure development

PBF-LB solidification occurs layer-by-layer

- When depositing (n+1)th layer, temperature of nth layer can cross critical temperatures (liquidus, solvus temperature for precipitation)
- Interfaces between layers: sites for formation of defects, intermetallics, residual stress etc.
- Some other temperature dependent phase transformations take place
 - Martensite formation

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- Secondary precipitation (ageing of powder bed)





AI-HS1 as-printed microstructure





Transient calculation of 5 layer deposition for Ti64 alloy (200 W, 1000 mm/s, 0.14 mm hatch and 0° scan rotation]. Time-temperature plot for probe shown

Heterogeneous nucleation via AM

Microstructure development



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1. Mehta, B., Frisk, K., & Nyborg, L. (2023). Advancing Novel Al-Mn-Cr-Zr Based Family of Alloys Tailored for Powder Bed Fusion-Laser Beam Process. Journal of Alloys and Compounds, 967, 171685. https://doi.org/10.1016/i.jallcom.2023.171685

 Durga, A., Pettersson, N. H., Malladi, S. B. A., Chen, Z., Guo, S., Nyborg, L., & Lindwall, G. (2021). Grain refinement in additively manufactured ferritic stainless steel by in situ inoculation using pre-alloyed powder. Scripta Materialia, 194, 113690. <u>https://doi.org/10.1016/j.scriptamat.2020.113690</u>

Home assignment

Steady state calculation of a melt pool in 316L stainless steel

Take from System definer \rightarrow Load Material \rightarrow 316L-StainlessSteel-UNS_S31603.xml provided to you. Define AM steady state calculation for this material

Laser power (W)	Speed (mm/s)	Layer thickness (µm)
215	1000	40

Heat source: Gaussian with 40 µm radius

- Consider fluid flow
- Consider both with/without keyhole model

Compare with experimental data and discuss

Experimental depth (µm)	Experimental half width (µm)
117.09 ± 5.8	69.6 ± 3.5

Experimental melt pools on 316 L Stainless steel printed at Chalmers University, Sweden On an EOS M290

