Simulations of Directed Energy Deposition process, High Speed Steel

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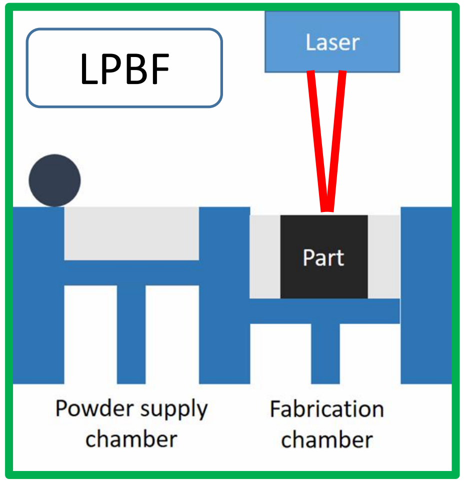
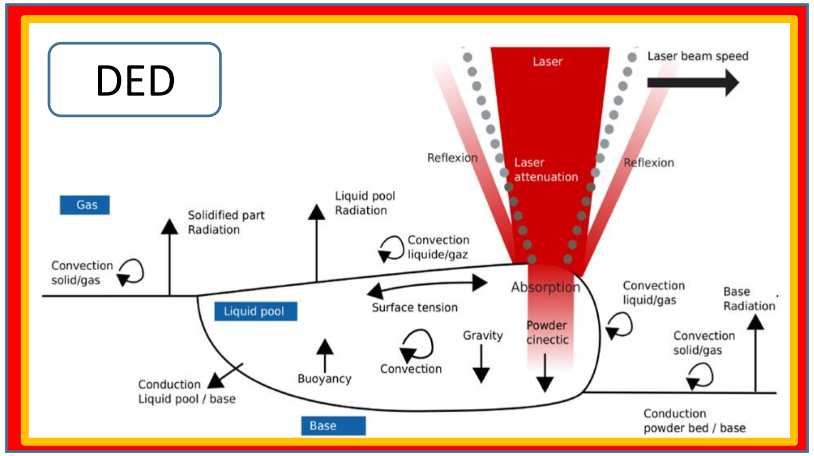
Content

- DED process
- M4 material
- Classical FE simulations
- Hybrid models coupling FE and Deep Learning
- What is next …



Additive Manufacturing a process family



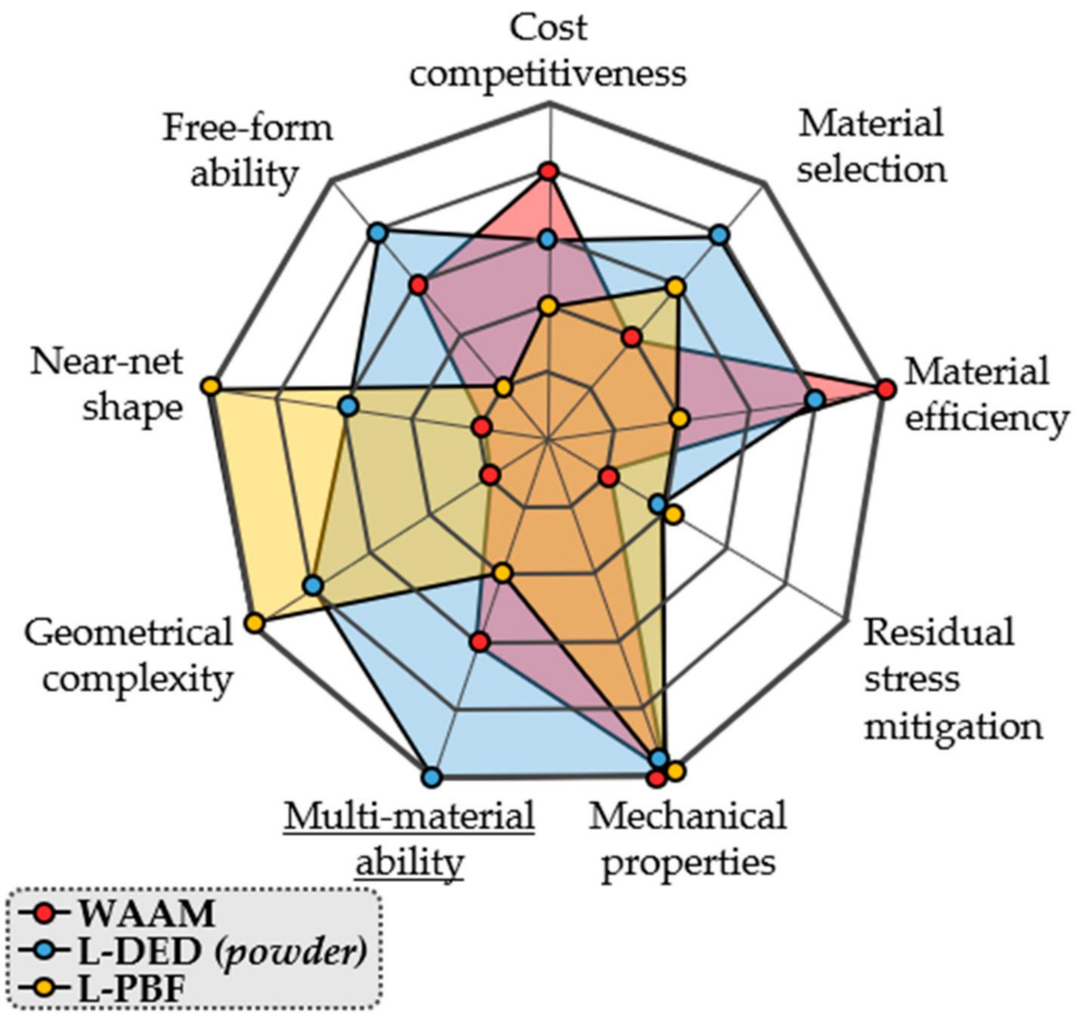
- Processes of metal AM
  - Powder
    - Powder bed
      - Laser → LPBF
      - Electron beam → EBM
    - Powder jet
      - Laser → **DED**
  - Wire
    - Electric arc → WAAM
    - Laser → DED-LW
    - Electron beam → EBAM

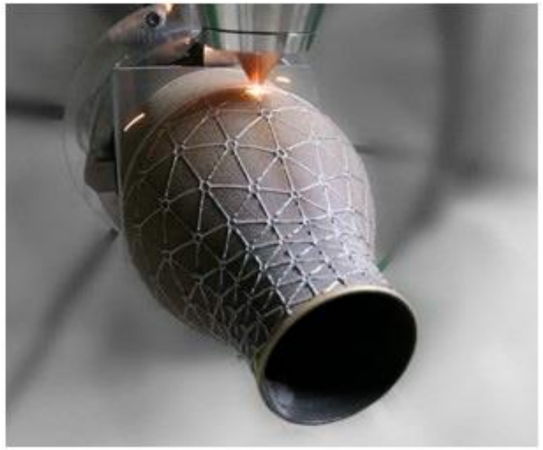
Material shape: Powder, Wire

Energy source: Laser, Electron beam, Laser, Electric arc, Laser, Electron beam

Fabrication process: LPBF, EBM, DED, WAAM, DED-LW, EBAM

DED advantages





Source: OPEN MIND Technologies AG

From Ostolaza, *Materials*, 2023

Feature	L-PBF	L-DED	WAAM
Part dimensions [mm]	max. 600 × 600 × 600	Virtually unlimited	Virtually unlimited
Surface finish, Ra [μm]	9–16	5–30	200
Dimensional accuracy [mm]	0.05–0.1	0.5–1.0	1.0–2.0
Build rate [g·min^{-1}]	3–4	6–50	300–400
Densification	>99%	>99%	>99%

Functionally graded materials German Aerospace Center (DLR)

Titanium blisk repairing

Nowotny *J. Therm. Spray Technol.*,2007

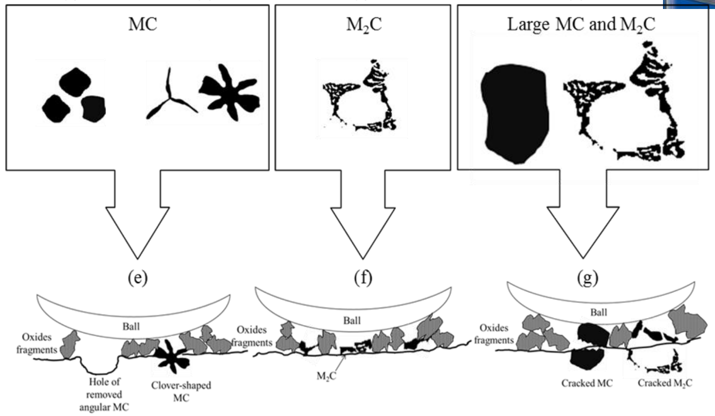
M4 material - High speed steel

- Fe-Cr-C-X alloys with X: carbide-forming element (i.e. V, Nb, Mo or W)

- Hard carbides ⇒ High hardness and wear resistance

→High speed machining cutting tools

→Cylinders
for hot rolling mills



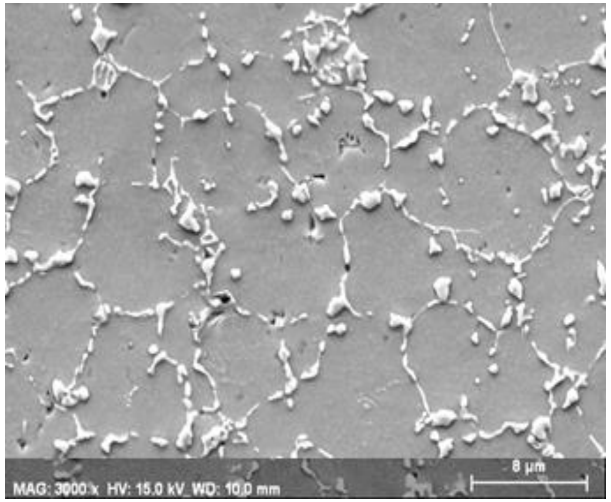
From Hashemi, *Surface & Coatings Technology*, 2017

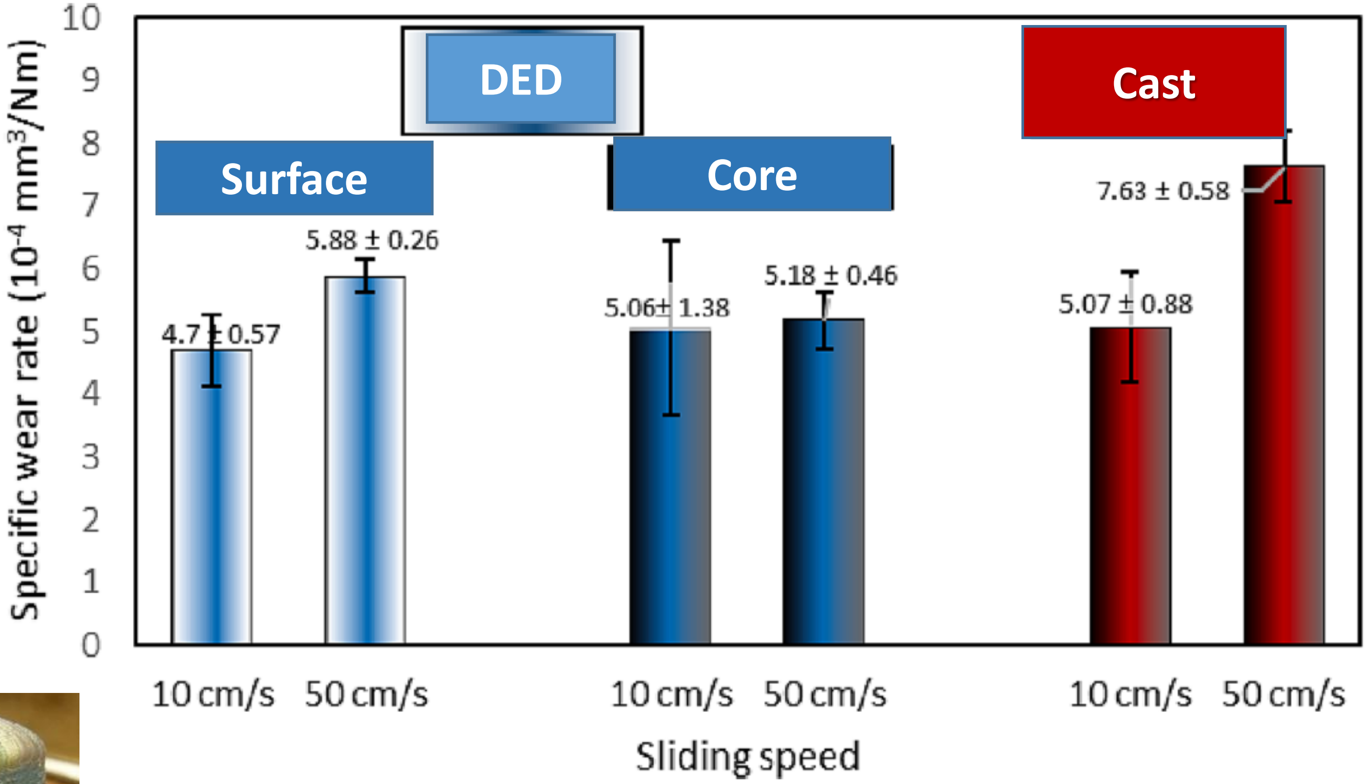
M4 powder composition

C	Mn	Cr	Mo	V	W	Ni	Si	Fe
1.35	0.34	4.30	4.64	4.10	5.60	0.9	0.33	Balance

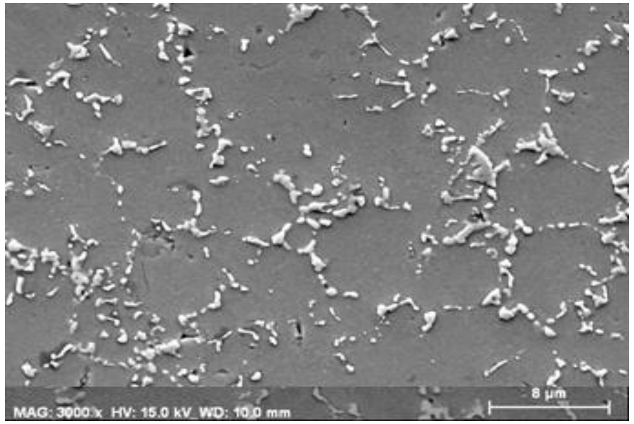
Motivation: Understand –Predict - Optimize

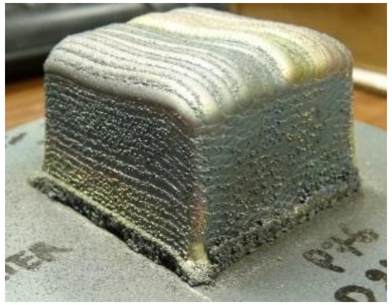
Near surface, Continuous M_2C network at grain boundaries





Middle height, Discontinuous network of M_2C





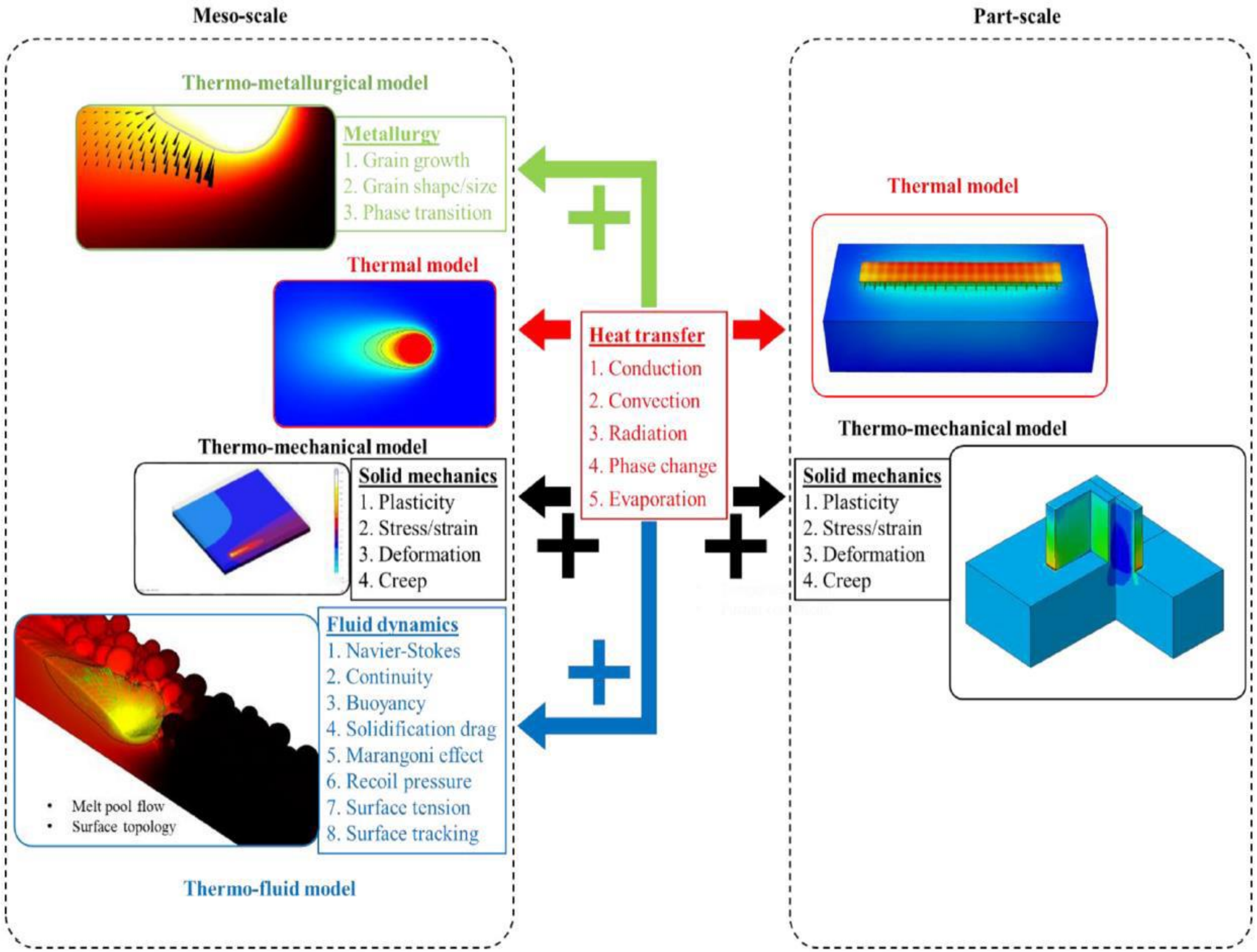
Process model to predict microstructure features

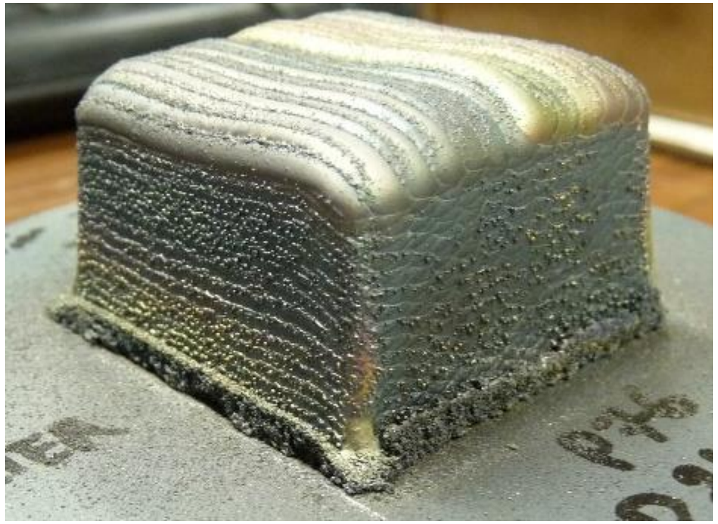
DED Model ?

AM Simulations : Priorities

1 Select your scale for your target

2 Predict an accurate thermal field



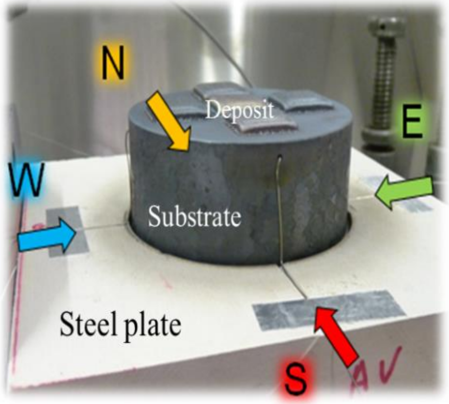


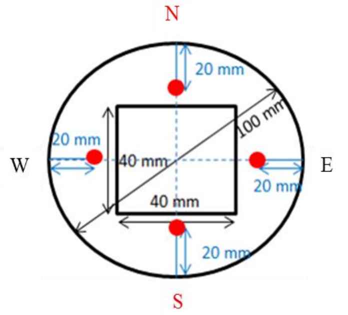
40 x 40 x 27.5 mm **(874 tracks)**

Goal = Homogeneous properties

→ Thermal 2D model enough

4 Thermocouples Tp(time)

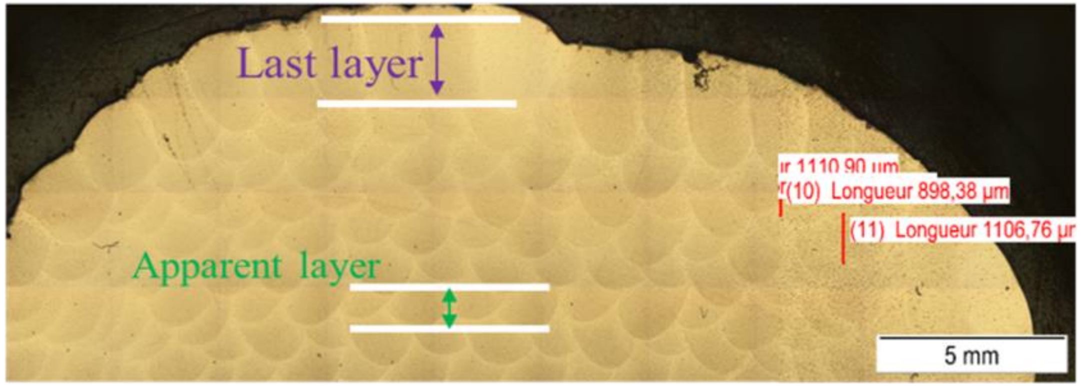




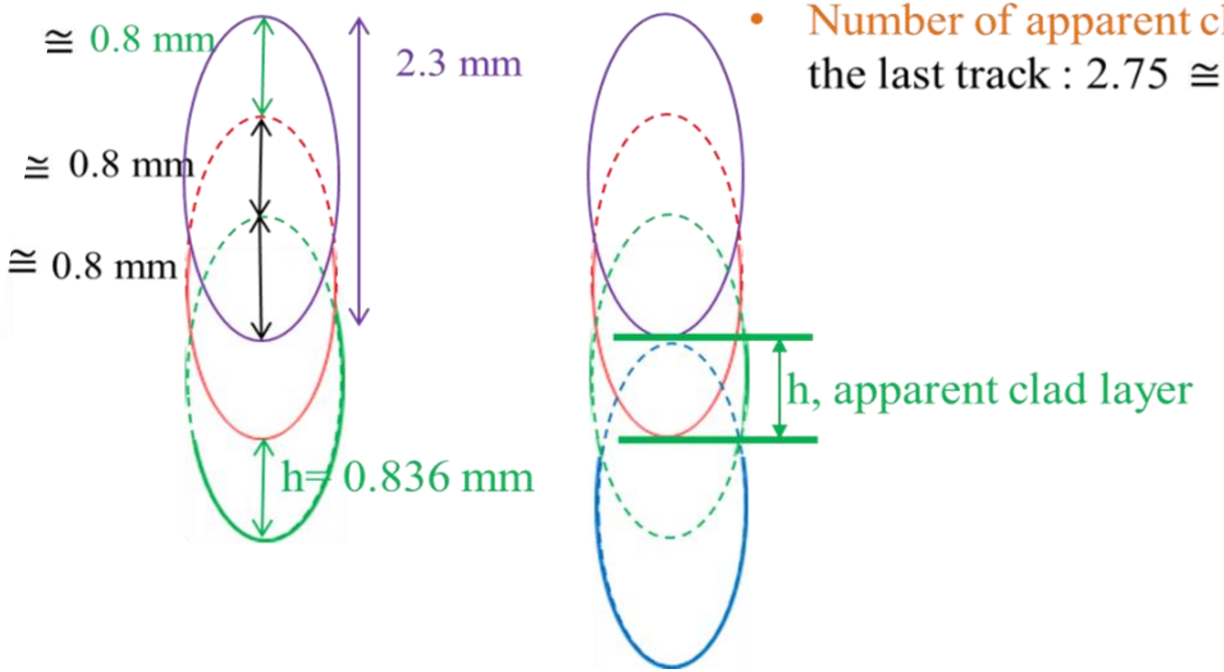
+ microstructure

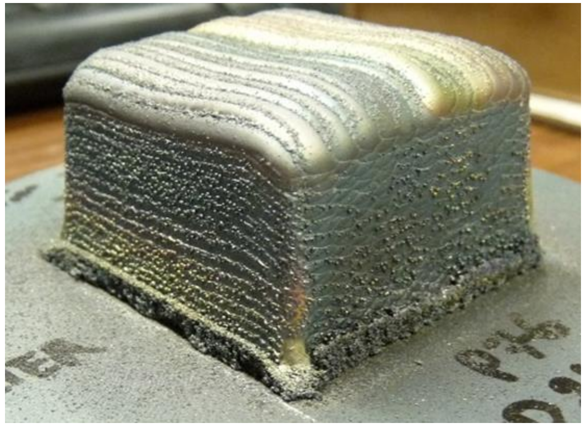
+ layer height

Layer height - Case of constant Laser Power



- Average height of the last clad layer (H_{layer}) (top of the deposit) : 2300 µm = 2.3 mm = real clad layer height
- Average height of apparent clad layer (h) : 836 µm = 0.836 mm
- Number of apparent clad layers in the last track : 2.75 ≅ 3





Mean height (H) of last layer : 2.3 mm

	Bulk Sample
Laser beam speed (mm/s)	6.67
Laser power (W)	1100
Pre-heating (°C)	300
Mass flow (mg/s)	76
Number of tracks per layer	27
Total number of layers	36

Thermal equations in FE home made code Lagamine

Heat transfer by conduction

$$\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+Q_{\text{int}}=\rho c_p\frac{\partial T}{\partial t}$$

Conductivity

Volume energy

Density

Heat Capacity

Heat transfer per convection and radiation

$$-k.(\nabla T.n)=-h(T-T_0)-\varepsilon\sigma(T^4-T_0^4)$$

Convection Coef.

Emissivity

Stefan-Boltzmann Constant

Solid FE Software
Many laws
Interfaces with Abaqus
with Metafor
In Fr, CL, NL, VTNM…

Melting latent Heat

$$C_p^{\;*}=\frac{L_f}{T_{em}-T_{sm}}+C_p$$

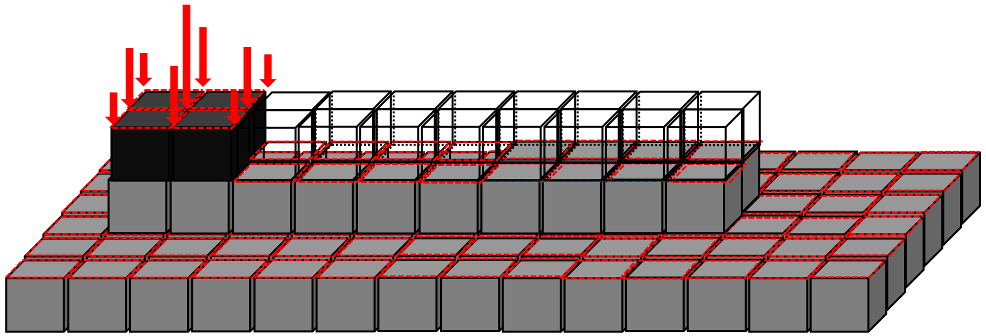
Enthalpic formulation

Enthalpy

$$H=\int\rho\cdot c(T)\mathrm{d}T$$

Software developed since 1984
in Uliege - Metals - Soil
http://www.lagamine.uliege.be/dokuwiki/doku.php

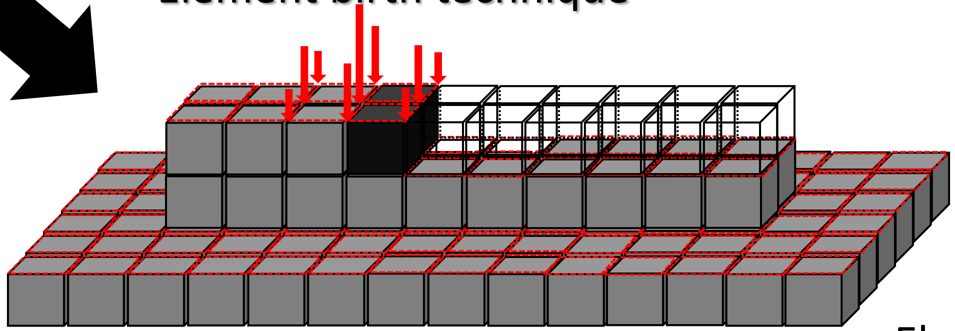
Element birth technique

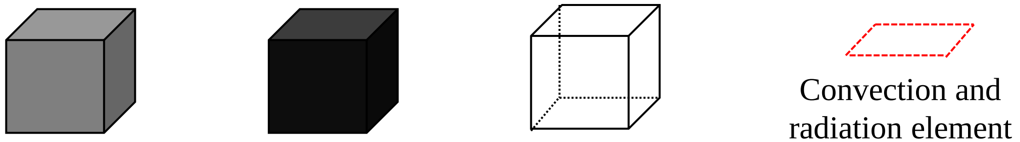


Variable number of elements, node, DOF
Heat flow and new material simulated by 2 to 9 elements
Boundary conditions = interface elements
adapted to solid element

For a thin wall 3D
Bulk Sample 2D

Element birth technique





Element size defined by laser beam size !
→ Direct mesh convergence
→ Mesh variable density by GMSH

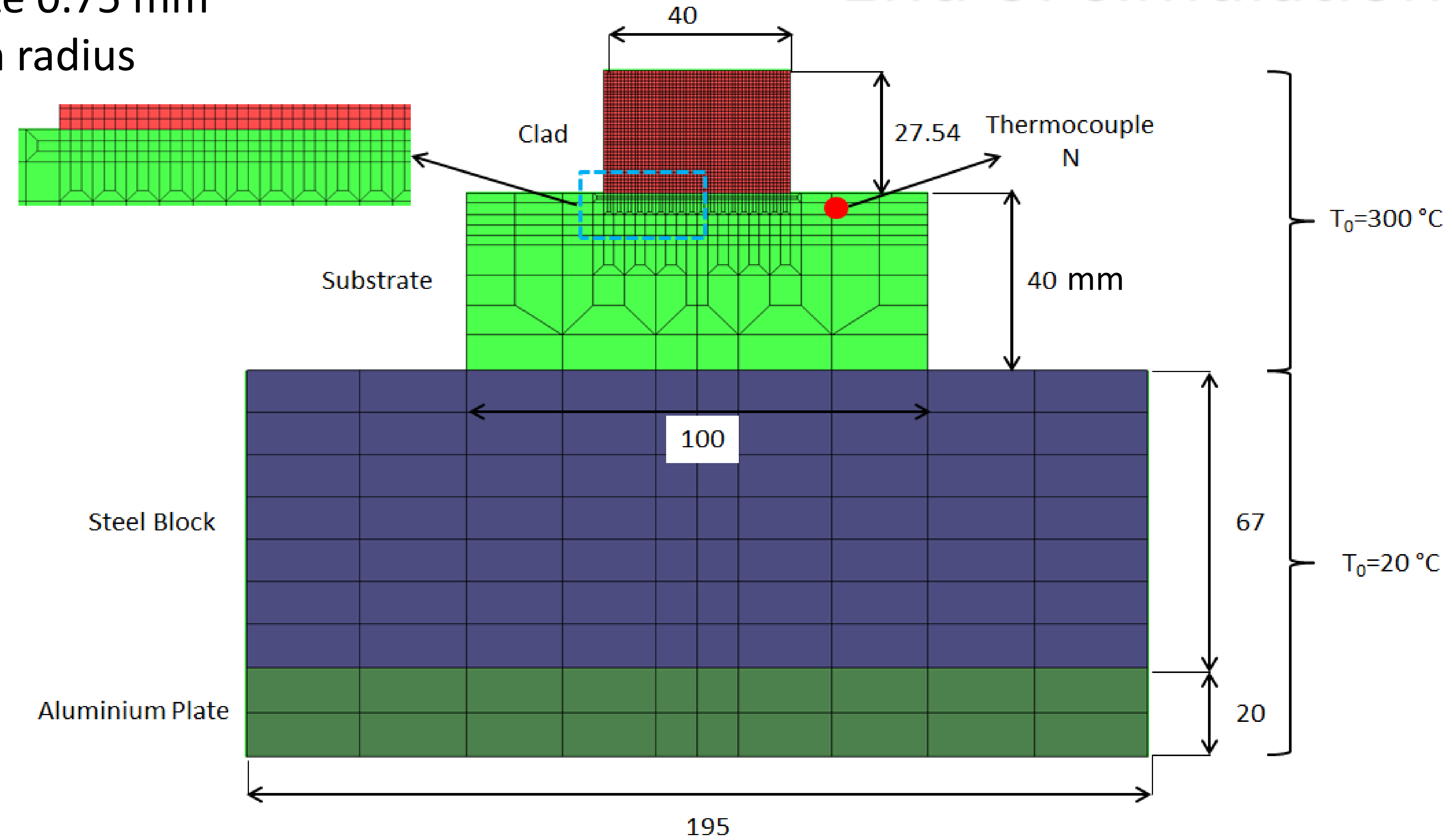
Convection-radiation elem. on vertical planes of the clad not drawn

FE thermal mesh of Bulk sample

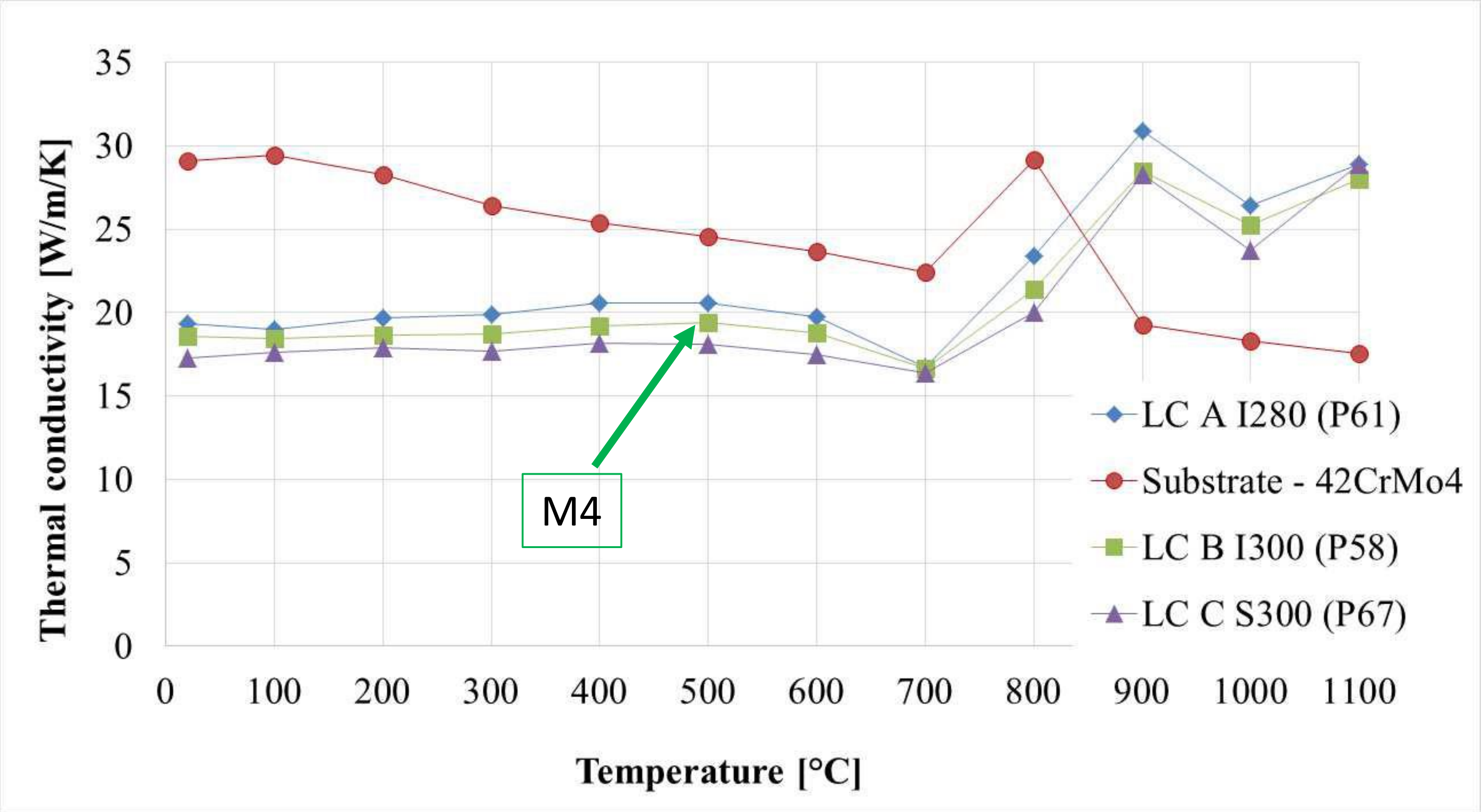
End of simulation

Element size 0.75 mm

Laser beam radius



Measured Thermo-physical parameters k c_p L_f ρ



Conductivity for the substrate
Three powder compositions
LC B = M4

Hashemi PhD Thesis Uliege 2017 measurements from bulk samples
Jardin Metals 2020 Thin wall samples (tables of data sets)

Experimental errors

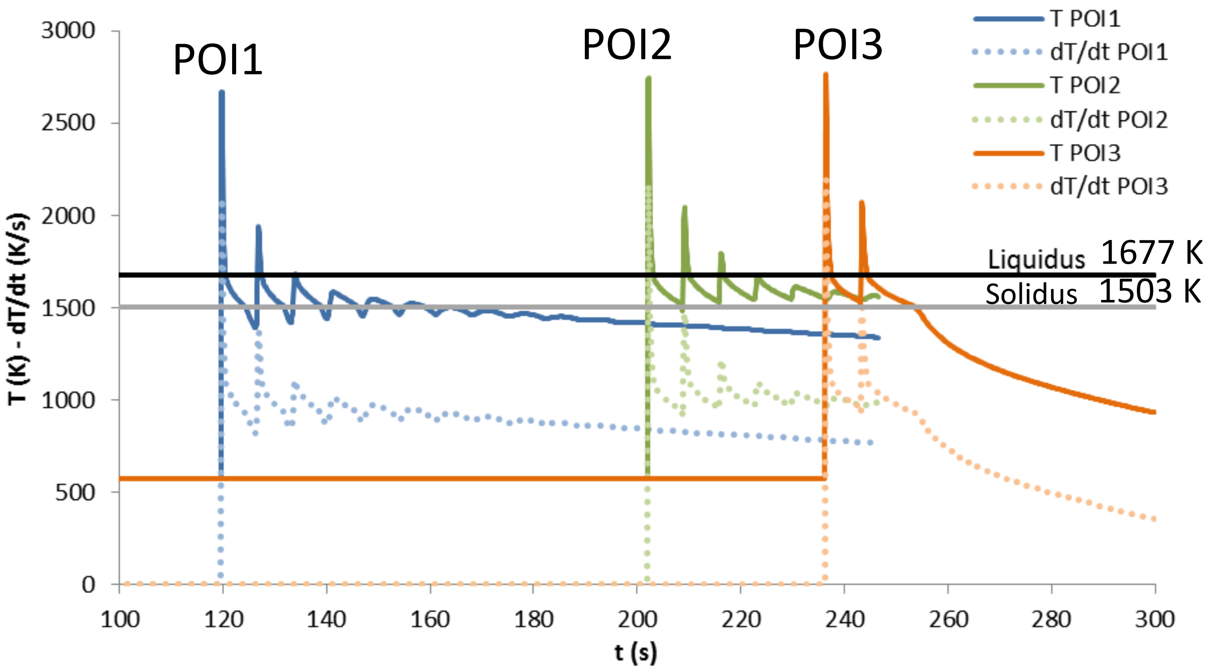
2% for density ρ
5 % enthalpy L_f
5% heat capacity c_p
2% on thermal diffusivity

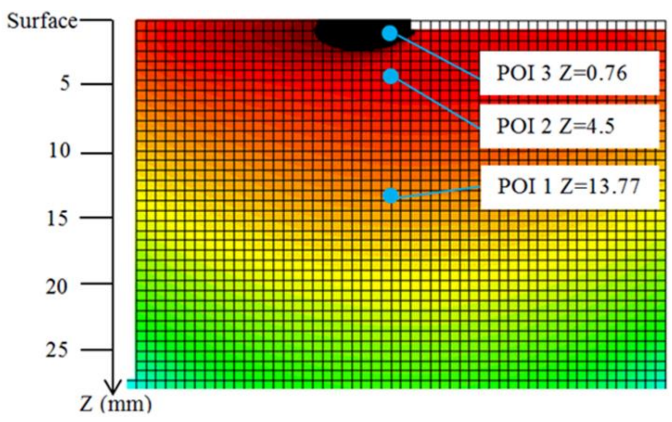
7 % for conductivity k

Differential Scanning Calorimetry Analysis, Laser Flash, Dilatometry, Pycnometer, Scale

FE predicted Tp at the substrate level
→Δ 44°C if reference data set or error affected ones

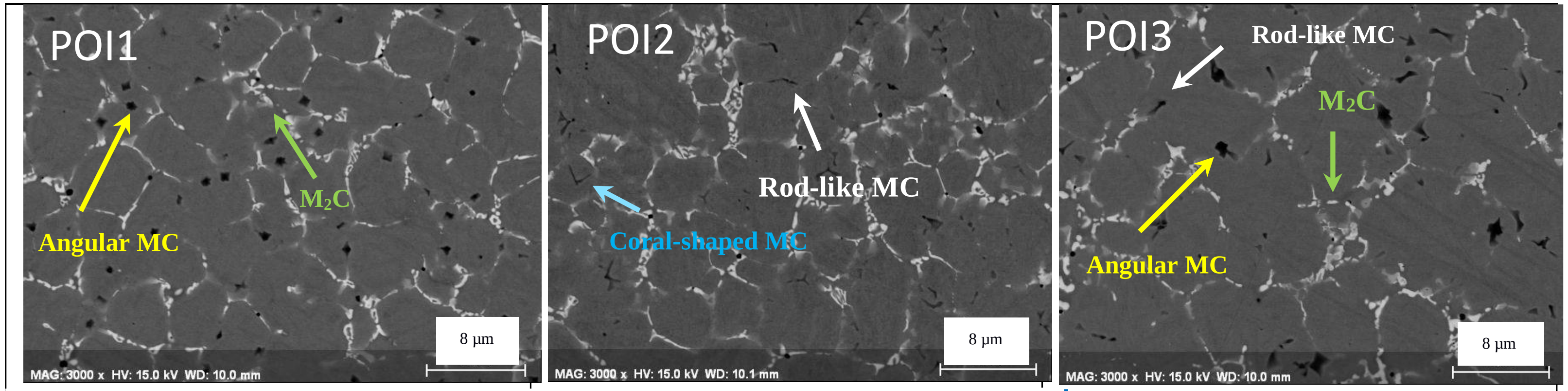
FE Tp field & history in the clad





Jardin Materials Letters 2019

-Number of full partial remelting
-Tp° Level between solidus and liquidus
- Superheating temperature

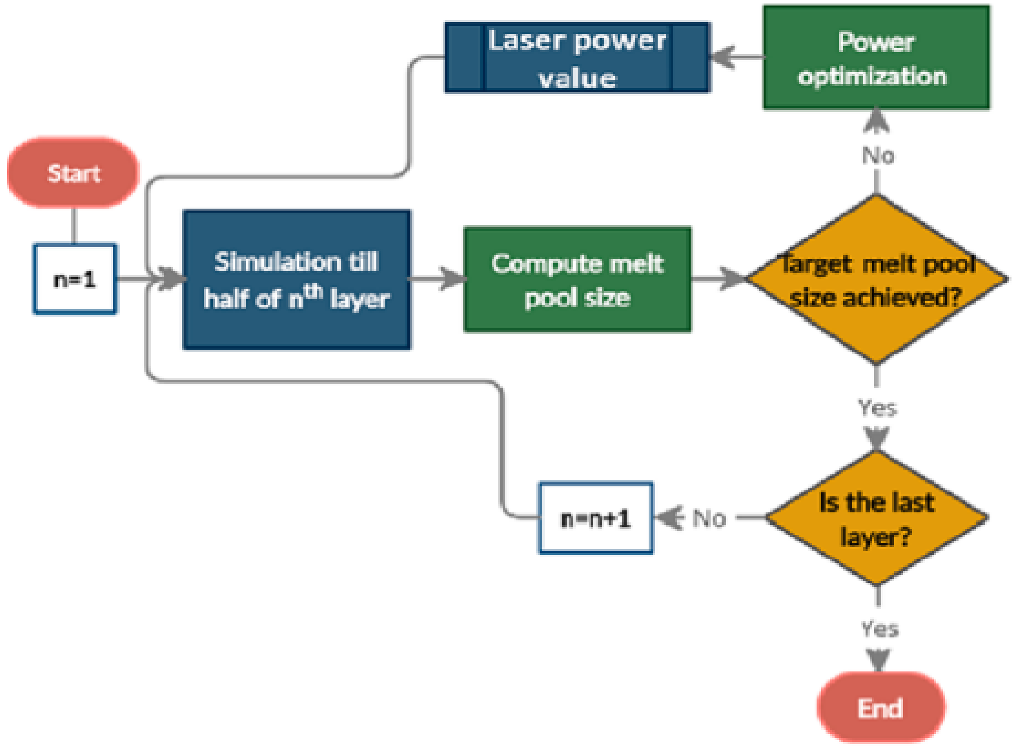


POI1	POI2	POI3
star-like MC lamellar eutectic M_2C intercellular carbides	coral-shaped **intra**cellular MC, intercellular eutectic M_2C and refined cells due to multiple melting	coarse angular MC eutectic M_2C within intercellular zones larger cell

Within DED process
substrate pre-heated in a furnace

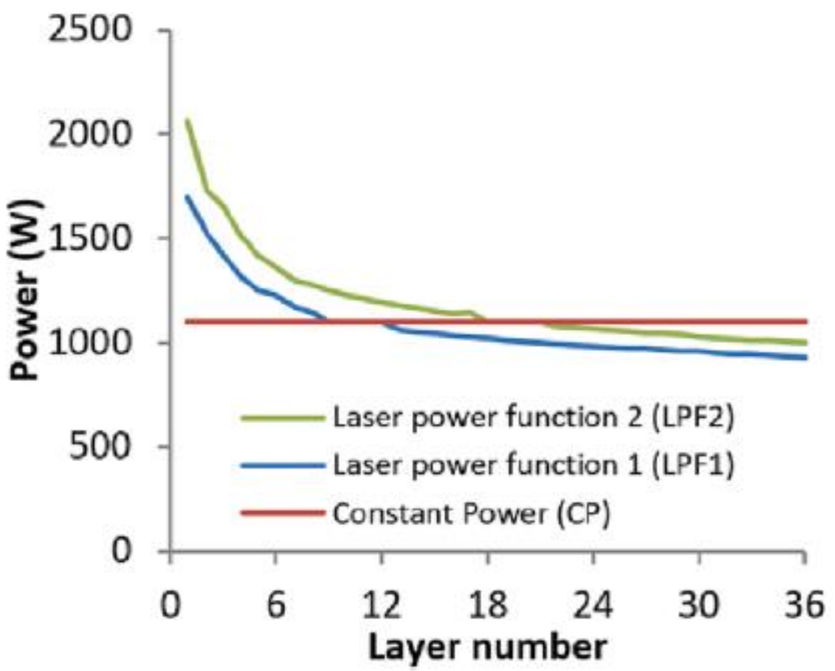
Laser power optimization

(↗ microstructure homogeneity)



Netwton Raphson algorithm to adjust Laser Power
To reach constant melt pool size (LPF1 LPF2)

LPF 1 → 1.4 mm depth, 4.4 mm length
LPF 2 → 1.8 mm 5.7 mm



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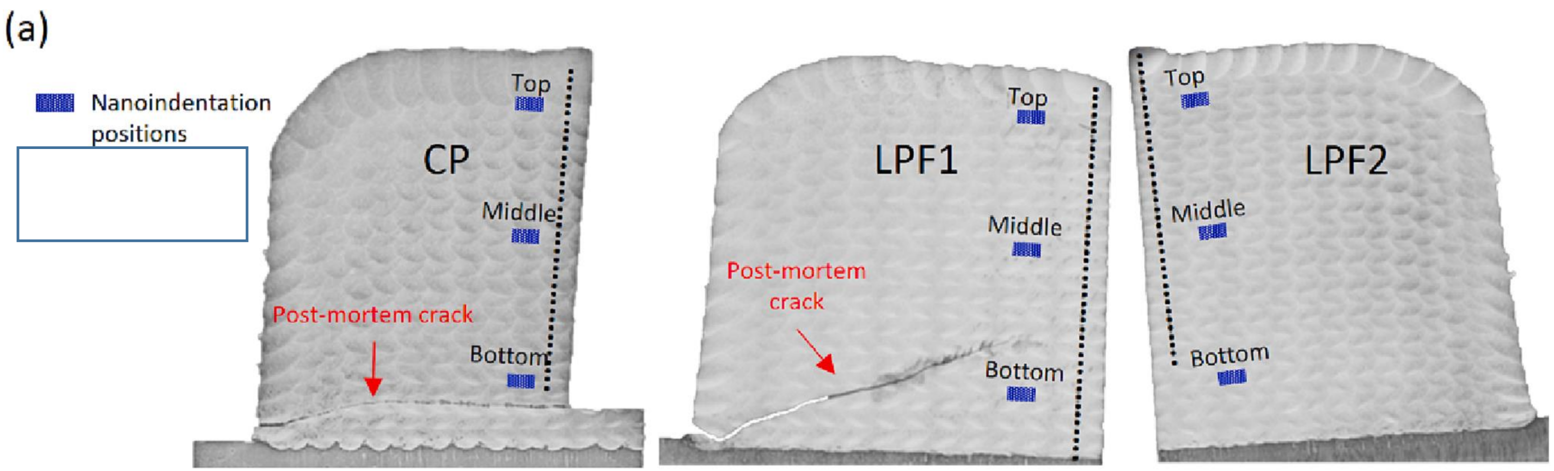
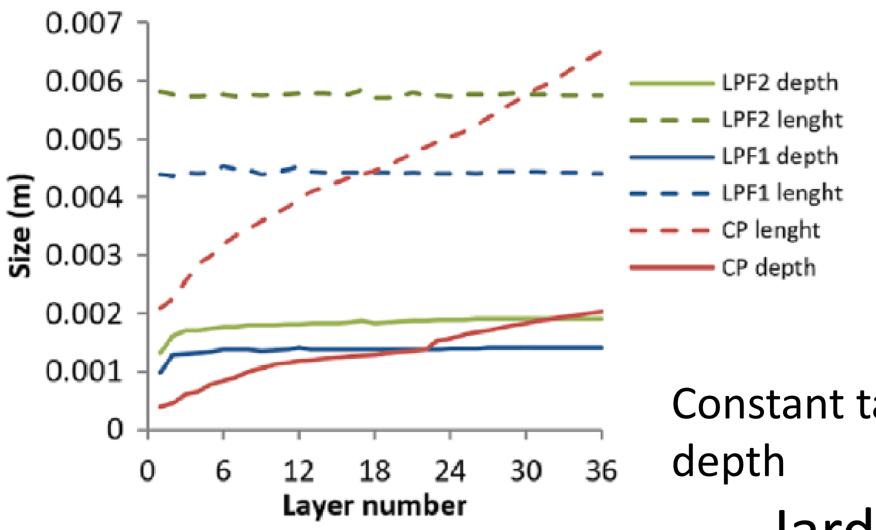
……. Vickers measurements

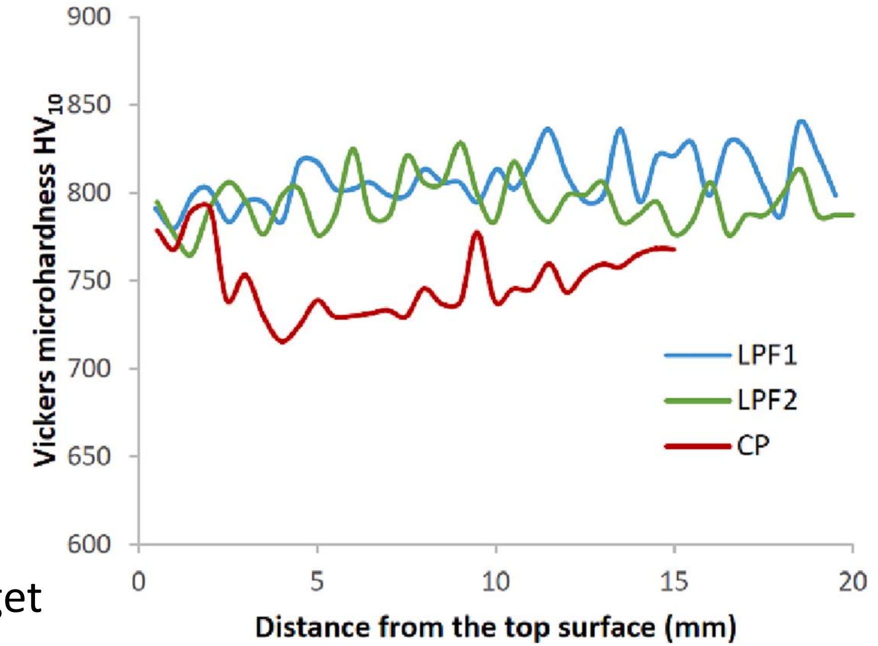
Hardness measurements → Homogeneity ?



Predicted melt pool depth & length



Constant target depth



Average values of Vickers microhardness of DED M4 steel	
Laser Power Function	HV_{10}
Constant	748 ± 19
LPF1	803 ± 15
LPF2	791 ± 14

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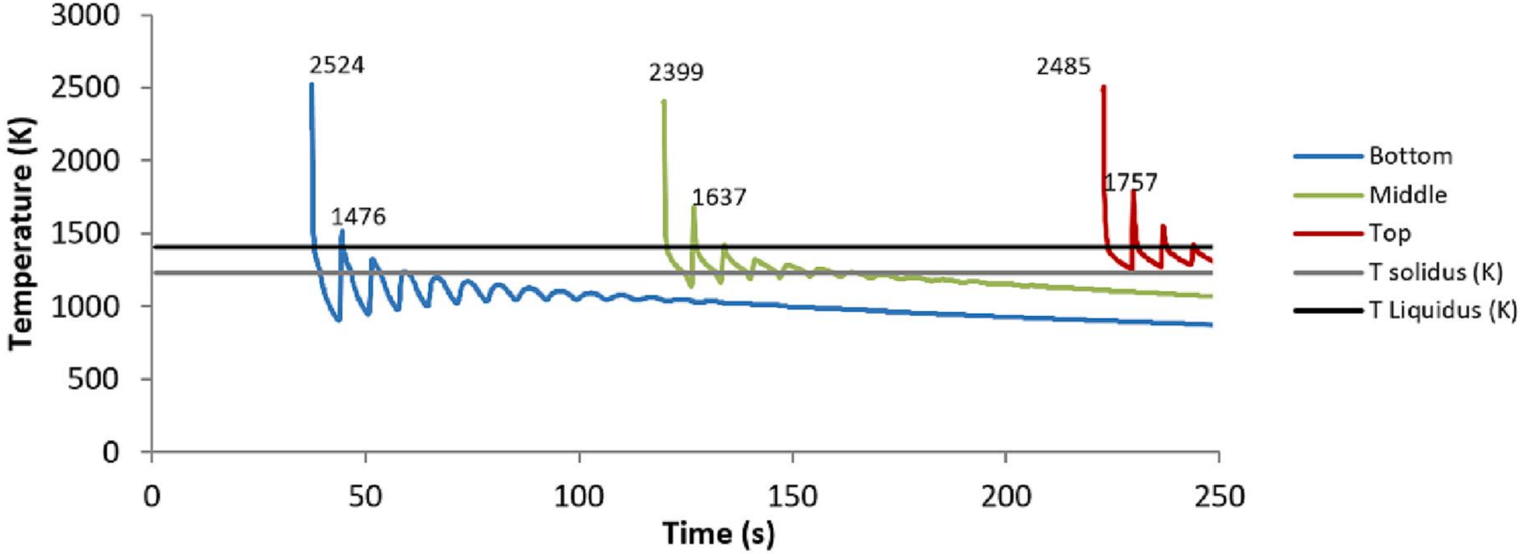
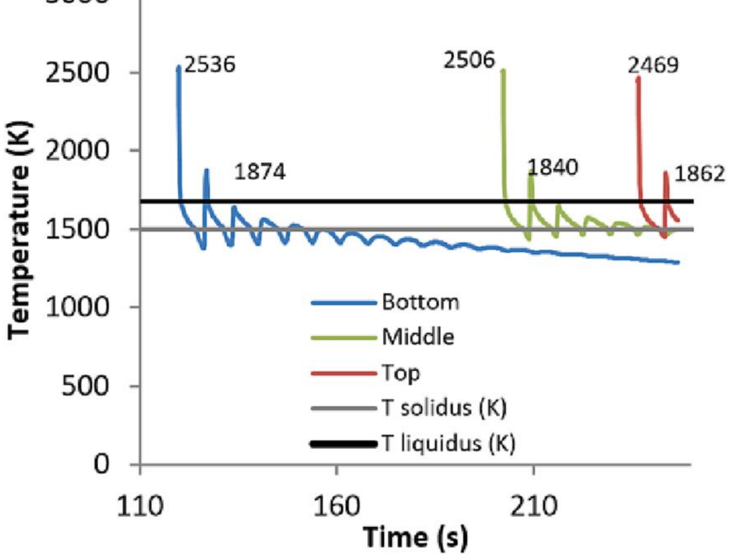
Result analysis

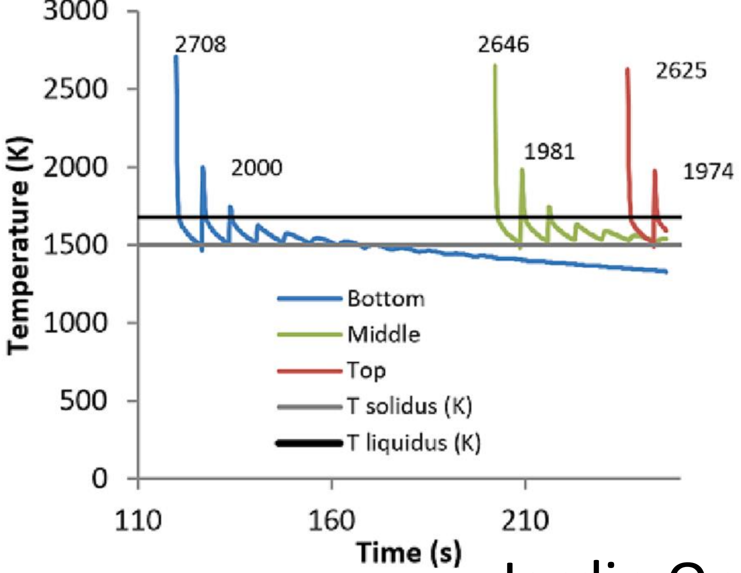
Constant Power



LPF1



LPF2



LPF2

Higher homogeneity

Higher in situ annealing Tp°

Average max peak Tp°

LPF2 : 2569 K

LPF1: 2505 K

CP : 2469 K

Higher accumulation of heat

→ slower cooling process

→ more homogenous microstructure

→ lower residual stresses

→ No crack in LPF2 sample at cutting.

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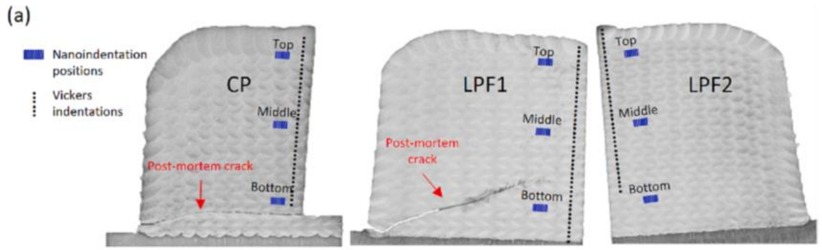
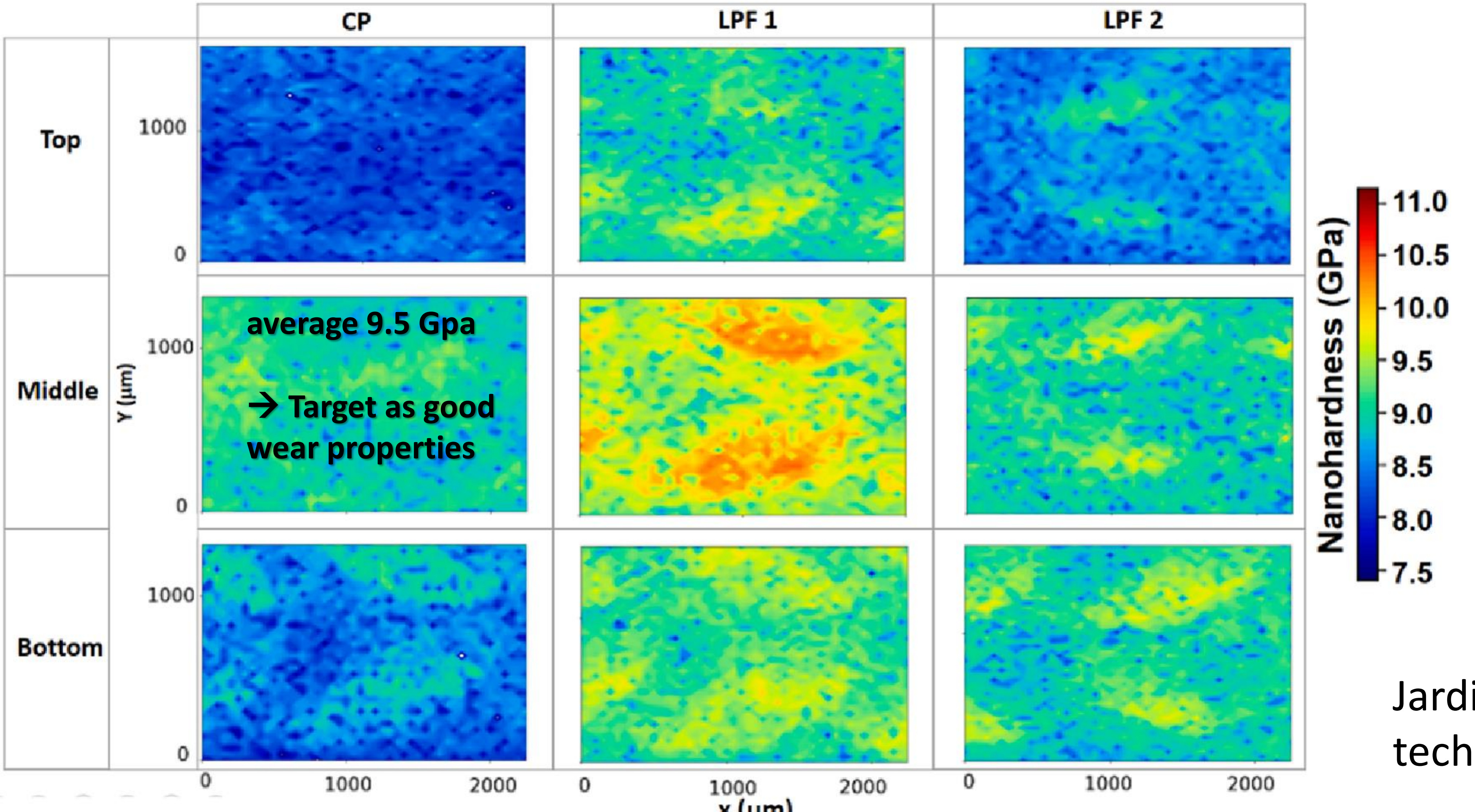
Nano indentation maps





Homogeneity of LPF2 confirmed + high level of hardness = optimum

Melt pool size
→ CFD needed

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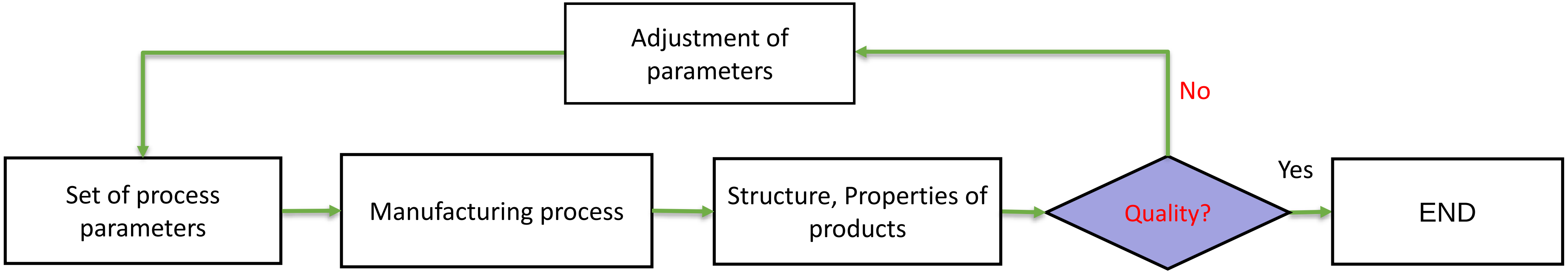
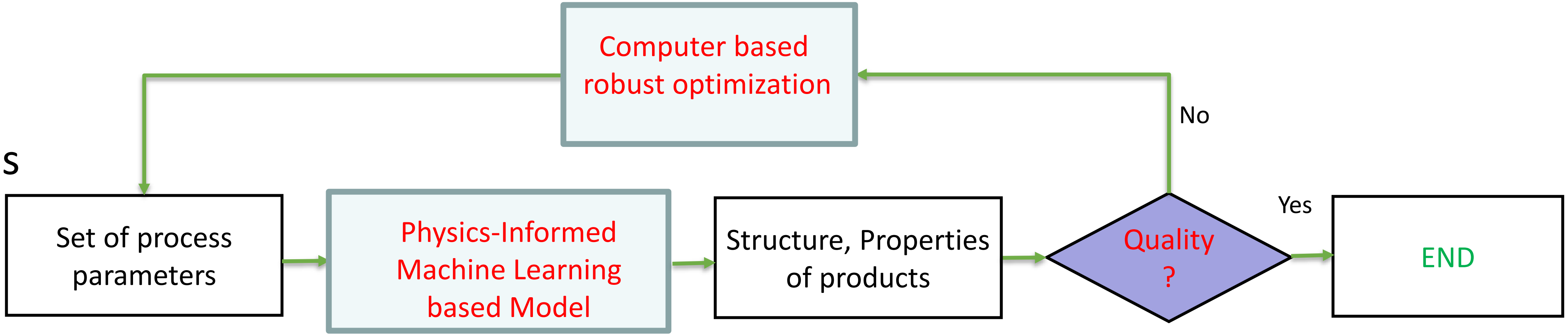
Process <u>robust</u> optimization
(it takes into account uncertainty)

Trials and Errors Without any FE or DL predictions



FE + DL predictions speed up the



Uncertainties, Optimisation, Robustness in DED?

For large amount of simulations interest of surrogate models DL

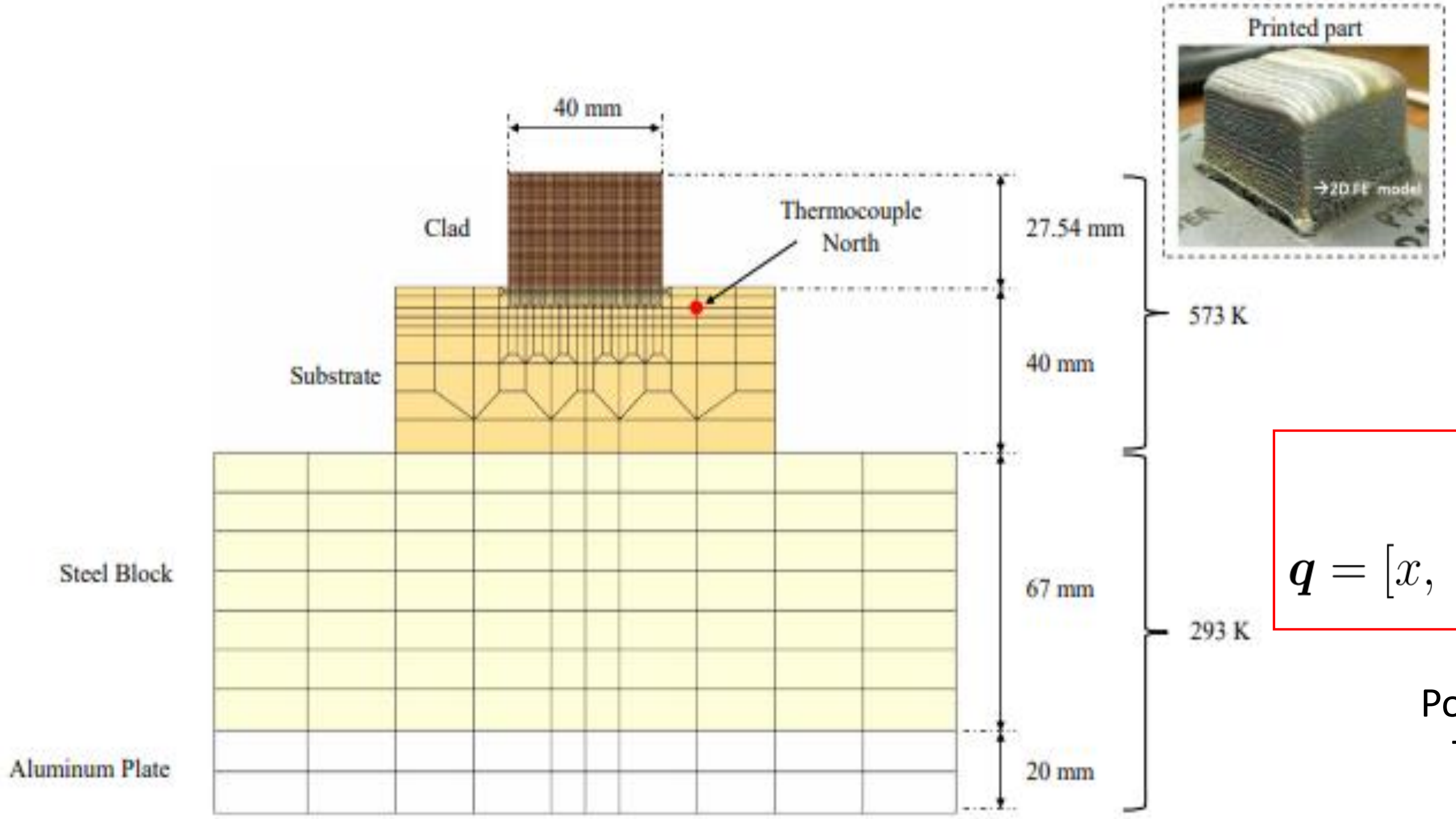
1. FFNN able to predict Tp° field *T.Q.D Pham Journal of Intelligent Manufacturing 2022*
2. Uncertainty effects *T.Q.D Pham Probabilistic-Engineering-Mechanics 2022*
3. Robust optimization (constant melt pool & energy minimum) *T.Q.D Pham Journal of Manufacturing Processes 2023*

Ongoing T.Q.D. Pham Phd

Develop physics computational model → Dataset & Machine Learning model → Uncertainty Quantification → Optimization under uncertainty, sensitivity analysis

1st paper | 2nd paper | 3rd paper

Feed Forward Neural Network (FFNN) replaces FE



Input ***q***

Output T

$$T = T(\boldsymbol{q}),$$

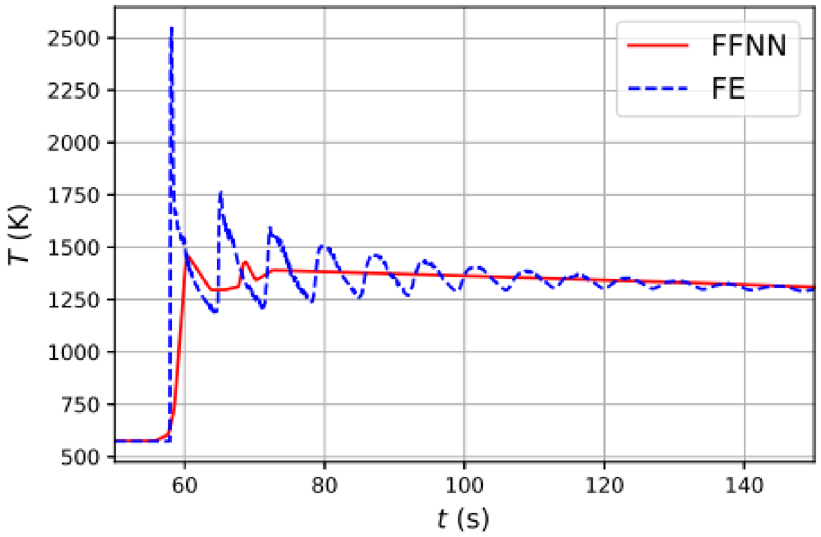
$$\boldsymbol{q} = [x,\ y,\quad t,\ m_1,\ \ldots,m_\mu,\ p_1,\ \ldots,p_\nu]$$

Position, Time	Material properties	Process parameters

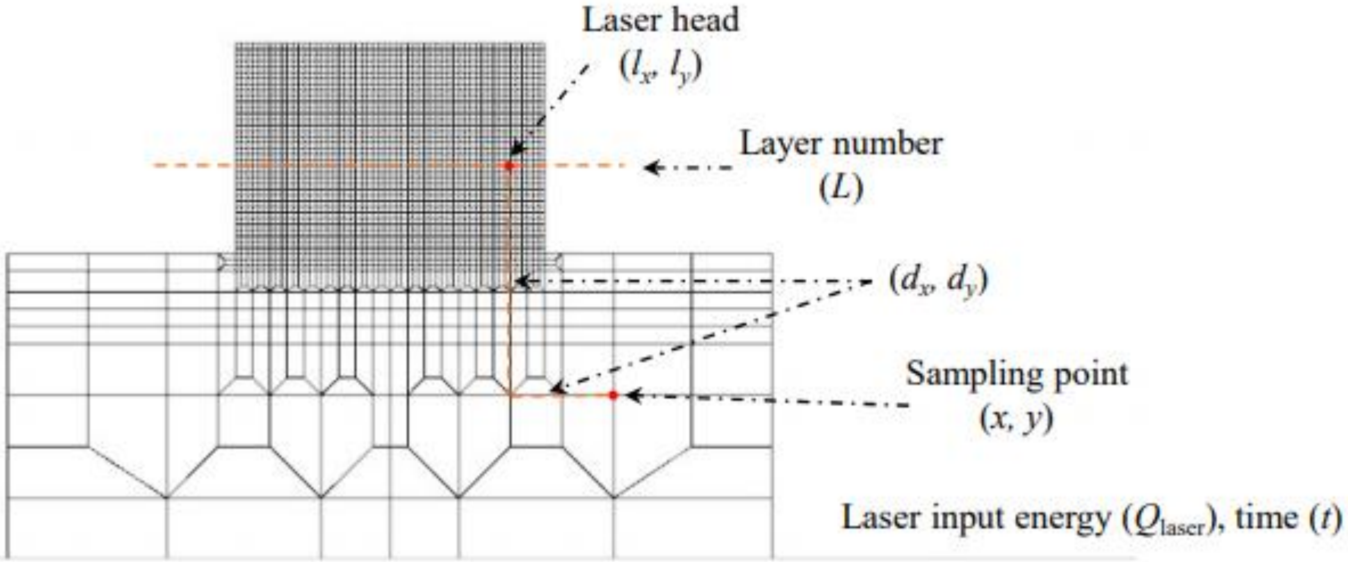
T.Q.D Pham Journal of Intelligent Manufacturing 2022

Feature selection *q*

Using only the $(x, y, t, Q_{\text{laser}})$



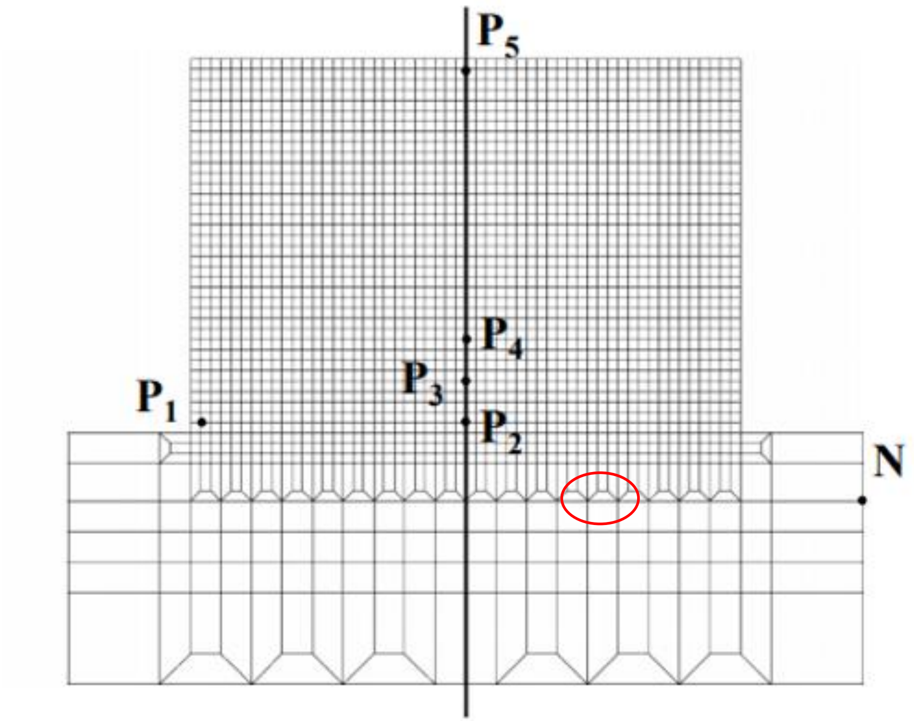
Integrate **physics**

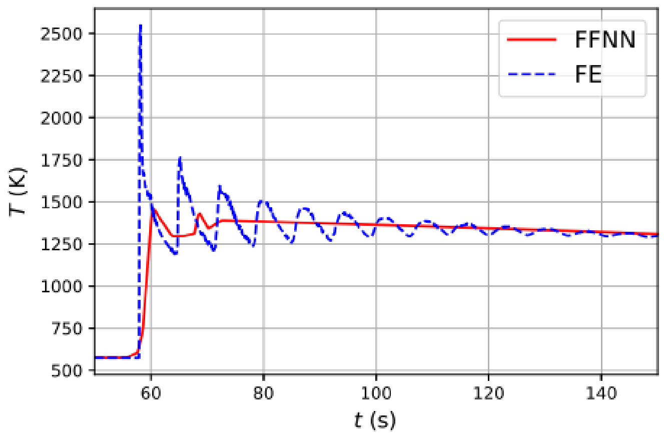


Model	Base model (BM)	Intermediate model (IM)	Full model (FM)
Input features	$x, y, t, Q_{\text{laser}}$	$x, y, t, l_x, l_y, Q_{\text{laser}}$	$x, y, t, l_x, l_y, d_x, d_y, L, Q_{\text{laser}}$
Number of input features	4	6	9
R^2	0.798	0.968	0.994

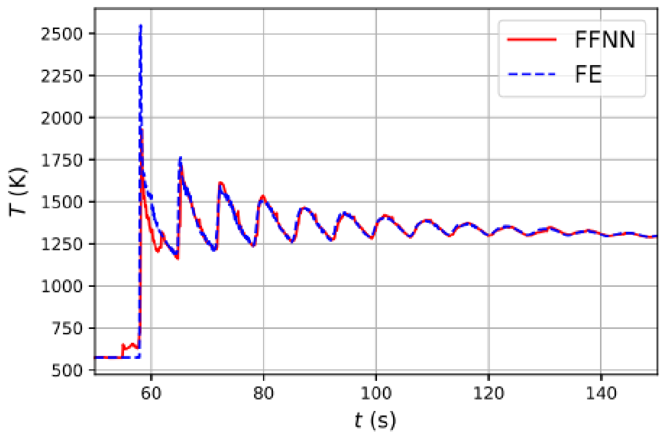
T.Q.D Pham Journal of Intelligent Manufacturing 2022

FFNN Result analysis Tp° at Point 2

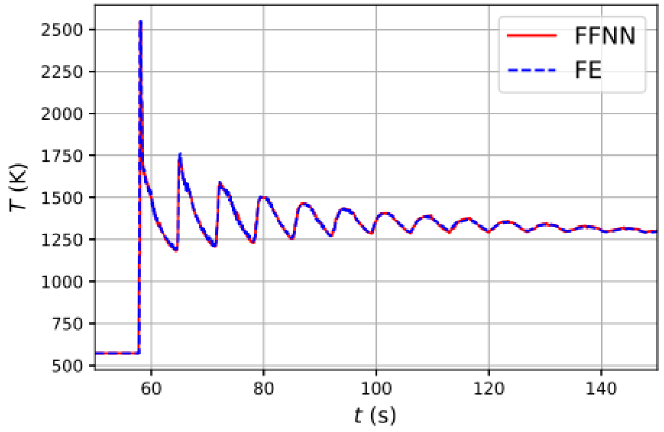




Base model (4)



Intermediate model (6)



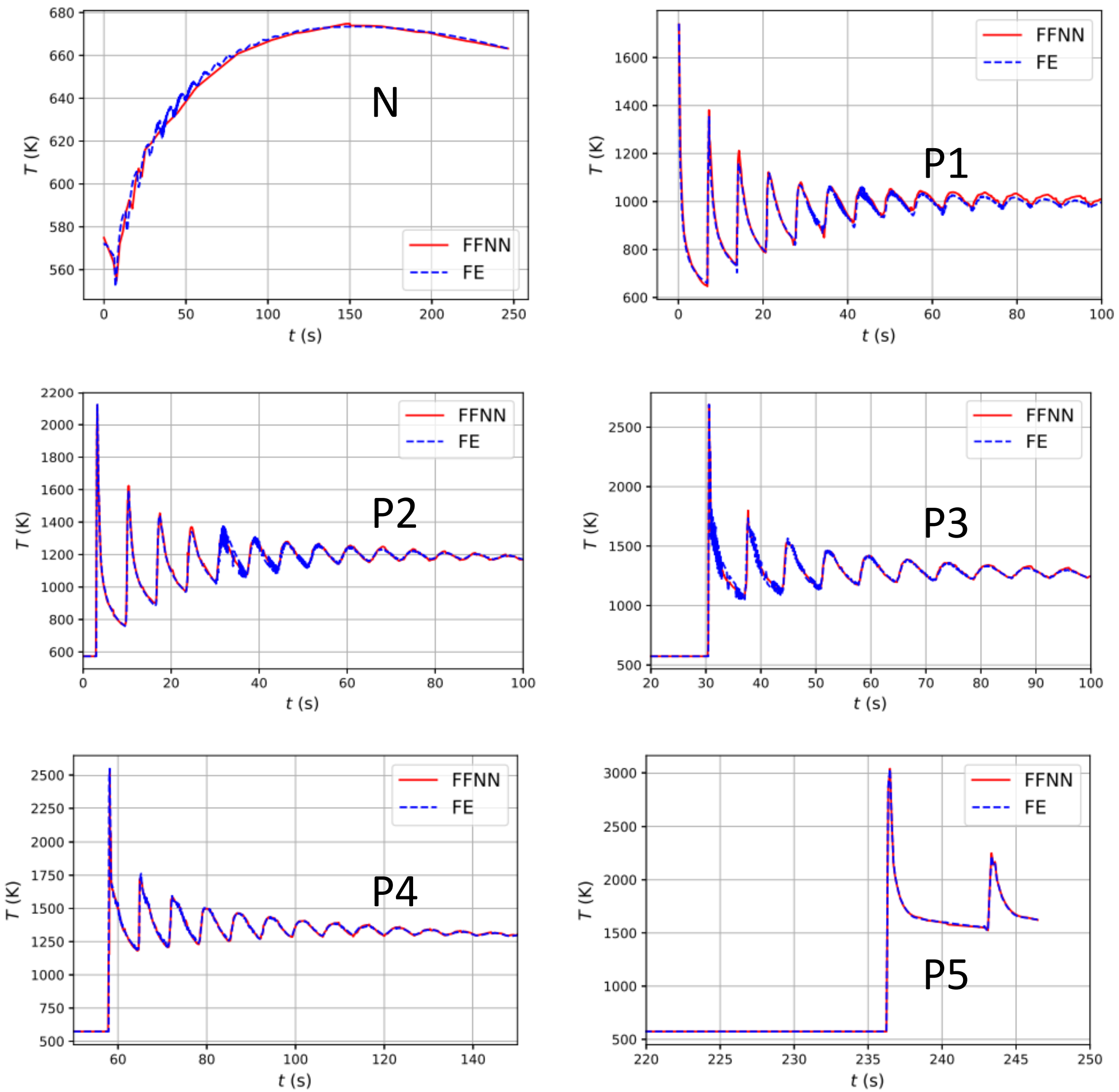
Full model (9)

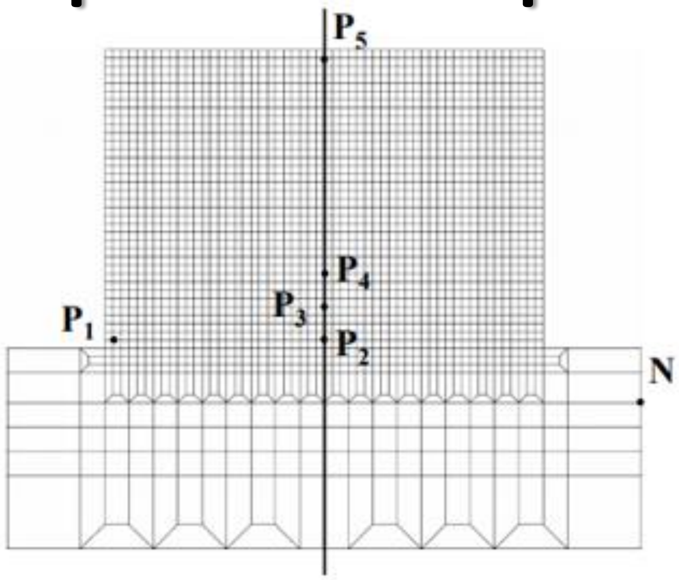
Integrating physics to the ML model to capture cycles and peaks

T.Q.D Pham Journal of Intelligent Manufacturing 2022

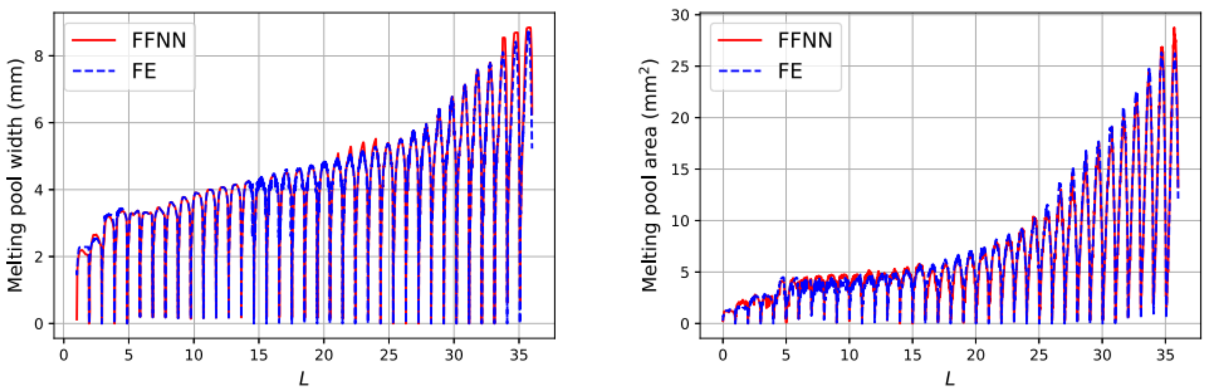
FFNN Result analysis Tp° + Melt pool size

Tp° history T(t)



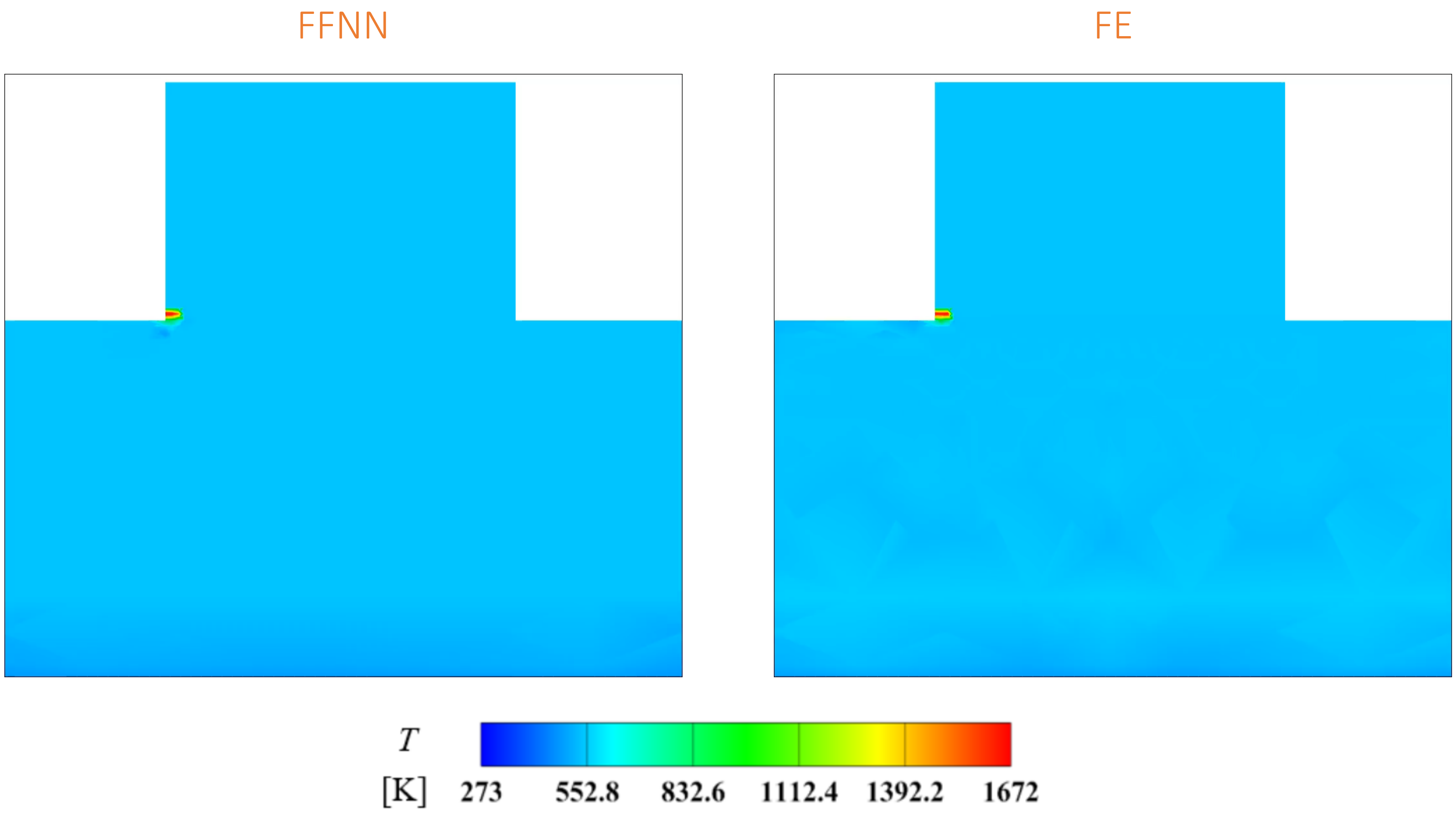


Melting pool

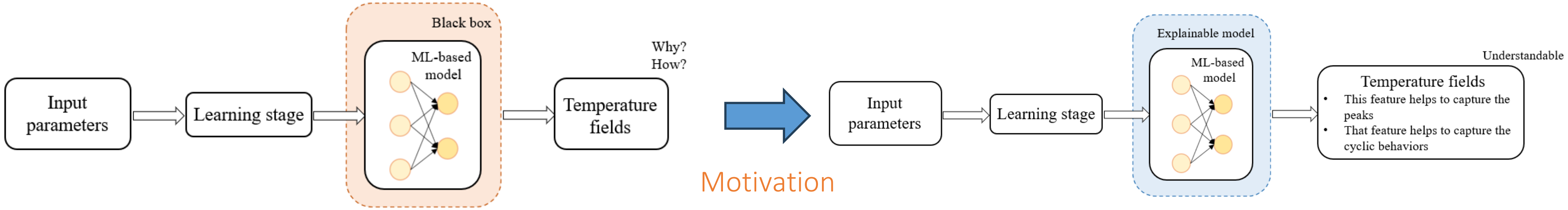


For each layer

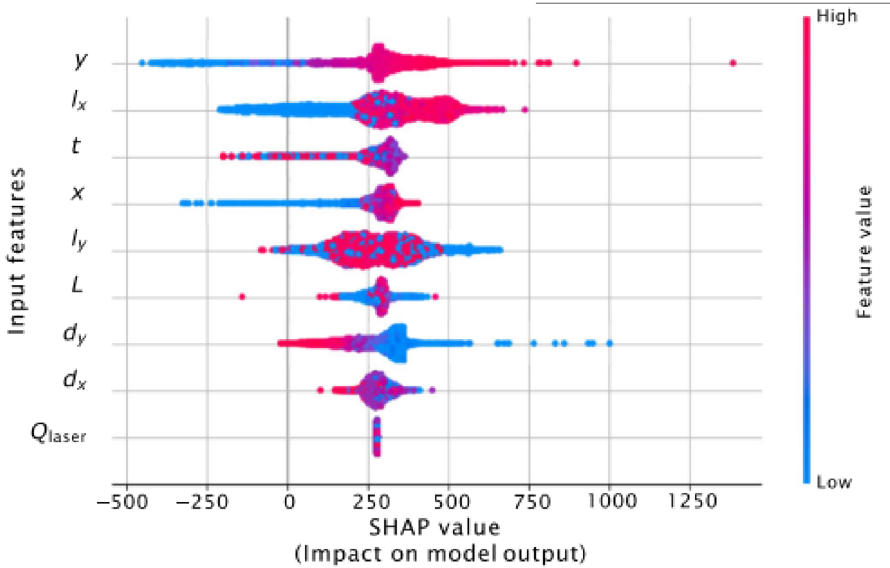
FFNN // FE Result analysis Tp°

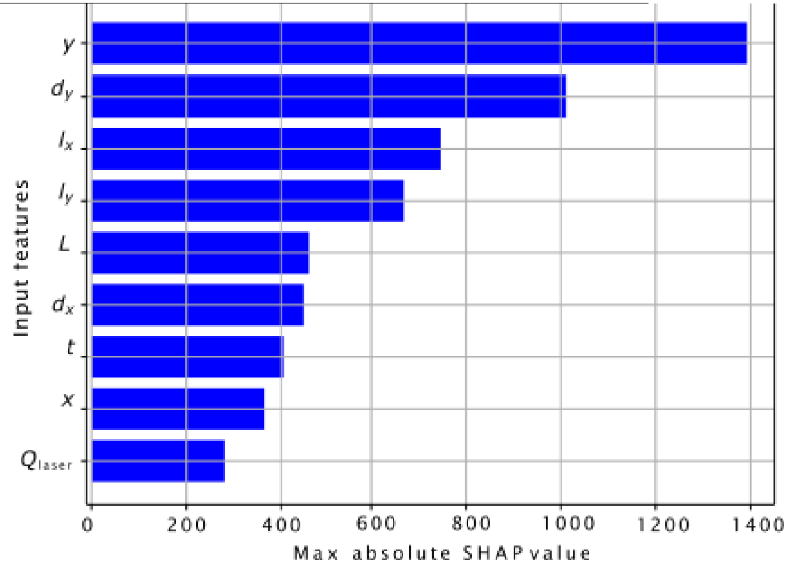


SHAP method to understand feature effects



Motivation





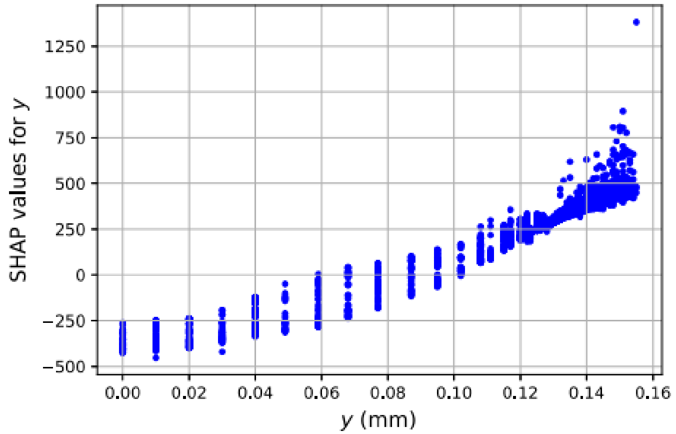
y vertical position

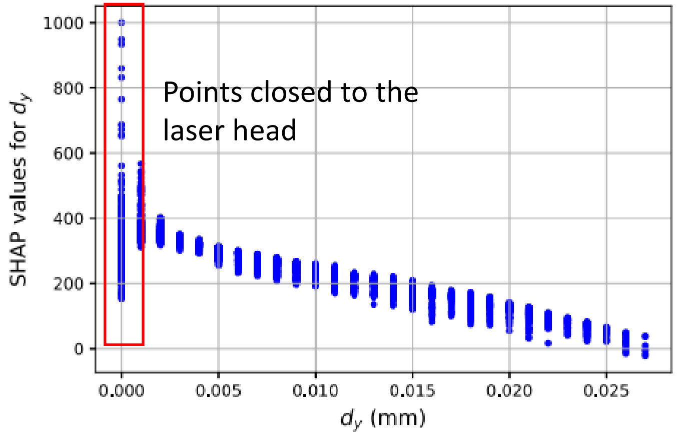
d_y vertical laser distance

l_x and l_y

laser position

= 4 most important features





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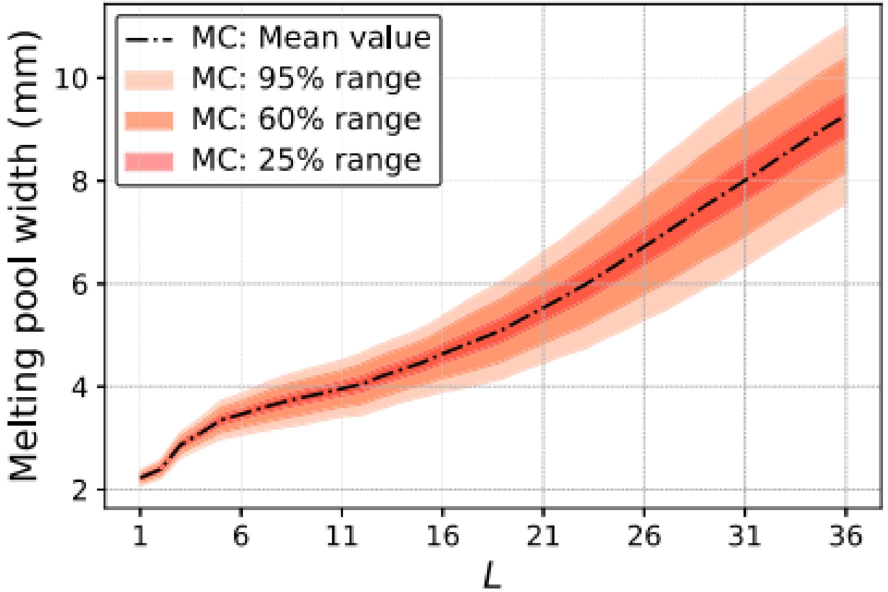
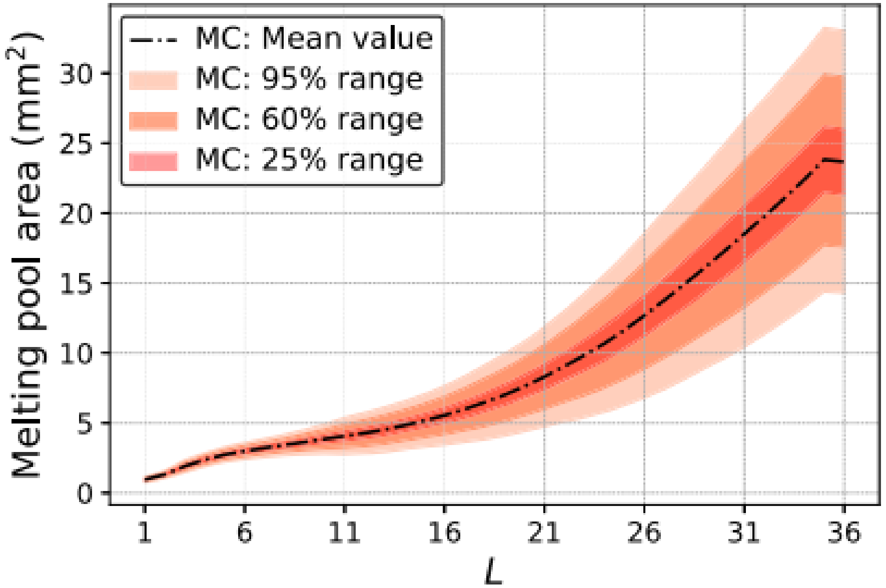
FFNN Result analysis

Extreme sensitivity of the melt pool to the uncertainty of $Q_{\mathbf{laser}}$





Computational cost

	Running FE simulations for creating training dataset	Training time	Single temperature field evaluation	1000 temperature fields evaluation
FE (h)	2.4	–	35→25 min	600
FFNN (h)	–	0.5	0.0033 (or 12 s)	3.3

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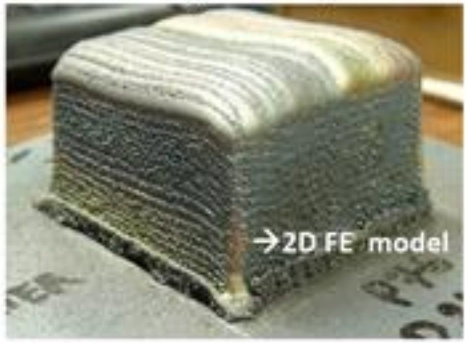

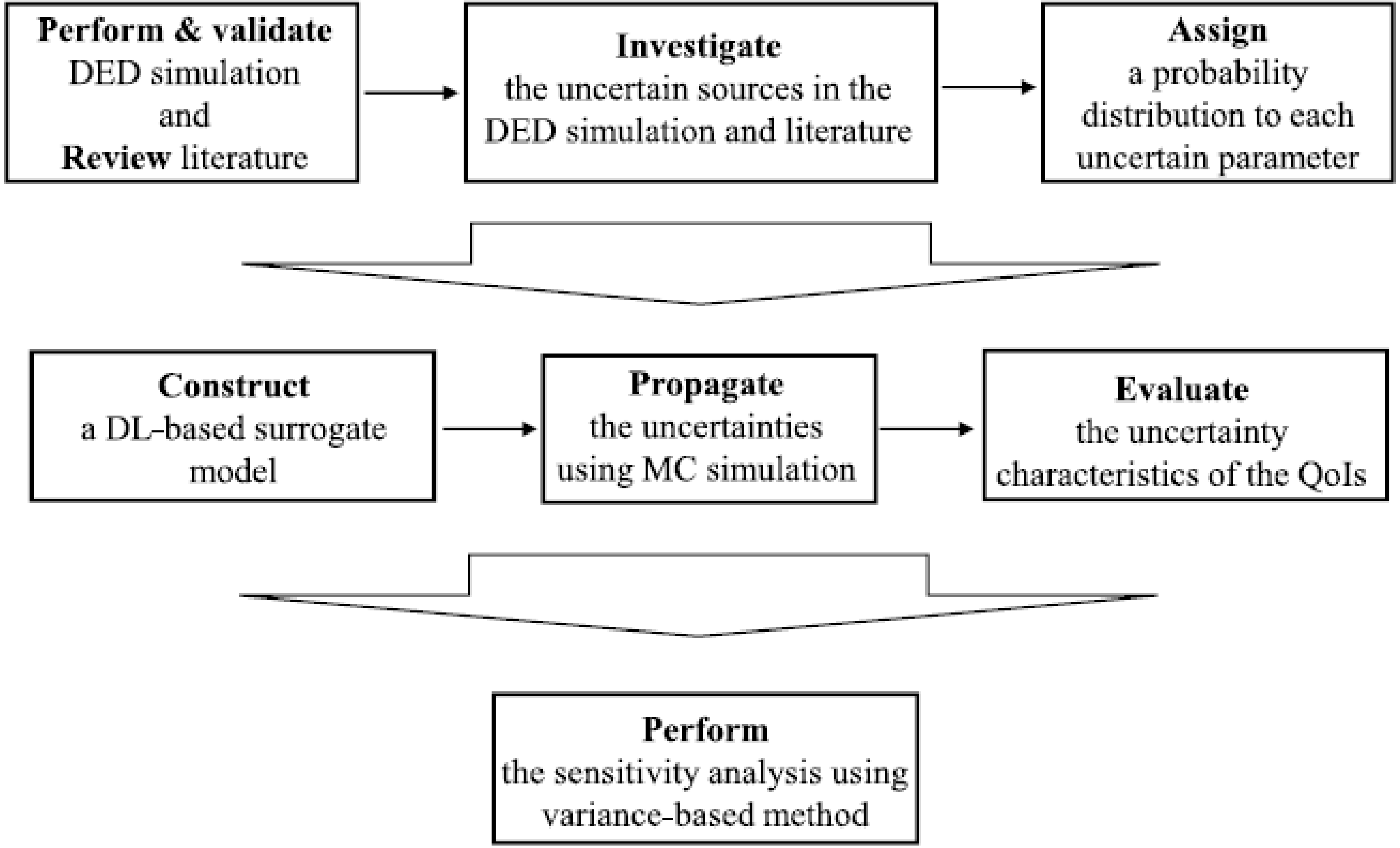

The uncertainty study

P_m: process parameter
$\mathcal{M}_m$: material properties
B_m: boundary conditions

→ DED simu →

Temperature field,
Cooling rate,
Melting pool sizes

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Parameter uncertainty based on literature review & domain knowledge

Input uncertain parameter		Notation	Reference	Minimum value	Maximum value	Distribution type	Unit
Process parameters	Effective laser power	$\mathcal{P}$	1	0.97	1.03	Uniform	-
	Scanning speed	v	350	335	365	Uniform	mm/min
	Controllable ambient temperature	T_a	298.15	284.15	312.15	Uniform	K
	Substrate preheating temperature	T_s	573.15	555.15	591.15	Uniform	K
Material properties	Convection	h	250	200	300	Uniform	$\mathrm{W/m^2K}$
	Radiation	ε	1	0.8	1	Uniform	-
Environmental conditions	Thermal conductivity	α_k	1	0.93	1.07	Uniform	-
	Heat capacity	α_c	1	0.95	1.05	Uniform	-

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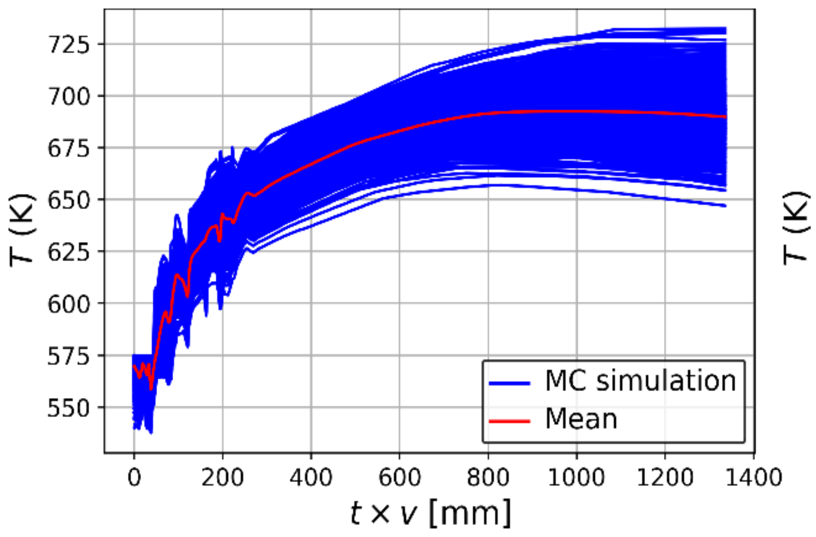
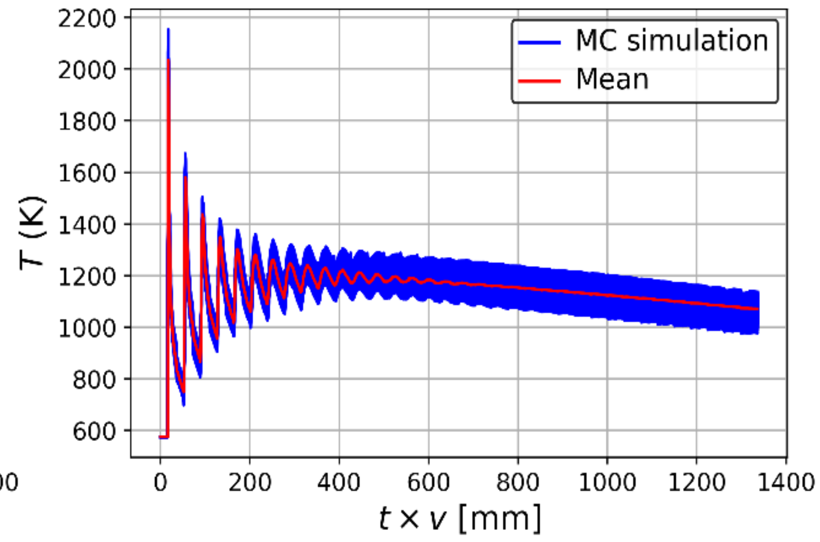
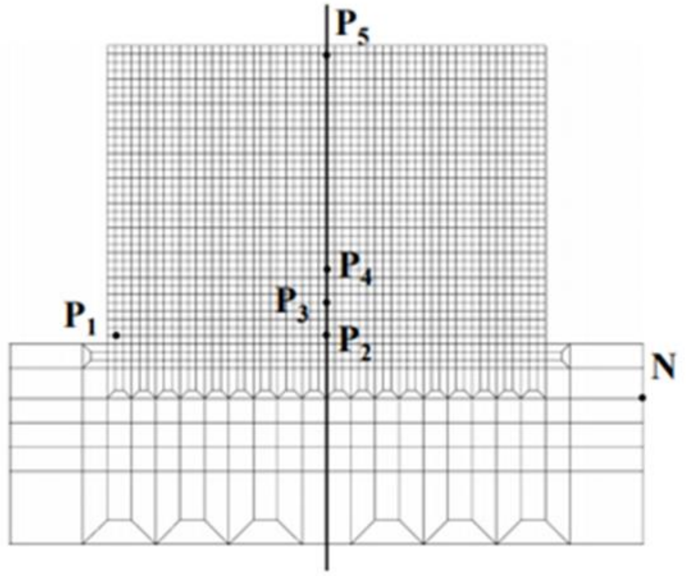
Propagation of uncertainty on Tp°

N



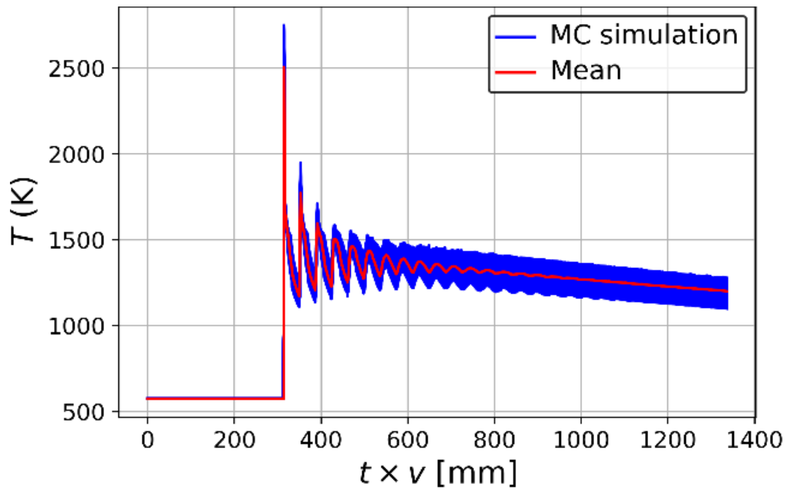
P1



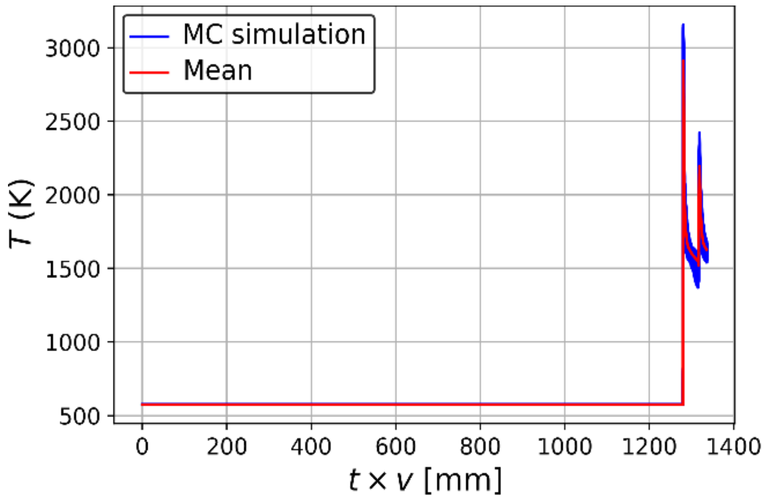


Montecarlo simulations to explore the space

P2



P4

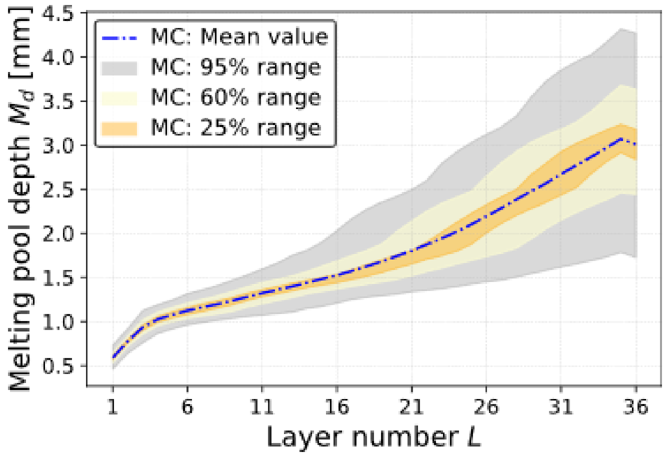


→ see details in: ***Characterization, propagation, and sensitivity analysis of uncertainties in the directed energy deposition process using a deep learning-based surrogate model***

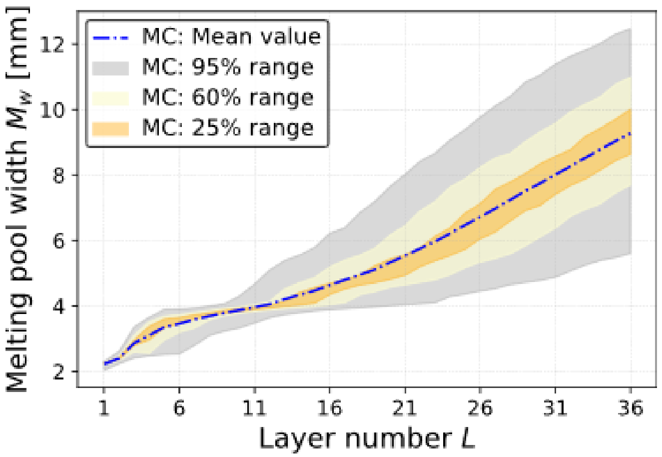
Thinh Quy Duc Pham, Truong Vinh Hoang, Xuan Van Tran, Seifallah Fetni, Laurent Duchêne, Hoang Son Tran, Anne-Marie Habraken

Probabilistic-Engineering-Mechanics, 2022

Prop. of uncertainty on melt pool size + CPU time



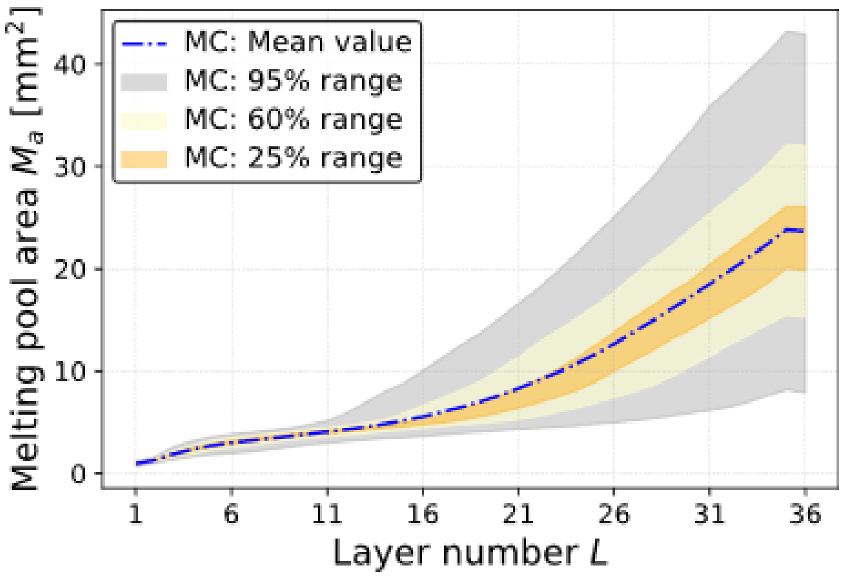
Depth



Width

→**Steady melting pool during DED process… a challenge !**

Need optimal laser power and minimum uncertainty



Area

Computational costs needed to perform a direct MC simulation, using the FE and FFNN-based surrogate model

Number of MC simulations	FE model (h)	FFNN-based surrogate model (h)
1	0.6	0.0033 (12 s)
1000	600	3.3

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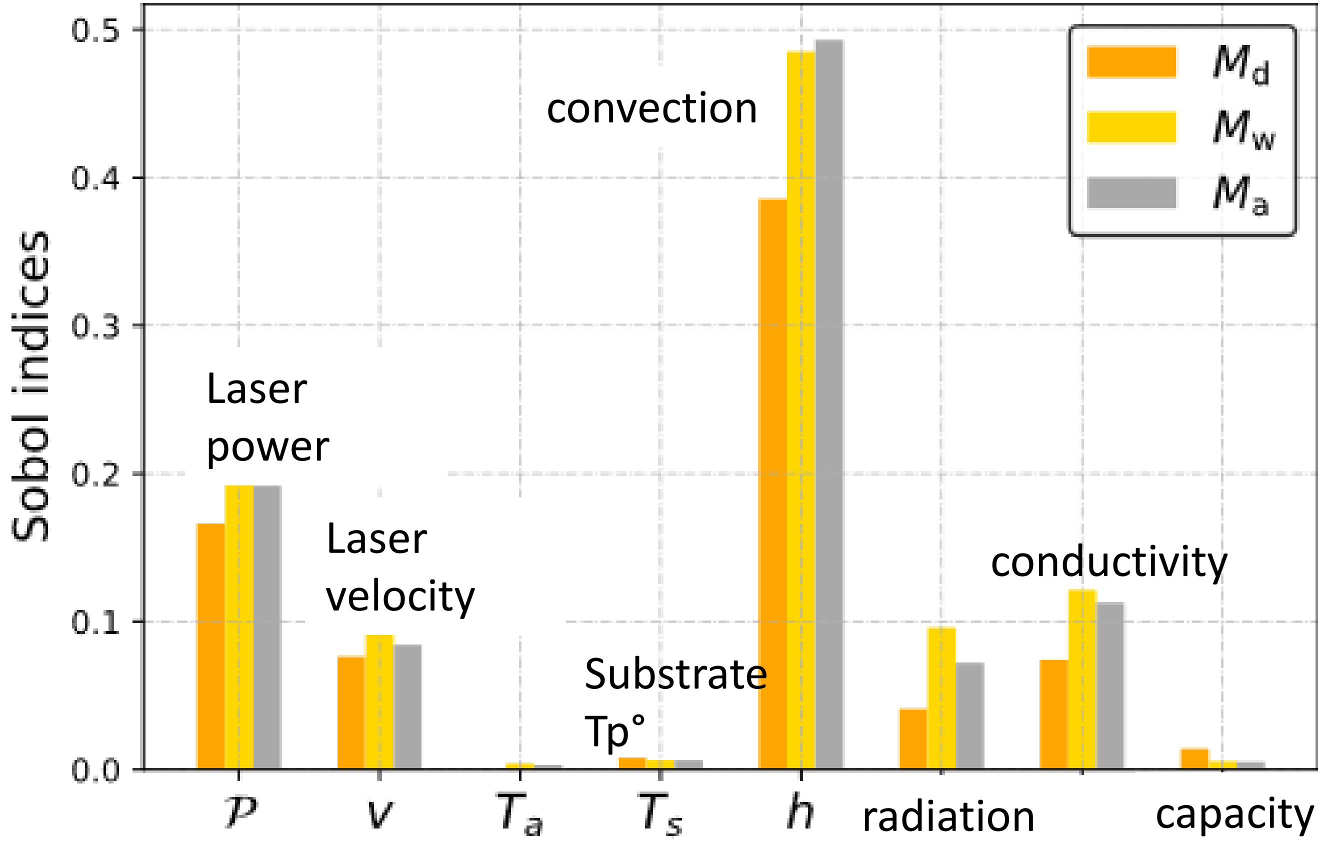
Conclusions about uncertainty study



Melt pool size M_d M_w M_a

→ Microstructure

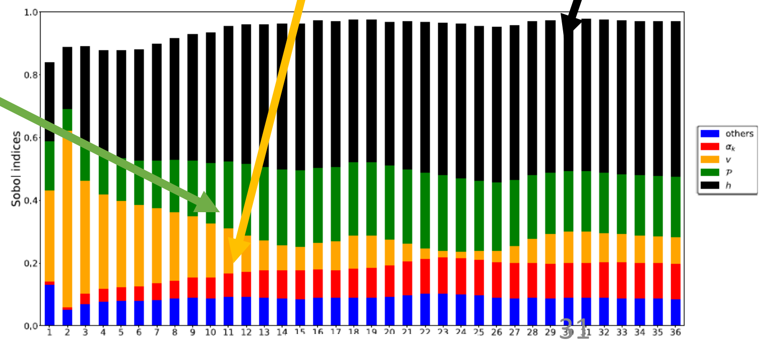
→ Product properties

Mostly modified due to Uncertainties on

-Convection h

-Laser power P

-Thermal conductivity



Layer

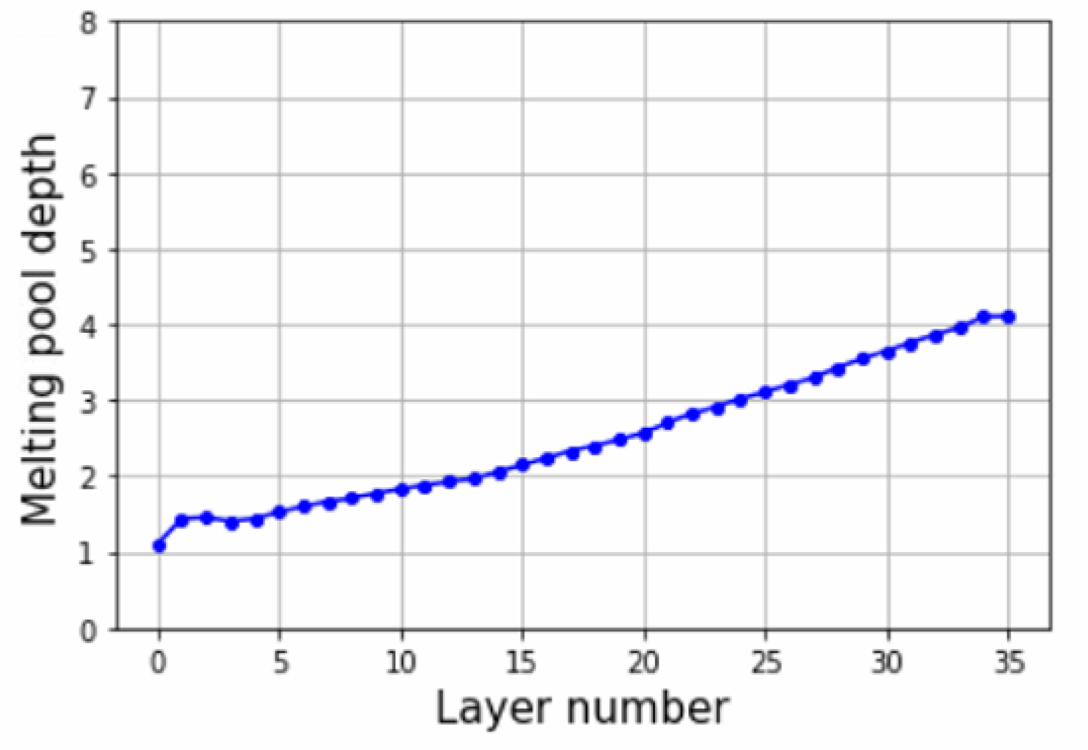
Need of stable input material properties and boundary conditions in industry

Material values input in model have a high impact

Remind: constant laser power → non constant M_d

Const power

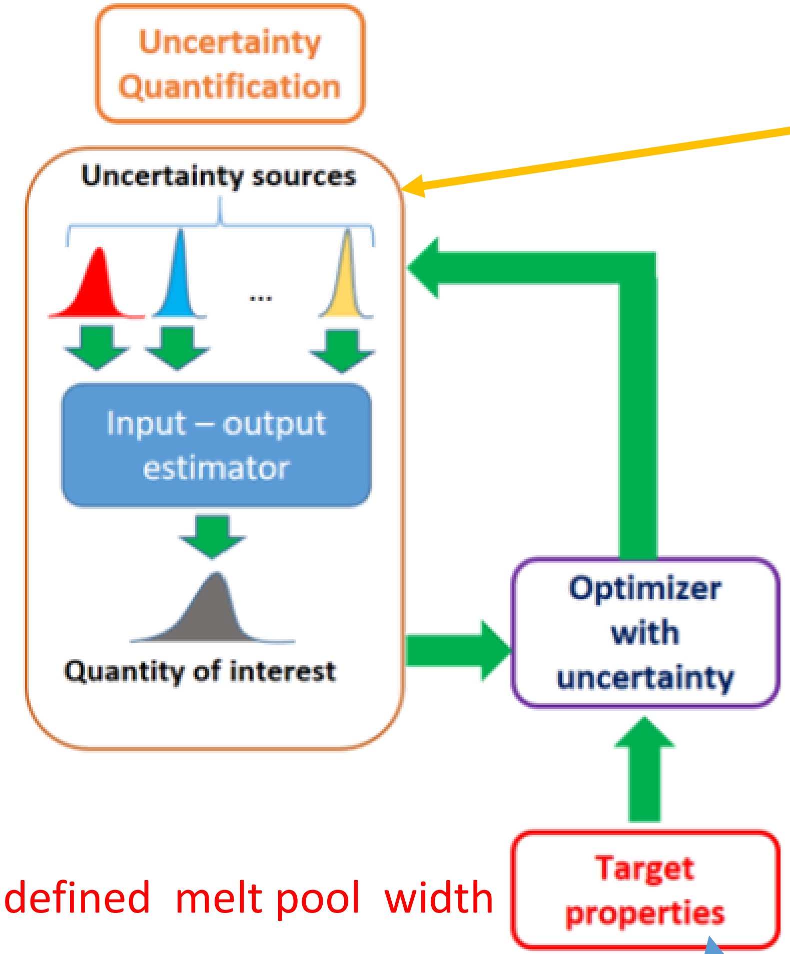
$P = 1100$ W



$\Rightarrow$ **Need to consider the laser power varying with layer number**

$\Rightarrow$ **More homogeneous melt pool and microstructure**

Optimization under uncertainty

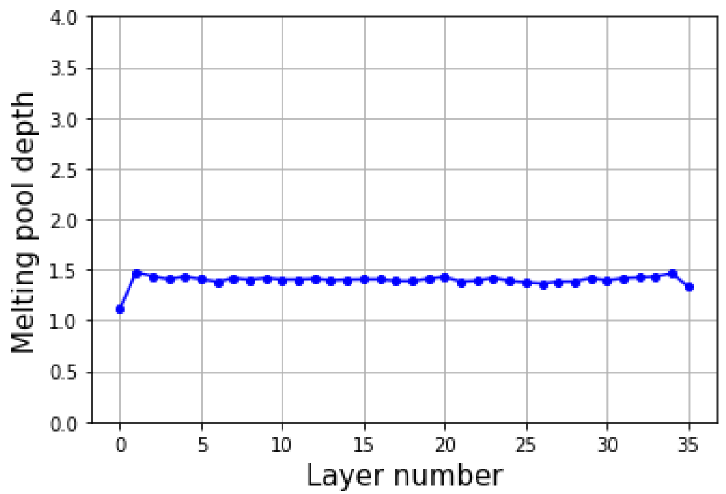


User defined melt pool width

Optimized parameter: Laser power

	Min	Max
Ambient temperature	284.15	312.15
Substrate preheating temperature	555.15	591.15
Convection	200	300
Radiation	0.8	1
Conductivity	0.93	1.07
Heat capacity	0.95	1.05

Range



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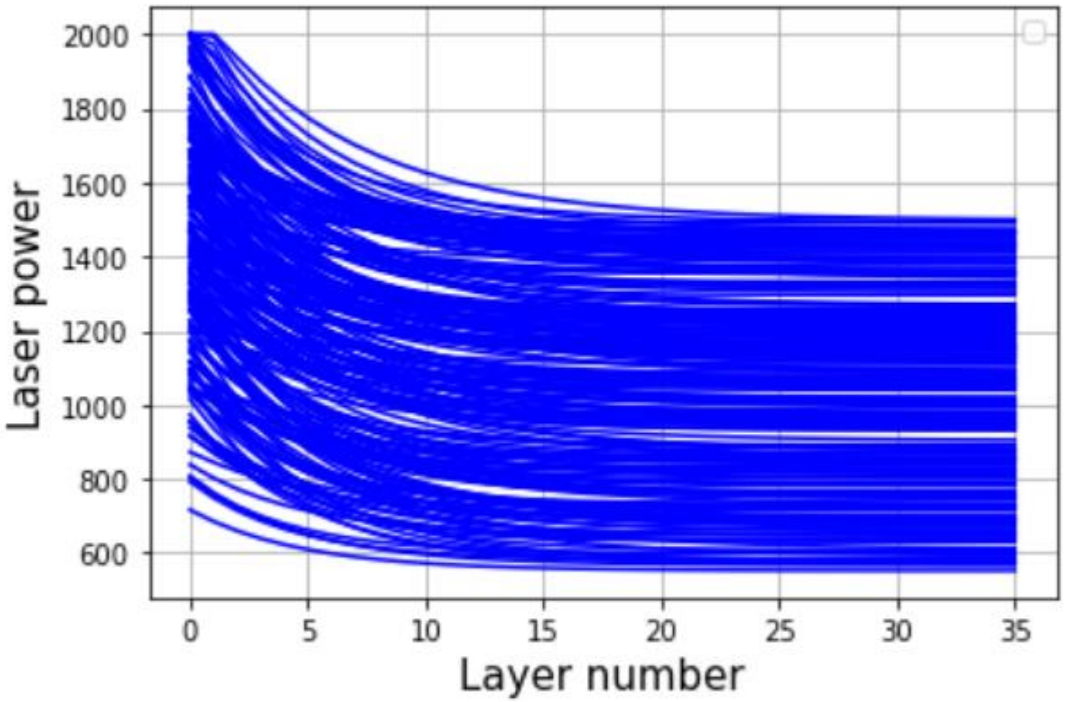
Laser power varying with layer number

$$f(x) = a \times e^{-kx} + b$$

$$a \in [200,800], b \in [550,1500], k \in [0.15,0.25]$$



a, b, k
also called
α_1 α_2 α_3
= the unkowns

If laser power value < 578 W, there will be no melting pool since the tp° is smaller than the melting temperature

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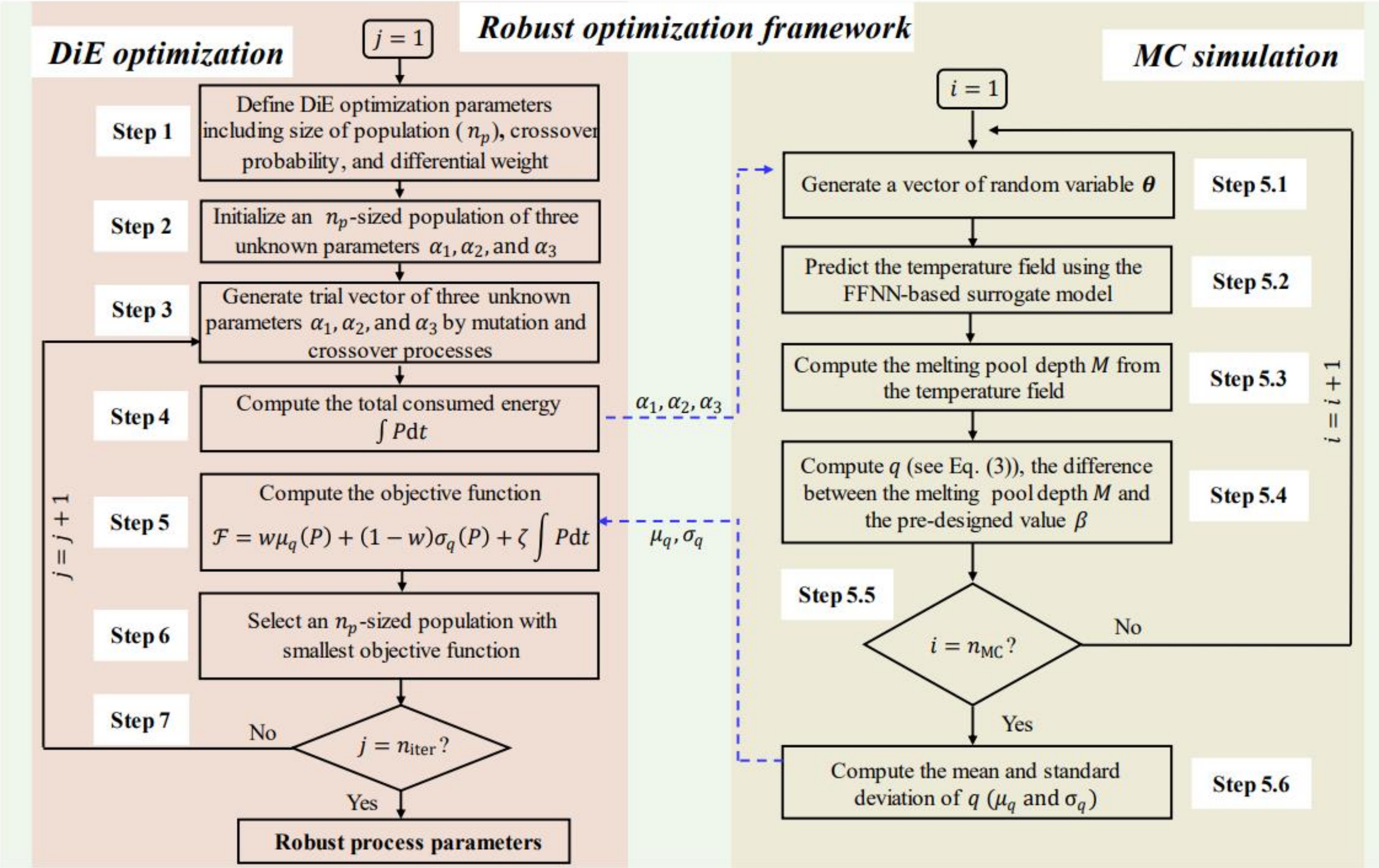
Optimal P(layers) under Minimal Energy

Objective function (step 5) :

Mean μ_q
& Standard deviation σ_q
of the difference
(computed melt pool size-user defined value)
+
Process Energy

(w weight and ζ scale factors)



Price KV.
Differential evolution, intelligent systems reference library 2013.

Bilal M *Eng Appl Artif Intel* 2020
Opara *Evol Comput* 2019

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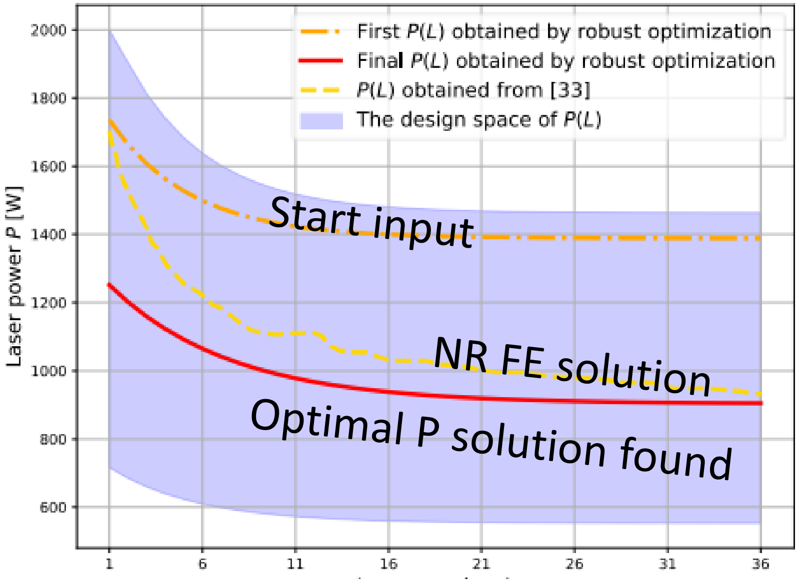
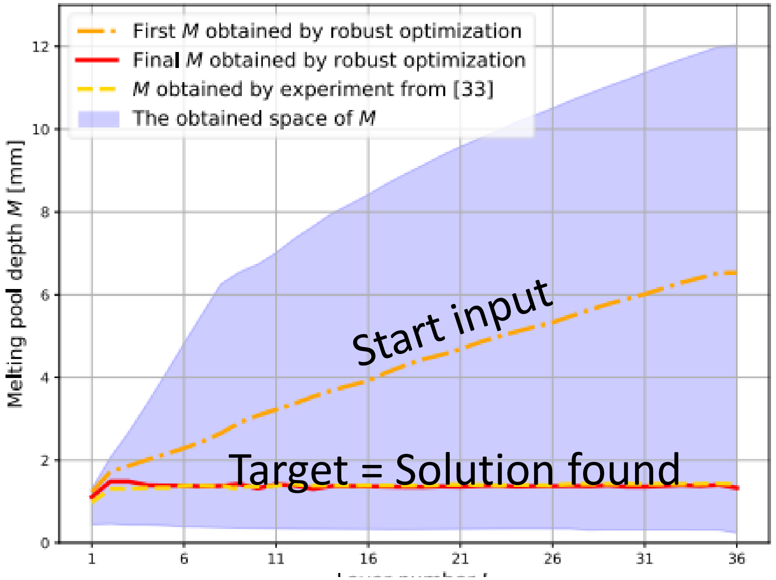
Differential Evolution (DiE)
Monte Carlo Simulations (MC)

Robust Results



Power Laser function versus layers



Melt pool depth versus layers

$$f(x) = a \times e^{-kx} + b$$

$a \in [200,800], b \in [550,1500],$
$k \in [0.15,0.25]$

→ Found:

$a = 407.1,$

$b = 910.16, k = 0.1498$

FE solution: Newton Raphson optimization without energy constraint

Jardin *Optic & Laser technology* 2023

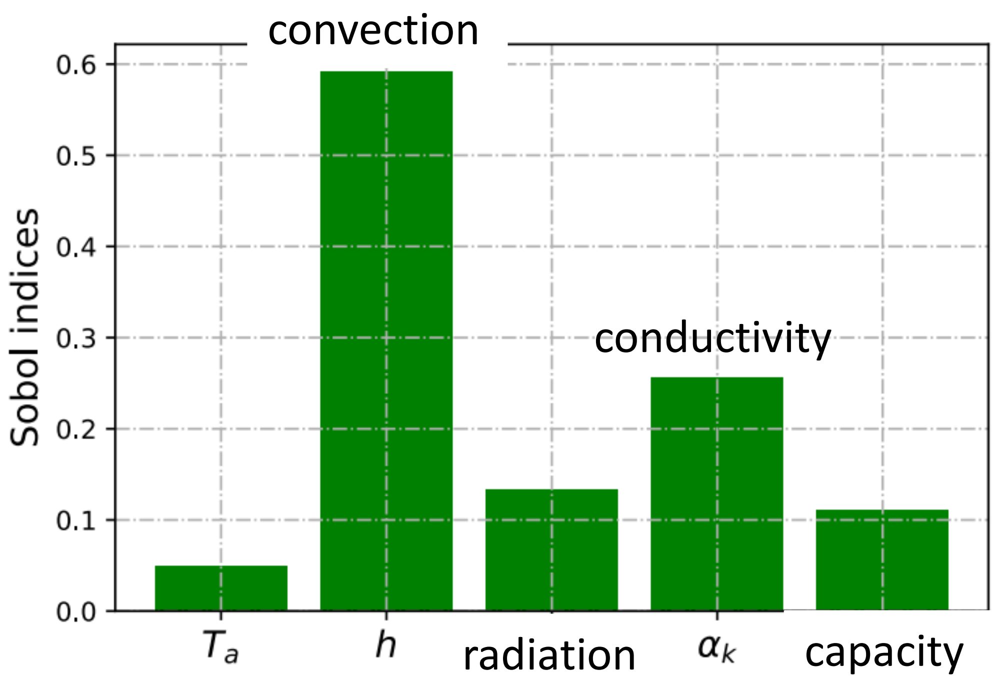
DL solution: Robust optimization - uncertainty & energy constraint added

T.Q.D Pham *Journal of Manufacturing Processes* 2023

Sensitivity analysis and computational cost

n_p = 60
size of the population to investigate the 3 unknown parameters defining power function (layer)

n_{MC} = 400
number of MC simu to evaluate the objective function within the iterative loop for one set of value of the unkown parameters



Why taking time to develop a surrogate model is worth

	Maximum number of DiE optimization iteration (n_{iter})	Number of predictions of the objective function ($n_{MC} \times n_p$)	Estimated time spent in FE model (h)	Estimated time spent in FFNN-based surrogate model (h)
	1	2400	1000	0.00166 (~6 s)
Nbr of iter before stabilisation	700	1,680,000	700,000	1.17
			29 days…	**1 hour 10 min**

What is next ?

Apply robust optimization framework to other material, other shape

Develop more efficient FE simulations (always validated by experiments)

-2D representative for 3D … accuracy ?

-couples FE method with Proper Orthogonal Decomposition to decrease CPU time ?

Leroy Dubief PhD (Estia & Univ Bretagne sud) 2023

Follow Particle FEM method coupling Computat. fluid Dynamics and Solid mechanics Bobach *Uliege Phd 2023*

Develop Microstructure predictions based on Tp°(t) :

-Phase Field model, Delahaye *Uliege Phd 2022*

-Time-phase Transformation-Block approach TTB, Tchuindjang *Metals* 2021,

-Phenomenological approach (JMAK, KM), Crespo *Scripta Materialia* 2010.

Exploit experiments to get material parameters:

-Thermo physical properties,

-Phase transformation kinetic from quenching dilatometer,

-% of phase from nanoindentation,

-% of phase by DL applied on optical images or EBSD map ….

Collaboration
Data sharing

Paper #1: ***Fast and accurate prediction of temperature evolutions in additive manufacturing process using deep learning***

Thinh Quy Duc Pham, Truong Vinh Hoang, Xuan Van Tran, Quoc Tuan Pham, Seifallah Fetni, Laurent Duchêne, Hoang Son Tran, Anne-Marie Habraken

Journal of Intelligent Manufacturing, IF: 6.498, 1-19, 2022

Paper #2: ***Characterization, propagation, and sensitivity analysis of uncertainties in the directed energy deposition process using a deep learning-based surrogate model***

Thinh Quy Duc Pham, Truong Vinh Hoang, Xuan Van Tran, Seifallah Fetni, Laurent Duchêne, Hoang Son Tran, Anne-Marie Habraken

Probabilistic-Engineering-Mechanics, IF: 3.784, 2022

Paper #3: ***A framework for the robust optimization under uncertainty in additive manufacturing***

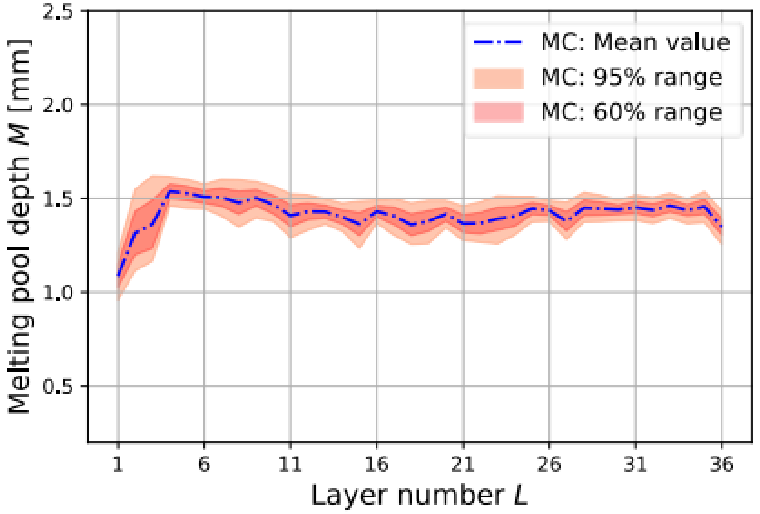
Thinh Quy Duc Pham, Truong Vinh Hoang, Xuan Van Tran, Seifallah Fetni, Laurent Duchêne, Hoang Son Tran, Anne-Marie Habraken

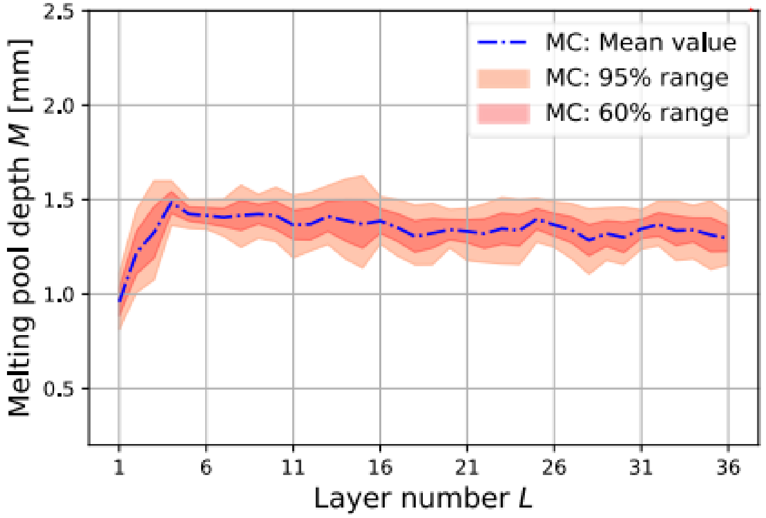
Journal of Manufacturing Processes, IF: 6.2, 2023

Robustness check

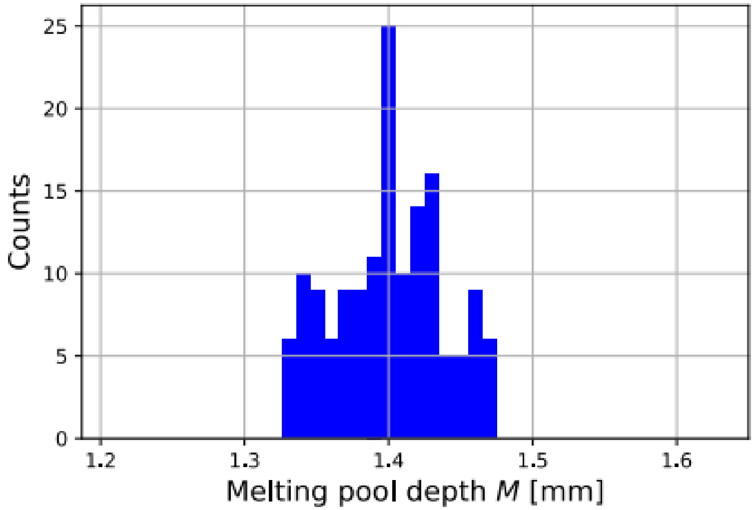
Robust optimization | **FE NR Deterministic method**

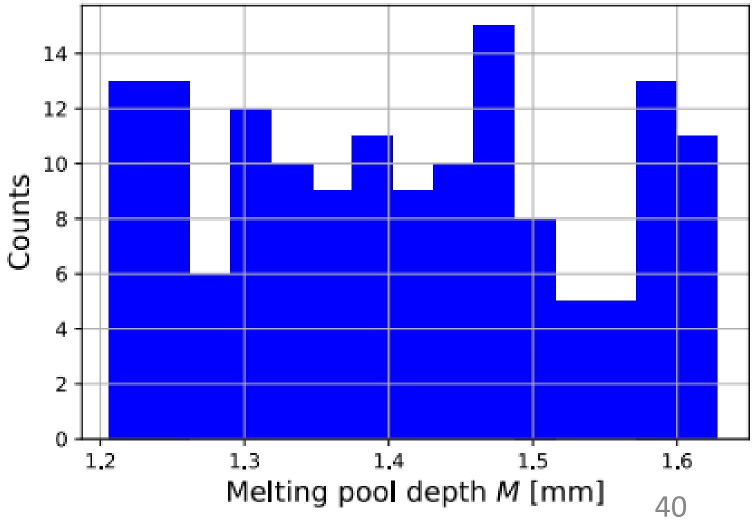
The mean value of the melt pool depth and its distribution obtained from 200 FE simulations



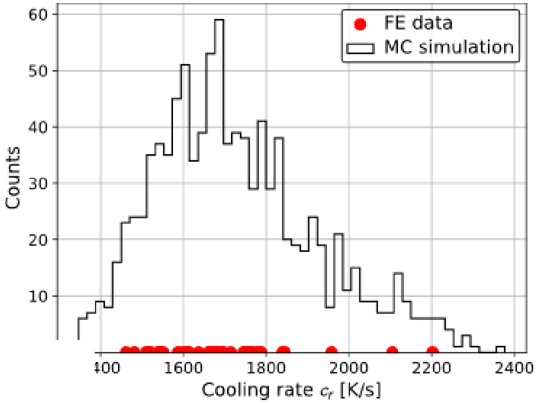


The empirical distribution of 200 melt pool depth data at layer 15

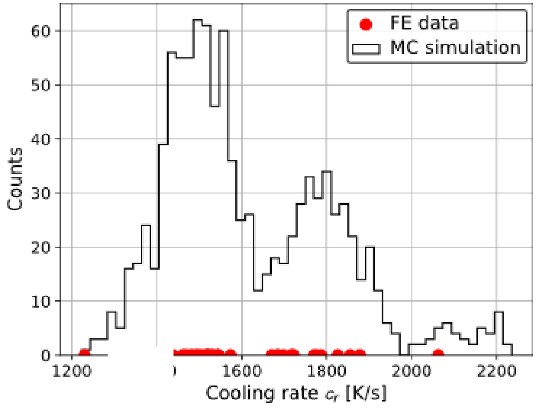




Propagation of uncertainty on cooling rate for middle point of the layers

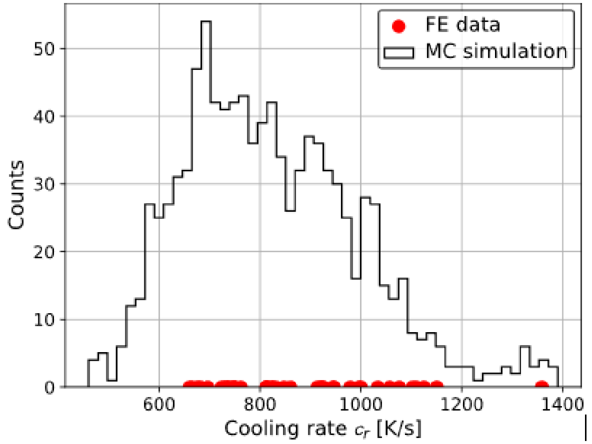


(a) Clad point P_1

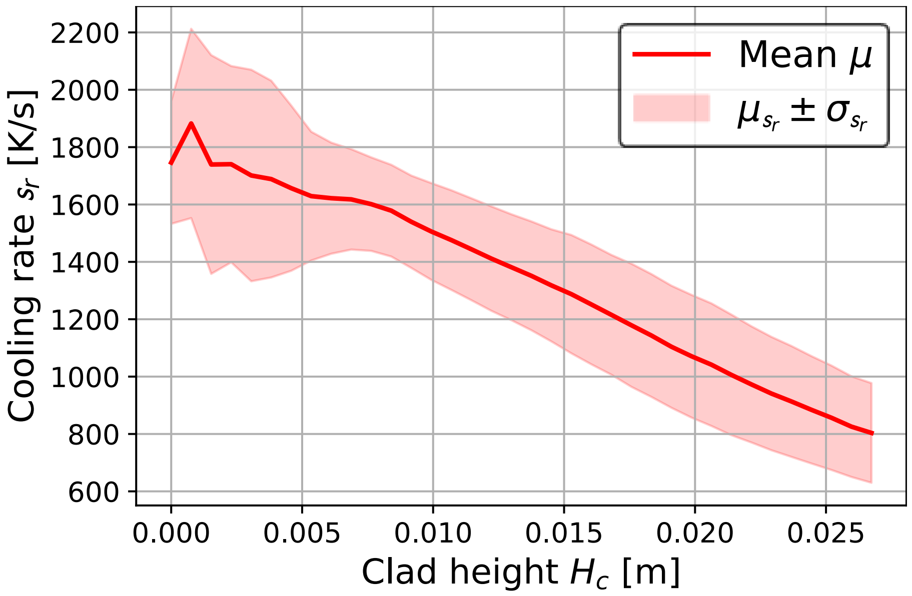


(b) Clad point P_2

Histogram of the 1000 MC and 100 FE simulations



(c) Clad point P_3



The mean gradually decreases with clad height, which is observed in several studies

T.Q.D Pham Probabilistic-Engineering-Mechanics 2022