M.S. Thesis 04/14/2020 1100 hrs. (CT)

Thermal modeling of additive manufacturing using graph theory:

Validation with directed energy deposition

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### Acknowledgements

#### The data for this work was requested from the publication at Pennsylvania State University (PSU)



J. C. Heigel, P. Michaleris, and E. W. Reutzel, "Thermo-mechanical model development and validation of directed energy deposition additive manufacturing of Ti–6Al–4V," Additive Manufacturing, vol. 5, pp. 9-19, 1/1/2015 2015.

### Outline

- Introduction
- Methodology
- Results
- Conclusions

### Outline

- Introduction
  - Background
  - Goal and Motivation
  - Current Efforts (Literature)
- Methodology
- Results
- Conclusions

### Background

Directed energy deposition (DED) is an additive manufacturing (AM) process.





### Why use directed energy deposition?



#### AGT 1500 (M1 Abrams Engine)

- Cost savings of over \$5M per year
- Added convenience for short interval maintenance

Source: Tom Cobbs, Product Manager at Optomec<sup>®</sup>

URL: https://optomec.com/how-3d-metal-printing-saves-time-and-lowers-costs-ded-for-repair-of-industrial-components/



### Why use directed energy deposition?

- 1. Produce complex geometries (e.g., satellites & spacecraft)
- 2. Repair rather than replace



#### After repair with DED



#### After machining



#### **Inconel Helical Gear Repair**

- Lead time reduction: 8 weeks to 1 day
- Enhanced material properties

Source: Tom Cobbs, Product Manager at Optomec<sup>®</sup>

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### Defects in AM occur at multiple scales.

#### The thermal aspects of the process affect the quality of the part.



W. J. Sames, F. List, S. Pannala, R. R. Dehoff, and S. S. Babu, "The Metallurgy and Processing Science of Metal Additive Manufacturing," International Materials Reviews, vol. 61, pp. 315-360, 2016.

### Thermal Aspects of DED

Certain heat transfer-related assumptions made in the context of the laser powder bed fusion (LPBF) must be relaxed for the DED process.





To mitigate severity of defects, the fundamental link between process parameters, thermal phenomena, and part properties must be understood.





# Graph theory approach for thermal modeling has been validated and published in the context of the LPBF process.



K. Cole, R. Yavari, P.Rao, *Computational heat transfer with spectral graph theory: Quantitative verification,* International Journal of Thermal Sciences, Volume 153, July 2020, (Accepted, in-press, available online). <u>doi: 10.1016/j.ijthermalsci.2020.106383</u>



### Goal

Validate the graph theory approach for thermal modeling for the DED process



Simulation (Literature)

Some, but not all, weld modeling principles fit well in the DED framework.

Transferrable Weld Modeling Principles?



### Simulation (Literature)

# Differences between welding and DED are demonstrated by considering the temperature of the base material and number of passes.



Source: metalsupplies.com

### Convection (Literature)

Researchers have assumed one of the following:

- 1. Convective heat loss is negligible (from weld modeling)
- 2. Uniformly distributed free convection loss
- 3. Uniformly distributed forced convection loss
- 4. Complex convection models (developed empirically or from CFD model)
- 5. Measurement-based convection models (Jarred Heigel)
- 6. Combination of free and forced convection (graph theory)





To increase computational efficiency, Michaleris proposed and tested two material deposition methods:

- 1. Quiet Elements: assigns scaled material properties to elements that have not been deposited
- 2. Inactive Elements: not included in analysis until they are deposited



P. Michaleris, "Modeling metal deposition in heat transfer analyses of additive manufacturing processes," *Finite Elements in Analysis and Design*, vol. 86, pp. 51-60, 4/28/2014 2014.

### Outline

- Context
- Methodology
  - Experiments
  - Simulation Procedure
    - $\rightarrow$  Graph Theory
    - $\rightarrow$  Implementation
  - Goldak's Double Ellipsoid Model
- Results
- Conclusions

Three Ti-6Al-4V single-track thin walls were deposited on separate clamped substrates of equal dimensions.





- Each substrate was clamped at one end
- A thermocouple collected thermal history at a specified location in the substrate
- Aluminum tape was used to shield TC 2 from forced convection loss in the first case



J. C. Heigel, P. Michaleris, and E. W. Reutzel, "Thermo-mechanical model development and validation of directed energy deposition additive manufacturing of Ti–6Al–4V," Additive Manufacturing, vol. 5, pp. 9-19, 1/1/2015 2015.



### Summary of Experiments

#### Temperature excursions are more prevalent with increased dwell time.



### Graph Theory



Step 1- Convert the part into a set of discrete nodes

M. R. Yavari, K. Cole, and P. Rao, "Thermal Modeling in Metal Additive Manufacturing using Graph Theory," *ASME Transactions, Journal of Manufacturing Science and Engineering*, vol. 141, pp. 071007-27, July 2019.



#### Step 1: Discretizing the part geometry into nodes and blocks

- Convert part into discrete nodes
- Number of nodes is set at a certain number per unit volume (called node density)
- Part is then divided into layers, hatches, and blocks





Step 2: Constructing a network graph from the cloud of discrete nodes

- Each node is connected to its nearest neighboring nodes
- Nearness is defined by  $\varepsilon$  (called the neighborhood distance)
- Matrix formed by placing  $a_{ij}$  in a row *i* and column *j* is called the adjacency matrix,  $\mathbf{A} = \begin{bmatrix} a_{ij} \end{bmatrix}$





#### Step 3(a): Heat loss through conduction

- Sole heat transfer mechanism between nodes is conduction
- A time step involves heating of nodes inside a block, one block at a time (t<sub>b</sub> = 0.922 s)



$$\mathbf{T}_c = \mathbf{\Phi} e^{-\alpha \mathbf{g} \mathbf{\Lambda} t_b} \mathbf{\Phi}' \mathbf{T}_0$$

Variable	Definition
<b>T</b> <sub>c</sub>	Temp. vector at time t (end of time step)
φ	Laplacian Eigenvector matrix
α	Thermal diffusivity of Ti-6Al-4V
g	Gain factor
Λ	Laplacian Eigenvalue matrix
$t_b$	Time step ( = 0.922 s)
T <sub>0</sub>	Temp. vector at time 0



#### Step 3(b): Heat loss through convection

• Heat loss through convection from the nodes on the surface of the part occurs in tandem with conduction

From Step 3(a):  $\mathbf{T}_{c} = \mathbf{\Phi} e^{-\alpha g \mathbf{\Lambda} t_{b}} \mathbf{\Phi}' \mathbf{T}_{0}$ 



#### Step 3(b): Heat loss through convection

•  $\beta$  is the inverse time constant can be related to the heat transfer coefficient

$$\mathbf{T}_b = \mathbf{T}_c e^{-\beta t_b}$$

$$\beta = \frac{h}{\rho \times L \times C_p}$$

Variable	Definition	Units
β	Inverse time constant	S <sup>-1</sup>
h	Heat Transfer Coefficient	W⋅m <sup>-2</sup> ⋅K <sup>-1</sup>
ρ	Density of Ti-6Al-4V	kg∙m⁻³
L	Block Length	m
$C_p$	Specific Heat	J·kg <sup>-1</sup> ·K <sup>-1</sup>



Step 3(c): Obtaining temperature at the end of a layer (after dwell)

- Heat is allowed to dissipate
- Identical to Steps 3(a) and (b), except iterative for a period equal to the dwell time (t<sub>d</sub>)





$$\mathbf{T}_{Lc} = \mathbf{\Phi} e^{-\alpha \mathbf{g} \mathbf{\Lambda} \mathbf{t}_{d}} \mathbf{\Phi}' \mathbf{T}_{b}$$

$$\mathbf{T}_{Lf} = \mathbf{T}_{Lc} e^{-\beta \mathbf{t}_d}$$

- $t_d = 20 \text{ s for Case A}$
- $t_d = 3$  s for Case B and Case C



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#### Step 4: Recording nodal temperatures in vector

- Steps 3(a), (b), and (c) are looped until the last layer is built
- The temperature of each node at each time step is recorded in a vector **T** (thermal history vector)



- Case A was used to calibrate the graph theory approach
  - Chosen because of the prominent temperature cycles
  - Combination of ε and g resulting in the lowest Mean Absolute Percentage Error (MAPE) was selected





Calibration was conducted at three node densities and three meltpool temperatures.

Nodes	Total	Number of	Node Density	Neighborhood	G	ain Factor (	g)
per Block	Number of Nodes	Nodes in Wall	(nodes/mm <sup>3</sup> )	Size, ε (mm)	T <sub>0</sub> = 1900 °C (mm <sup>-2</sup> )	T <sub>0</sub> = 2200 °C (mm <sup>-2</sup> )	T <sub>0</sub> = 2450 °C (mm <sup>-2</sup> )
1	2830	310	0.2355	4.5	8	10	12
2	5660	620	0.4709	4.75	1	1.5	1.95
3	8490	930	0.7064	5.5	0.12	0.15	0.17





Heat transfer coefficients are estimated in the calibration step and are held constant throughout all simulation cases.





Free convection was estimated first by observing the prediction during the initial rising action of the experiment.



$$\boldsymbol{\beta} = \frac{h}{\rho \times L \times C_p}$$

Heat	Inverse Time Constant	Equivalent Heat
Transfer	in Graph-theoretic	Transfer Coefficient
Coefficient	Method [s <sup>-1</sup> ]	[W·m <sup>-2</sup> ·K <sup>-1</sup> ]
Clamp	0.05 (200× free)	981.2
Forced	0.0025 (10× free)	49.1
Free	0.00027	5.3



Estimated heat transfer coefficients were compared to Heigel's measurement-based convection model.





- The Cartesian coordinates of one node, called the sensor node, are defined with the coordinates of the thermocouple
- How do we account for aluminum tape used to shield the thermocouple from forced convection?
  - Sensor node is "buried" at a depth of 0.1 mm below the surface of the substrate



Sensor Location



- Material properties change with temperature
- A linear function was fit to approximate thermal diffusivity
- A new thermal diffusivity value,  $\alpha_{Layer}$ , is based on the average temperature in the layer before it,  $T_{Layer}$

T [°C]	k [W∙m⁻¹∙°C⁻¹]	C <sub>p</sub> [J·kg <sup>-1</sup> ·°C <sup>-1</sup> ]	Calculated $\alpha$ [m <sup>2</sup> ·s <sup>-1</sup> ]
20	6.6	565	2.64
93	7.3	565	2.92
205	9.1	574	3.58
250	9.7	586	3.74
315	10.6	603	3.97
425	12.6	649	4.38
500	13.9	682	4.60

$$\alpha_{\text{Layer}} = 0.0042 \times T_{\text{Layer}} + 2.612$$

$$\mathbf{T}_{c} = \mathbf{\Phi} e^{-\boldsymbol{\alpha} \mathbf{g} \mathbf{\Lambda} t_{b}} \mathbf{\Phi}' \mathbf{T}_{0}$$

#### **Transient Material Properties**



### Goldak's Double Ellipsoid Heat Source

- The laser penetrates further into the part than just one layer
- Blocks below the meltpool must also be given an elevated temperature
- Layers below the deposition layer are called sublayers





Goldak's model is taken from weld modeling and applied to laser-based processes.



#### Moving Heat Source Model



### Goldak's Double Ellipsoid Heat Source

- The unitless scaling factor, C, was used to set an upper limit on the temperature profile
- C is dependent on the meltpool temperature

$$T_0(x, y, z, t) = \mathbf{C} \times \mathbf{P} \times \frac{1}{2\pi K \sqrt{x^2 + y^2 + z^2}} \times \exp\left[-\frac{v}{2\kappa} \times \left(x + \sqrt{x^2 + y^2 + z^2}\right)\right]$$

Variable	Units	Value
С	Dimensionless	0.125 to 0.191
Laser Power (P)	[W]	415
Laser Velocity (v)	[m•s <sup>-1</sup> ]	8.5 × 10 <sup>-3</sup>
Thermal Conductivity (K)	[W•m <sup>-1</sup> K <sup>-1</sup> ]	6.8
Thermal Diffusivity ( $\kappa$ )	[m <sup>2</sup> • s <sup>-1</sup> ]	2.7228 × 10 <sup>-6</sup>

#### Scaling Factor: Justification



The best way to validate is through experimentation, but some inconsistencies remain.

Geometry	Laser Power (P) [W]	Scan Speed [mm·s <sup>-1</sup> ]	Method	Meltpool Temperature (T <sub>0</sub> ) [°C]
Thin Wall	300	12.7	Pyrometer	~1850
Thin Wall	290	12.7	Pyrometer	1900-2000
L-shaped Thin Wall	450	10.6	IR Camera	$2485 \pm 161$
Cylinders	350	16.9	Pyrometer	2100 - 2500
Rectangular Thin Wall	300	2.0	Quiet Element Technique	2447
Cube	800	10.0	In-house Code (GAMMA)	2500
Thin Wall	425	8.5	Inactive Element Technique	1800 - 2000
My Values:	415	8.5		

Three meltpool temperatures selected in this work to represent the range of values observed: 1900 °C, 2200 °C, and 2450 °C.



### Goldak's Double Ellipsoid Heat Source

- Starting point: Liquidus temperature (1630 °C) is reached at the periphery of the meltpool
- Center of the meltpool is hotter since it receives highest laser intensity and is surrounded by molten Ti-6Al-4V



Scaling Factor: Profiles



Once the laser profile is consistent with reality, temperatures are found with respect to depth.



Scaling Factor: Depths



The implementation of Goldak's model is distilled into three steps.

<u>Step 1</u>

- Set reference point
- Determine distance to the center of each sublayer

### Implementing Goldak



### Outline

- Context
- Methodology
- Results
  - Definitions
  - Case A Results
  - Case B Results
  - Case C Results
  - Summary
- Conclusions

- Mean Absolute Percentage Error (MAPE)
- Root Mean Square Error (RMSE)
- Each simulation is repeated three times, and the uncertainty is quantified in terms of the standard deviation of error

$$MAPE = \frac{100\%}{n} \times \sum_{i=1}^{n} \left| \frac{T_i - \hat{T}_i}{T_i} \right|$$

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{\left(T_i - \hat{T}_i\right)^2}{n}}$$

Variable	Definition
n	Number of data points
i	Current instant of time
$T_i$	Measured temperature
$\widehat{T}_i$	Simulated temperature



Case A Results

Due to the programmed 20-second dwell time, this case results in the lowest peak temperature (200 °C).



2200 °C

Prediction accuracy improves with increasing meltpool temperature.



1900 °C



### Case A Results



N

- For the simulation using one node with T<sub>0</sub> = 2200 °C, the MAPE is found to be 10.75%, and RMSE is 23 °C
- Can compute in 9 minutes on a desktop computer
- Build time: 25.6 minutes

Node Density [nodes∙mm <sup>-3</sup> ]	Computation Time [min]	ation $T_0 = 1900 ^{\circ}C$		T <sub>0</sub> = 2200 °C		T <sub>0</sub> = 2450 °C	
		MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]
0.2355	9	13.1	25.9	10.8	23.2	10.1	21.5
(1 node)		(1.4)	(1.6)	(2.0)	(2.8)	(4.5)	(6.9)
0.4709	82	9.8	22.8	7.7	18.8	7.6	17.7
(2 nodes)		(0.6)	(1.0)	(1.3)	(2.1)	(2.3)	(3.8)
0.7064	194	8.0	20.7	6.6	18.4	6.0	16.5
(3 nodes)		(1.6)	(1.7)	(1.1)	(1.4)	(2.6)	(2.9)



# Without the dwell time, this case results in the highest peak temperature (500 °C).



2200 °C

Prediction begins to exceed experiment when the same geometry is deposited without a dwell time.



1900 °C



### Case B Results





- For the simulation using one node with T<sub>0</sub> = 2200 °C, the MAPE is found to be 17%, and RMSE is 75 °C
- Can compute in 9 minutes on a desktop computer
- Build time: 5.2 minutes

Node Density [nodes∙mm <sup>-3</sup> ]	Computation Time [min]	tion T <sub>0</sub> = 1900 °C		T <sub>0</sub> = 2200 °C		T <sub>0</sub> = 2450 °C	
		MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]
0.2355	9	26.5	114.4	17.3	<mark>75.0</mark>	10.5	48.5
(1 node)		(2.6)	(11.5)	(1.6)	(5.3)	(2.8)	(11.6)
0.4709	82	24.5	105.2	<b>12.7</b>	59.5	10.5	49.5
(2 nodes)		(1.9)	(8.2)	(0.5)	(2.4)	(0.9)	(3.6)
0.7064	194	22.6	98.0	12.5	57.8	12.4	53.3
(3 nodes)		(0.5)	(1.6)	(0.9)	(3.8)	(0.5)	(3.1)



## With the increased wall height and no dwell time, this case reaches a peak temperature of 300 °C.



Prediction is not as accurate when given a new part geometry.



1900 °C

0.4709 nodes/mm<sup>3</sup>



### Case C Results



- For the simulation using one node with T<sub>0</sub> = 2200 °C, the MAPE is found to be 28%, and RMSE is 78 °C
- Can compute in 21 minutes on a desktop computer
- Build time: 10.1 minutes

Node Density [nodes∙mm <sup>-3</sup> ]	Computation Time [min]	<b>T</b> <sub>0</sub> = 19	900 °C	T <sub>0</sub> = 22	T <sub>0</sub> = 2200 °C		T <sub>0</sub> = 2450 °C	
		MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]	MAPE [%]	RMSE [°C]	
0.2355	21	31.6	84.9	28.2	<mark>78.6</mark>	16.7	45.7	
(1 node)		(4.0)	(10.7)	(2.0)	(5.5)	(0.5)	(1.6)	
0.4709	188	32.0	84.0	<b>19.7</b>	<b>51.7</b>	12.5	35.0	
(2 nodes)		(1.1)	(2.7)	(0.2)	(0.9)	(1.2)	(5.2)	
0.7064	650	21.8	55.3	10.0	26.1	9.3	28.0	
(3 nodes)		(1.1)	(3.4)	(0.7)	(3.3)	(3.4)	(14.6)	



### Summary



Simulation Snapshots



### Outline

- Context
- Methodology
- Results
- Conclusions
  - Takeaways
  - Future Work



### Takeaways

The graph-theoretic approach can provide valid thermal predictions for the DED process at a relatively low computational expense.





### Takeaways

- Computation time reported for Heigel's model is for the part's half-symmetry
- A calculated error of approximately 20% was attainable for each case while simulating the entire part

Data	Case A		Case B		Case C	
	Time [min]	MAPE [%]	Time [min]	MAPE [%]	Time [min]	MAPE [%]
Finite Element (Heigel Model)	136	10.4	136	2.4	No Report	4.1
Graph Theory	82	7.59	82	11.94	188	19.79
Build Time	25.6 minutes		5.2 minutes		10.1 minutes	



### Future Work

#### 1. Obtain meltpool temperature directly from the experiment

 This would allow for a better calibration and corresponding prediction



- 2. Resolve disproportionate boundary node quantities
  - Extra heat losses associated with convection and radiation are applied to the boundary nodes
  - 15% more heat loss in the lowest node density case

A.C. Gaikwad, R. Yavari, M. Montazeri, K. Cole, L. Bian, P. Rao. Toward the Digital Twin in Metal Additive Manufacturing – Integrating Thermal Simulations, Sensing, and Analytics to Detect Process Faults, IISE Transactions (Accepted, in-press, available online) doi: 10.1080/24725854.2019.1701753



- 3. Implement more rigorous radiative heat loss approximation
  - A new radiation approximation appeared to improve the prediction accuracy for only Case B



- 4. Develop method for changing node density in the substrate
  - Lower node count will reduce computation time



### Obtaining Eigenvectors ( $\phi$ ) and Eigenvalues ( $\Lambda$ ) <sup>65</sup>

Adjacency matrix  $A \stackrel{\text{\tiny def}}{=} [a_{ij}]$ 



Sum each row of the Similarity matrix, and put it on the diagonal

Laplacian matrix

$$\mathcal{L} \stackrel{\text{\tiny def}}{=} (\mathcal{D} - A)$$

 $\mathcal{L}\phi = \Lambda\phi$ 

M. R. Yavari, K. Cole, and P. Rao, "Thermal Modeling in Metal Additive Manufacturing using Graph Theory," *ASME Transactions, Journal of Manufacturing Science and Engineering*, vol. 141, pp. 071007-27, July 2019.

