Building blocks for a digital twin of additive manufacturing
- a path to understand the most important metallurgical variables

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Thanks to: Manvatkar V., De A., Zuback J.S., Knapp G.L., Blecher J.,
Zhang W., Elmer J.W., DOE-NEUP, America Makes, AWS
Digital twin of additive manufacturing

Why digital twin of AM?
- Save time and money
- Minimizing trial and error optimization
- Expediting product qualification
- Reducing/alleviating defects

Components developed at Penn State
i. Heat transfer and fluid flow simulation
ii. Solidification, grain structure and texture evolution
iii. Residual stress and distortion simulation considering convective heat transfer
iv. Reduced order modeling - Back of the envelope calculations

i. Heat transfer and liquid metal flow

Prediction of deposit geometry
Temperature and velocity distributions
Cooling rates and solidification parameters
Heat transfer and fluid flow model

Solve equations of conservation of mass, momentum and energy

**INPUT**
Process parameters
Material properties

**OUTPUT**
Transient temperature & velocity fields, cooling rate, solidification parameters ...

Calculation domain: about 250,000 cells
Five main variables: three components of velocities, pressure & enthalpy
1.25 million algebraic equations (250000 x 5)
100 iteration at any time step => 0.125 billion equations/time step
1000 time steps => 125 billion total equations

Manvatkar, De, DebRoy, J. Appl. Phys., 2014
3D transient temperature distribution

<table>
<thead>
<tr>
<th>Laser power (W)</th>
<th>Beam radius (mm)</th>
<th>Scanning speed (mm/s)</th>
<th>Layer thickness (mm)</th>
<th>Substrate thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>210</td>
<td>0.5</td>
<td>12.5</td>
<td>0.38</td>
<td>4</td>
</tr>
</tbody>
</table>
**Multiple thermal cycles**

![Diagram of multiple thermal cycles](image)

Numerical and experimental monitoring locations (thermocouple) are shown.

### Table

<table>
<thead>
<tr>
<th>Material</th>
<th>Laser power (W)</th>
<th>Beam radius (mm)</th>
<th>Scanning speed (mm/s)</th>
<th>Powder flow rate (g/s)</th>
<th>Substrate thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti-6Al-4V</td>
<td>2000</td>
<td>2.0</td>
<td>10.6</td>
<td>0.4</td>
<td>10</td>
</tr>
</tbody>
</table>

Why considering convective flow?

- Heat conduction models neglect the mixing of the hot and the cold liquids.
- Heat conduction models overestimate cooling rates.

<table>
<thead>
<tr>
<th>Alloy</th>
<th>SS 316L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam radius (mm)</td>
<td>2.0</td>
</tr>
<tr>
<td>Scanning speed (mm/s)</td>
<td>10</td>
</tr>
<tr>
<td>Powder flow rate (g/s)</td>
<td>0.42</td>
</tr>
<tr>
<td>Substrate thickness (mm)</td>
<td>10</td>
</tr>
</tbody>
</table>
- Peak temperature increases at high power as in welding.
- Pool volume increases with heat input. Pool volume is larger in upper layers due to heat accumulation during the building process.
Cooling rate decreases with linear heat input, as in welding.

Cooling rate is lower in upper layers, because of significant heat accumulation during the depositing process.
The ratio of temperature gradient to solidification rate, \( G/R \), determines the morphology of the solidification structure.

- \( G/R \) decreases in upper layers, due to the decease of temperature gradient \( G \).
- \( G/R \) decreases with linear heat input, due to the decease of temperature gradient \( G \) or increase of solidification rate.
ii. Microstructure and grain growth

Temporal evolution of grain structure
Spatial distribution of grain shape and size
Effect of scanning strategy on solidification texture
3D Transient heat transfer and fluid flow model

Temperature field, thermal cycles, solidification parameters

Material properties

Temporal evolution, spatial distribution of grain structure.

Visualized grain growth process

Grain morphology size, and topology.

Wei, Elmer, DebRoy, Acta Mater, 2016; Wei, Elmer, DebRoy, Acta Mater (Cu), 2017
Temporal evolution of grain structure

<table>
<thead>
<tr>
<th>Material</th>
<th>Laser power (W)</th>
<th>Beam radius (mm)</th>
<th>Scanning speed (mm/s)</th>
<th>Layer thickness (mm)</th>
<th>Substrate thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>IN 718</td>
<td>250</td>
<td>0.5</td>
<td>15</td>
<td>0.4</td>
<td>4</td>
</tr>
</tbody>
</table>
The morphology and size of the grains varies significantly with the longitudinal sectional planes as well.

The grain structure varies significantly with the horizontal sectional planes.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017
The cross-sectional area of the grains are larger in the sectional planes near the top surface.

Grain sizes are smaller at the locations away from the center of the molten pool.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017
The grains appear in the form of columnar grains near the top surface, and the longitudinal central plane.

The columnar grains appear in the form of equiaxed grains near the edge of the fusion zone, which may be misleading.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017
Grains with six edges have highest frequencies, which is similar to the topological features of grains in isothermal systems.

The topological class distributions of the grains are unaffected by the pronounced spatial and temporal variations of the temperature in the heat affected zone.

Wei, Elmer, DebRoy, Acta Mater (Al), 2017
Role of laser scanning strategy

Unidirectional laser scanning

Bidirectional laser scanning

Multiple-layer, single-pass, directed energy deposition of IN718

Calculated temperature field of longitudinal sections at various locations

Three dimensional melt pool - Temperature and velocity fields

Magnification of temperature field with maximum heat flow directions

Bidirectional laser scanning

For unidirectional scanning, the angle of the primary dendrites is about 60° to the horizontal line.

For bidirectional scanning, there is 15° deviation of between the primary dendrites and the maximum heat flow direction. The angle between primary dendrites of neighboring layers is 90°.

iii. Residual stresses and distortion considering convective heat transfer

Thermo-mechanical model based on accurate temperature calculations considering flow of liquid metal

Calculation of residual stresses and distortion

Effects of layer thickness and heat input
Thermo-mechanical model

3D Transient heat transfer and fluid flow model

Temperature and velocity distribution for the domain

Abaqus database (.odb) file

Residual stress, strain, deformation for the domain

Geometry, mesh and temperature field

Python script
Calculated strain from temperature field

Temperature, K

Alloy: Inconel 718, Laser power: 300 W, Speed: 15 mm/s


Longitudinal strain during deposition
Scanning direction is along the positive x-axis
10 x magnification
Calculation of residual stresses

Scanning direction is along the positive x-axis
10 x magnification

Alloy: Inconel 718,
Laser power: 300 W,
Speed: 15 mm/s

Thinner layer thickness and lower heat input are helpful. Residual stresses can be decreased as much as 30% by doubling the number of layers to build the same height. Doubling the heat input reduces the residual stresses by about 20% and enhances the distortion by about 2.5 times.

iv. Reduced order modeling -
Back of the envelope calculations
Why dimensionless numbers?

- Reduce the number of parameters that need to be investigated
- Groups of variables provide important insights unlike individual variables
- Calculated using the heat transfer fluid flow model

Peclet number

\[ Pe = \frac{UL}{\alpha} \]

- Thermal diffusivity \( \alpha \)
- Pool length \( L \)
- Characteristics velocity \( U \)

Relative importance of heat transfer by convection and conduction

Mukherjee, Manvatkar, De, DebRoy, J. Appl. Phys., 2017
Marangoni number

\[ Ma = -\frac{d\gamma}{dT} \frac{w\Delta T}{\eta \alpha} \]

- Surface tension gradient: \( d\gamma/dT \)
- Pool width: \( w \)
- Temperature difference: \( \Delta T \)
- Viscosity: \( \eta \)
- Thermal diffusivity: \( \alpha \)

- Represents the effects of Marangoni stress on molten metal velocity
- High Marangoni no. => Active circulation => Wider molten pool
- Higher Marangoni no. => more efficient convective heat transfer

Mukherjee, Manvatkar, De, DebRoy, Scripta Mater., 2017
Fourier number

Heat dissipation rate

Heat storage rate

\[ F_o = \frac{\alpha}{V \cdot L} \]

- Thermal diffusivity: \( \alpha \)
- Pool length: \( L \)
- Scanning speed: \( V \)

- Laser power: 190-270 W, scanning speed: 15 mm/s
- High Fourier no. => Fast heat dissipation => Rapid cooling
- Ti-6Al-4V has the highest thermal diffusivity among 3 alloys

Mukherjee, Manvatkar, De, DebRoy, J. Appl. Phys., 2017
**Prediction of thermal strain**

\[
\varepsilon^* = \frac{\beta \Delta T}{EI} \frac{t}{F \sqrt{\rho}} H^{3/2}
\]

- High Power and low speed
- High peak temperature and large pool
- More solidification shrinkage
- High thermal strain and distortion

<table>
<thead>
<tr>
<th>Variables</th>
<th>Symbols</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal expansion coefficient</td>
<td>( \beta )</td>
</tr>
<tr>
<td>Temperature difference</td>
<td>( \Delta T )</td>
</tr>
<tr>
<td>Fourier number</td>
<td>( F )</td>
</tr>
<tr>
<td>Heat input per unit length</td>
<td>( H )</td>
</tr>
<tr>
<td>Total time</td>
<td>( t )</td>
</tr>
<tr>
<td>Flexural rigidity of substrate</td>
<td>( EI )</td>
</tr>
<tr>
<td>Density</td>
<td>( \rho )</td>
</tr>
</tbody>
</table>

Research needs for building a digital twin

- More rigorous validation of component models
- Including convective heat transfer to make models more realistic
- Scale-up of models for real life components
- Solid state transformations for common engineering alloys
- Reverse modeling
Thank you!

http://www.matse.psu.edu/modeling

**Modeling of welding and 3D printing**

We develop models of welding and 3D printing that are useful to produce defect free, structurally sound and reliable parts. They compute the most important factors that affect metallurgical product quality such as temperature and velocity fields, cooling rates and solidification parameters by solving tens of billions of equations efficiently. Specially structured for integration with genetic algorithms and other search engines, these simulations can be made bi-directional, switching traditional input and output variables, tailoring product attributes and optimizing production variables.