On August 10-11, the HPC4Manufacturing (HPC4Mfg) Program hosted the Modeling of Powder Dynamics in Metal Additive Manufacturing meeting in Austin, Texas at the Hilton Austin Hotel. The organizing committee united 100 participants from industry, laboratory, and academia. Presentations from keynote and plenary lecturers focused on the following topics:

- needs from models for powder spreading; flowability,
- spreadability, and segregation;
- effects of particle size, particle size distribution, and particle morphology;
- recycle and re-use of materials, and
- effects of environmental conditions.

Breakout sessions were held to discuss each topic and gather feedback in areas such as scientific challenges and priority research directions.
Organizing Committee

- A group of organizers served as note takers and facilitators

- From left to right:
  - Wayne King, Lawrence Livermore National Laboratory
  - Dan Bolintineanu, Sandia National Laboratories
  - Vijay Jagdale, United Technologies Research Center
  - Lang Yuan, GE Global Research
  - Ben Brown, Kansas City National Security Campus
  - Srdjan Simunovic, Oak Ridge National Laboratory
  - Jeremey Lechman, Sandia National Laboratory
  - Kartik Shah, Applied Materials
  - Eric Herbold, Kansas City National Security Campus
  - Otis Walton, Lawrence Livermore National Laboratory
  (not pictured)
The attendance was maximized to room capacity; it was a very hot topic!
### Executive Summary: Priority Research Directions

<table>
<thead>
<tr>
<th>Topic</th>
<th>Priority Research Direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>What is needed for models of powder spreading?</td>
<td>Calibrate and validate DEM contact/motion/flow models</td>
</tr>
<tr>
<td>Flowability, Spreadability, Segregation</td>
<td>Connect layer quality to part performance</td>
</tr>
<tr>
<td>Effects of Particle Size, Particle Size Distribution, and Particle Morphology</td>
<td>Bring part level performance requirements to powder layer level metrics</td>
</tr>
<tr>
<td>Recycle and Re-Use of Materials</td>
<td>Identify connection between powder evolution and processing productivity and part performance to inform limits on powder reuse</td>
</tr>
<tr>
<td>Effects of Environmental Conditions</td>
<td>Apply physics and surface chemistry (theory and characterization) to understand the effects of powder properties to inform DEM</td>
</tr>
</tbody>
</table>

The above priority research directions received the largest number of votes from the participants. Some votes were close, so it is best to see the details that follow.
Collection of Priority Research Directions (PRDs)

Using a live interactive audience participation tool, Poll Everywhere, participant votes for Priority Research Directions (PRDs) were collected in real time.

- The outcome of each breakout group was displayed on a slide
- The participants used their mobile devices to vote in real time on the PRDs
- Each participant received 1 vote for their top priority research direction on each topic
### Definitions of Advanced Manufacturing

<table>
<thead>
<tr>
<th><strong>Powder Flowability</strong></th>
<th>The ease with which a powder will <em>flow</em> under a specified set of conditions. Normally, powders ‘flow’ within an internal geometry (e.g., a channel, pipe, hoppers, silos, etc.)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Powder Spreadability</strong></td>
<td>The ease with which a powder will <em>spread</em> under a specified set of conditions. Normally, powders are ‘spread’ within a sliding contact (i.e., relatively moving surfaces).</td>
</tr>
<tr>
<td><strong>‘Flowability’ and ‘Spreadability’</strong></td>
<td>Qualitative attributes which, in addition to the powder’s characteristics, depend on the size and configuration of the ‘system’ in which they are evaluated, as well as on the rate of deformation (i.e., inertial effects may influence the value assigned to the attribute).</td>
</tr>
</tbody>
</table>
Keynote Lectures

Otis Walton
Lawrence Livermore National Laboratory
Livermore, California

Stefan Luding
University of Twente
Enschede, Netherlands

Mustafa Megahed
ESI Group
Paris, France
DEM (i.e., particle-scale simulations) can provide insight not modeled by continuum approaches, like FE (such as size-segregation).

Traditional DEM for >100μm particles, only has liquid-bridge or cemented-joint cohesion.

<30μm AM powders have high van der Waals cohesion effects (e.g., JKR & DMT models).

Smallest particles’ cohesion causes plastic deformation at contacts ➔ high rolling resistance.

DEM simulation models for AM need to include:
  — Size & Shape distributions;
  — normal-direction Repulsion & cohesion;
  — sliding-friction;
  — rolling ‘friction’;
  — twisting-‘friction’;
  — viscous or hysteretic energy ‘dissipation’;
  — and perhaps(?) interstitial-air effects.

Important to calibrate model parameters to mimic bulk behavior under similar conditions

Need improved calibration procedures (sensitivity analyses can provide some guidance)
Particle Simulations for Additive Manufacturing
Stefan Luding, University of Twente, Enschede, Netherlands

- DEM simulation codes: mercuryDPM.org and mercuryLab.org
- From micro/contact-mechanics to macro-behavior (coarse-graining)
- Calibration and Validation of cohesive, frictional contact models and DEM
- Choice of calibration tests and relevant parameters - depending on (flow) regime(s) and application - continuum modeling & dimensionless variables
- CPU-time when running moderate to large DEM -> mercuryCloud
- Apply modern and novel experimental techniques for additional information not available otherwise ...
Modeling Powder Spreading for Additive Manufacturing
Mustafa Megahed, ESI Group, Paris

- The characteristics of the powder layer affect material quality
- Part manufacturability is affected by delivery system in many ways
- Modeling powder spreading is a central component of ESI-AM
Plenary Lectures and Breakout Groups
What is Needed for Models for Powder Spreading
Fred Higgs, Rice University

- **Predictions based on comprehensive powder properties.** Spreading models need to be able to simulate spreading behavior by incorporating the thermal, tribological, mechanical, rheological, and morphological properties of powder particles.

- **Motivation.** AM machine users have reported two powders appearing to be identical yet exhibiting radically different spreading behavior.

- **Connectivity between single particle and full powder spreading behavior.** Between the spreader geometry and the build plate are the dynamic powders being spread and fused or bound. Models need to integrate the 3D printer’s design parameters and the powder’s behavior to yield predictable metrics about powder spreadability.

- **Short- and long-range effects from multi-layer spreading.** Models need to provide not just single spread layer information, i.e., short-range effects, but also the long-range effects from multi-layer spreading predictions and spreading on top of previously spread layers.

- **Tractable information for machine operators.** Results from spreading models need to be rapidly converted to reduced-order models, look-up tables, process maps, etc. to provide actionable guidance for 3D printer operators.
What is Needed for Models for Powder Spreading
Current Status and Recent Advances

- There is a gap in understanding what the models can provide in terms of actionable information
- Particle models are mature
- The need is for developing the parameters that describe realistic AM powders
- There is not a general understanding of the importance of coater technology to the process

- Models can do particle dynamics simulations for realistic situations such as spreading over realistic surfaces
- DEM has the potential to positively impact the cost of metal AM
- There may be useful information to be obtained from other fields such as pharmaceuticals, ceramics, metal injection molding, roofing tiles

https://www.youtube.com/watch?v=MUr3H-M-nRk
What is Needed for Models for Powder Spreading
Scientific Challenges and Opportunities

- DEM should be used to inform realistic machine designs including spreading, dispensing, coater technology, coater speed, coater wear/life
- Need a measure for the similarity of DEM predictions with experiment

- Coater blades may not be the best way to recoat. Investigations should be made into alternate coater technologies
- There is a need for reduced order powder dynamics models for practical use on the shop floor
What is Needed for Models for Powder Spreading
Priority Research Directions

Based on 89 Responses
Key Parameters and Issues: Flowability, Spreadability, Segregation
Jeremy Lechman, Sandia National Laboratories

- Particle description
  - Shape, Composition
  - Surfaces – structure, composition
    - Particle-particle interactions: friction, adhesion/cohesion

- Index flow measures
  - Relevance to varying conditions, types of flow – e.g., very thin flows, segregation
  - Hall Flow, flowdex, rotating drum, rheometers, ...
    - Which relevant for model selection, parameter estimation, and calibration?
    - Best practices for model validation and uncertainty quantification?

- Bulk flow measures
  - How to measure bulk friction coefficient and cohesion in limit of low confining stress?
  - Role of Van der Waals attraction/adhesion, humidity, electrostatics, ... in determining effective cohesion?

- Other issues: role of air, vibration, etc.
Key Parameters and Issues: Flowability, Spreadability, Segregation
Current Status and Recent Advances

- The terms flowability and spreadability, while descriptive, is not quantitative
- There is no standardized technique for model calibration and validation
- Get Bryan Ennis to give input on particle measurement methods

- Spreading thin layers may not correlate with today’s standard powder characterization methods; What are the right measurement methods
- What characteristics of the powder control flowability and spreadability
Key Parameters and Issues: Flowability, Spreadability, Segregation
Scientific Challenges and Opportunities

- Is the layer quality affected by the presence of parts in a powder bed
- Is there a way to quantify the morphology of a powder layer
- What is the standard test that would be relevant to spreadability
- What are the relevant DEM parameters/models that affect spreadability
- Are there reduced order models that could be applied?
- Is there a multiscale analogy for DEM?
Key Parameters and Issues: Flowability, Spreadability, Segregation

Priority Research Directions

Based on 88 Responses

- Develop a standard for flowability and spreadability: (1) definition, (2) powder characteristic metrics, (3) measurement techniques: 30%
- Document and prioritize the physical models required to model AM: 6%
- Replace calibration with physics-based models: 16%
- Develop better standard testing for layer quality (e.g., flatness, density/porosity variation): 8%
- Connect layer quality to part performance: 33%
- Understand how spatial variations in the powder bed affect sintering process: 6%
- Quantify segregation in powder layer: 2%

Poll locked. Responses not accepted.
There is limited information on whether powder should be mixed and also in regards to other sources of variability in PSD. Experiments at NIST have shown spatial variability of PSD of 17-4SS nitrogen atomized powder to be minimal (less than 2 μm) in an as-received condition (in container) and in a loose, partless, spread powder bed (50 mm deep spread in 20 μm layers). Significant PSD variability has been seen while spreading over solidified LPBF surfaces. From these findings mixing of powder is not warranted, but this must be confirmed with more studies.

Calibrated DEM model is allowing the above-mentioned variability to be further investigated in the LPBF process. Initial findings suggest the loose powder/part interface may be the culprit.

In-situ validation of DEM models can be challenging and is usually not conducted. At NIST a spreading testbed using cross-sectional imaging and digital image correlation is used to validate DEM models produced at the University of Arkansas as well as to conduct a general analysis of the spreading process providing a means to identify primary variables.

Powder rheology is potentially an insightful tool, but prior to its acceptance as an ex-situ powder characterization technique it must be evaluated in terms of uncertainty. Static charging has been seen in experiments and may be a concern for certain materials and apparatuses.

Techniques for particle sizing of AM precursor materials often do not provide comparable results. Methods developed at NIST Boulder allow for more accurate 3D morphological representations of powder particles using XCT imaging and can serve as a means for comparing results from several other PSD measurement techniques.
Key Parameters and Issues: Effects of Particle Size, Particle Size Distribution, and Particle Morphology

Current Status and Recent Advances

- We do not currently understand why variations in PSD can be compensated for with process parameters: in absence of a prediction, the need to modify the process is undesirable in a production setting.

- We know that the spreading process can produce segregated layers. What is the impact?

- What is the critical morphology measure that is important to the process?

- There is not agreement on whether to report in number or volume frequency which is likely due to difference in measurement methods.
Key Parameters and Issues: Effects of Particle Size, Particle Size Distribution, and Particle Morphology

Scientific Challenges and Opportunities

- Large spatter can have a big effect on defect formation in a given layer
- What is the optimal method for powder production: nozzle design, droplet flow
- There are computational challenges associated with large powder layers, complicated morphologies
- Model is needed to predict/optimize PSD, morphology, and density in atomization systems
- Can particles be separated by morphology
Key Parameters and Issues: Effects of Particle Size, Particle Size Distribution, and Particle Morphology

Priority Research Directions

Based on 84 Responses
Recycle and Re-Use of Materials
Andrew Carter, Stratasys Direct Manufacturing

- **Status:** Material usage in additive manufacturing can be very efficient if 100% of unconsolidated metal powder is recycled back into the process. This work aims to strengthen the sentiment that any change in feedstock properties (i.e. PSD, morphology, and chemistry) does not manifest as poor mechanical properties in the final additive material.

- **Powder Reuse Study:**
  - Compared 7 EOS M280 Machines, 2 Material Providers, 8 Material Lots.
  - Data represents 385 production builds over an 8 month period.

- **Testing Included:** 210 tensile bars (tests performed approx. every 4 builds), 14 Chemical, 20 Metallography

- **Summary:** Regardless of powder age and times recycled the mechanical properties and material microstructure showed no sign of degradation or increased variation. There was negligible difference in room temperature tensile properties or microstructure across the build plate, across the 7 machines, or between the 2 material providers.

### Comparisons

*Table Key: Tensile Property: Max. Difference in Mean, Max Difference in Coefficient of Variance*

<table>
<thead>
<tr>
<th>Recycled Powder (Difference between Virgin to 60 times recycled)</th>
<th>Build location</th>
<th>Machine to Machine</th>
<th>Material Provider</th>
</tr>
</thead>
<tbody>
<tr>
<td>UTS: 0.5ksi, 0.83 % YS: 0.1ksi, 0.97% Elongation 0.50%, 0.50%</td>
<td>UTS: 0.15ksi, 0.08% YS: 0.16ksi, 0.25% Elongation: 0.05%, 0.14%</td>
<td>UTS: 1.53ksi, 0.34% YS: 1.06ksi, 1.40% Elongation: 4.70%, 2.23%</td>
<td>UTS: 3.2ksi 0.02% YS: 0.3ksi, 0.28% Elongation: 1.01%, 4.76%</td>
</tr>
</tbody>
</table>
Recycle and Re-Use of Materials
Current Status and Recent Advances

- For certain materials, there are indications that recycle and reuse may be less of a problem than previously thought
- We have not seen fatigue data using recycled powder
- Terminology: blending, mixing
Recycle and Re-Use of Materials
Scientific Challenges and Opportunities

- There is a need to integrate kinetic thermodynamic models into DEM models to simulate the “aging” of powder (temperature history needed)
- DEM could be used to understand if powders remaining in the dispenser need to be mixed before the next build
- DEM could be used to prescribe the optimal steps in sieving and mixing of powders
Recycle and Re-Use of Materials
Priority Research Directions

Based on 82 Responses
Effects of Environmental Conditions
Rainer Hebert, University of Connecticut

- Humidity affects Hall flow behavior in a non-linear fashion (Fig. 1a), but initial experiments with Ti-6Al-4V powder did not confirm a similar behavior with raking over a build plate (Fig. 1b).

- Variations in Hall flow with relative humidity are attributed to surface films of hydroxides and hydrated oxides. Limited knowledge exists about the stability of hydroxides and hydrated oxides on typical additive manufacturing powders as a function of temperature and partial pressures of gases and water vapor.

- Vibrations of powder beds have been demonstrated to induce patterns that appear to be counter-productive to dense powder beds sought for additive manufacturing (for example, F. Melo, P.B. Umbanhowar, H.L. Swinney, “Hexagons, Kinks, and Disorder in Oscillated Granular Layers”, Phys Rev Lett, vol. 75(21), pp. 3838-3842 (1995))

- Total pressures in build chambers appear not to impact powder dynamics with the possible exception of vacuum levels low enough to induce desorption of adsorbates on powder particles.

- New research directions should revolve around computational and experimental studies of powder particle surface chemistries and phases to provide input to DEM models.

- An experimental set up to control the raking system and environment, coupled with in-situ X-ray tomography will provide data sets for the DEM community to help validate simulation predictions.

Fig. 1a: Flow time vs relative humidity for Cu powder. From: G. Matei, N. Claussen, H.H. Hausner, Electronic design: circuits and systems, vol. 8, pp. 5-11, 1974

Fig. 1b: Ti-6Al-4V powder size distribution after raking in 62 % relative humidity and in dry condition, taken from left and right sections on build plate.
Effects of Environmental Conditions
Current Status and Recent Advances

- Are environmental effects on layer quality affected by the presence of parts in a powder bed?

- Despite the long history of study of environmental effects on powders, there is not much information for the AM community.

- Can we benefit from the experience in the powder metallurgy community?

- Can we benefit from the DoD experience in powders?
Effects of Environmental Conditions
Scientific Challenges and Opportunities

- Can we understand the “oscillatory” behavior that has been observed as a function of humidity?
- Understanding environmental effects requires a distinctly different set of modeling and experimental tools.
- What is the effect of humidity of layer quality?
- Is there an opportunity in modifying the surfaces of powder to improve performance?
Effects of Environmental Conditions
Priority Research Directions

Based on 86 Responses

- Model vibration induced particle motion/redistribution for mixed particle size distribution: 9%
- Standardize methods (experimental) to capture the impact of environmental variation on powder and part level metrics and performance: 13%
- Apply physics and surface chemistry (theory and characterization) to understand the effects of powder properties to inform DEM: 43%
- Develop standard procedures at the operating floor level from model investigations of sensitivities and experimental observations: 8%
- Develop understanding of laser interactions with surface chemistry and its effect on part performance: 17%
- Develop reduced order models to simulate long term environmental and chemistry effects: 6%
- Use modeling and simulation surface modify powders to improve applicability to AM: 3%
Action Items

- Set up seminar on multiscale modeling suggested by Jim Belak (Invitation sent to Madhava Syamlal of NETL)

- WebEx by Bryan Ennis (October 17, 2017, 9:00am Pacific Time)

- Conduct vote limited to practitioners -Completed

- Make contact with International Fine Particle Research Institute (IFPRI) -joint research portfolio ifpri.net -Completed
Poll Results from Practitioners
What the models need: Priority research directions

- Understand Impact of gas flow on powder dynamics: 21%
- Calibrate and validate DEM contact/motion/flow models: 26%
- Identify model/parameter sensitivity: 21%
- Continue parallel development of discrete and continuum/reduced order models
- Develop datasets for model validation and calibration Guide metrology for AM for in-situ and ex-situ characterization: 5%
- Optimize feedstock specifications and processes: 16%
- Employ models to identify/prioritize physics to include in simulations: 11%

Based on 19 Responses
Flowability, Spreadability, Segregation: Priority research directions

- Develop a standard for flowability and spreadability: (1) definition (2) powder characteristic metrics (3) measurement techniques: 47%
- Document and prioritize the physical models required to model AM
- Replace calibration with physics-based models
- Develop better standard testing for layer quality (e.g., flatness, density/porosity variation): 5%
- Connect layer quality to part performance: 37%
- Understand how spatial variations in the powder can affect AM process: 5%
- Quantify segregation in powder layer: 5%

Based on 19 Responses
Based on 18 Responses

- Identify the effect of powder delivery method on layer quality: 44%
- Quantify surface effects on powder interactions: 17%
- Develop methodology to quantify particle morphology: 11%
- Quantify impact of trapped gas in powder on part performance: 6%
- Bring part level performance requirements to powder layer level metrics: 17%
- Evaluate plausibility of using nonspherical powder: 6%
Recycle and Re-Use of Materials: Priority Research Directions

Poll locked. Responses not accepted.

- Identify connection between powder evolution and processing productivity and part performance to inform limits on powder reuse: 80%
- Characterize the effect of sintering that occurs in electron beam AM on recycling: 7%
- Employ DEM to inform spatial and statistical variability in powder layer formation: 13%
- Use models to inform process and application aware specifications for recycled powders.
- Integrate chemical thermal kinetic models into DEM simulation:

Based on 15 Responses
Effects of Environmental Conditions: Priority Research Directions

Poll locked. Responses not accepted.

Based on 17 Responses