HPC and AM:

Overcoming the barriers to material qualification

Workshop on Predictive Theoretical and Computational Approaches for Additive Manufacturing

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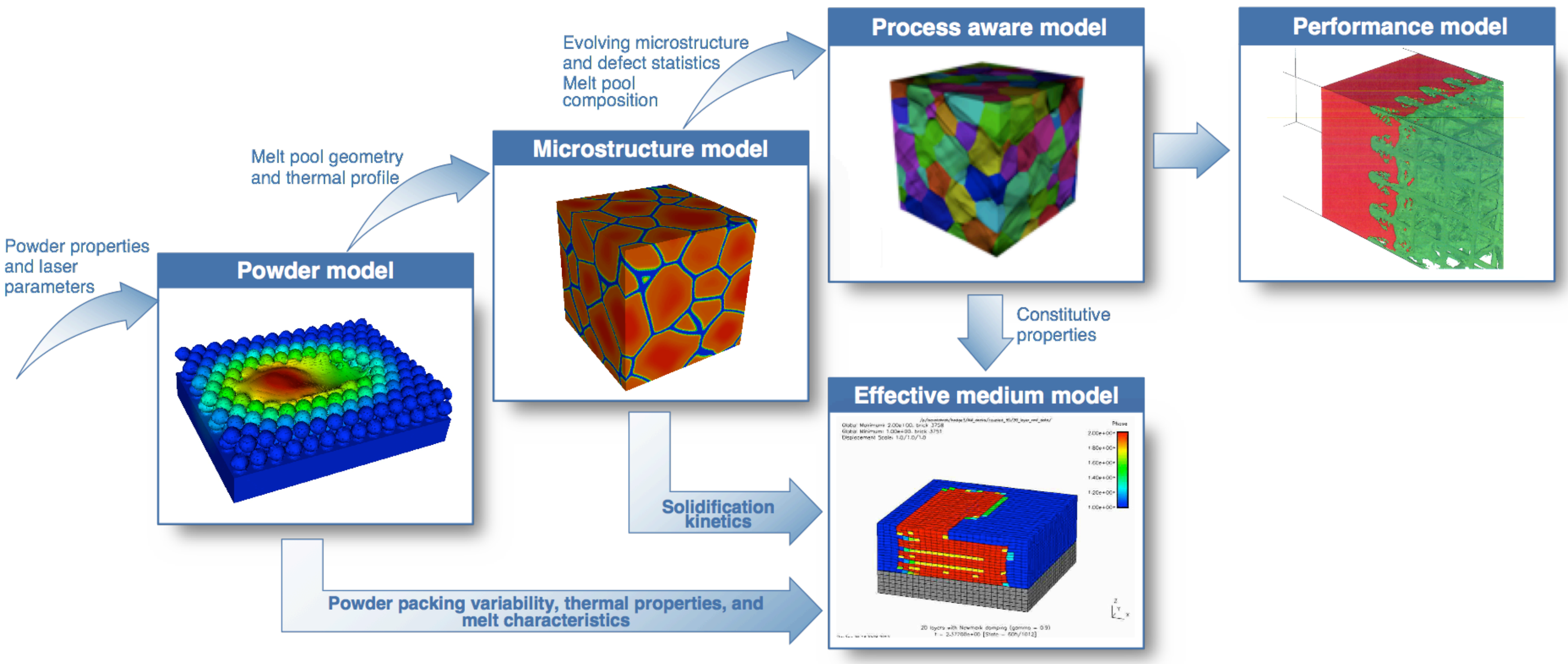
Questions

- Computational methods and approaches for simulating materials processing, properties and performance relationships for materials design using additive manufacturing as well as key process parameter identification and process mechanics.
- How to leverage high performance computing spanning scientific discovery to ensembles of engineering solutions?
- How can AM benefit from fundamental advances in verification, validation and uncertainty quantification methodologies? (Prelude to In-Situ Monitoring & Diagnostics theme)
- Is there sufficient funding in the US for fundamental research and development (TRL1 through TRL3) for additive manufacturing?
- Most US academic institutions house their additive manufacturing programs in mechanical engineering departments, and materials departments remain largely disengaged. How can we better involve our top-tier MS&E students and faculty in additive manufacturing?

Multiscale modeling approaches provide key insights into AM metal processes that will inform performance simulations



Metal AM process covers a broad range of length and time scales, making modeling challenging

Modeling of the AM process dates back to 1998

- Metal thermal models
  - Contuzzi, N., Campanelli, S., Ludovico, A.D., 2011. 3D Finite Element Analysis In The Selective Laser Melting Process. Int. J. Simul. Model 10, 113-121
  - Dai, K., Li, X.X., Shaw, L.L., 2004. Comparisons between thermal modeling and experiments: effects of substrate preheating. Rapid Prototyping Journal 10, 24-34
  - Kolossov, S., Boillat, E., Glardon, R., Fischer, P., Locher, M., 2004. 3D FE simulation for temperature evolution in the selective laser sintering process. International Journal of Machine Tools and Manufacture 44, 117-123
  - Roberts, I.A., Wang, C.J., Esterlein, R., Stanford, M., Mynors, D.J., 2009. A three-dimensional finite element analysis of the temperature field during laser melting of metal powders in additive layer manufacturing. International Journal of Machine Tools and Manufacture 49, 916-923
- Metal thermo mechanical models
  - Hussein, A., Hao, L., Yan, C., Everson, R., 2013. Finite element simulation of the temperature and stress fields in single layers built without-support in selective laser melting. Materials & Design 52, 638-647
  - Matsumoto, M., Shiomi, M., Osakada, K., Abe, F., 2002. Finite element analysis of single layer forming on metallic powder bed in rapid prototyping by selective laser processing. International Journal of Machine Tools and Manufacture 42, 61-67
- Polymer powder bed fusion
  - Williams, J.D., Deckard, C.R., 1998. Advances in modeling the effects of selected parameters on the SLS process. Rapid Prototyping Journal 4, 90-100

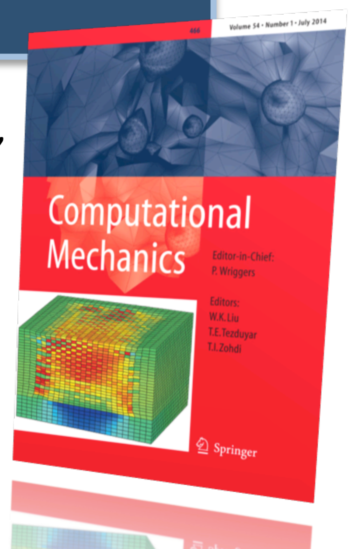
Modeling of the AM process dates back to 1998

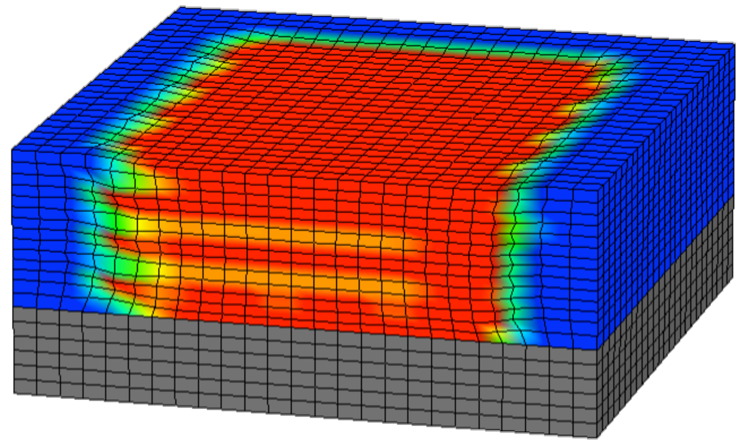
- Residual stress modeling
  - Zaeh, M., Branner, G., 2010. Investigations on residual stresses and deformations in selective laser melting. Production Engineering 4, 35-45
- Laser-powder interaction
  - Fischer, P., Romano, V., Weber, H.P., Karapatis, N.P., Boillat, E., Glardon, R., 2003. Sintering of commercially pure titanium powder with a Nd : YAG laser source. Acta Materialia 51, 1651-1662
  - Gusarov, A.V., Smurov, I., 2010. Modeling the interaction of laser radiation with powder bed at selective laser melting. Physics Procedia 5, 381-394
  - Tolochko, N.K., Arshinov, M.K., Gusarov, A.V., Titov, V.I., Laoui, T., Froyen, L., 2003. Mechanisms of selective laser sintering and heat transfer in Ti powder. Rapid Prototyping Journal 9, 314-326

Effective Medium Modeling is carried out at the part scale using LLNL's DIABLO code

DIABLO allows prediction of material behaviors and is suitable for complex structural response and temperature-driven deformations

Hodge, N.E., Ferencz, R.M., Solberg, J.M., 2014. Implementation of a thermomechanical model for the simulation of selective laser melting. Comput Mech, 1-19.

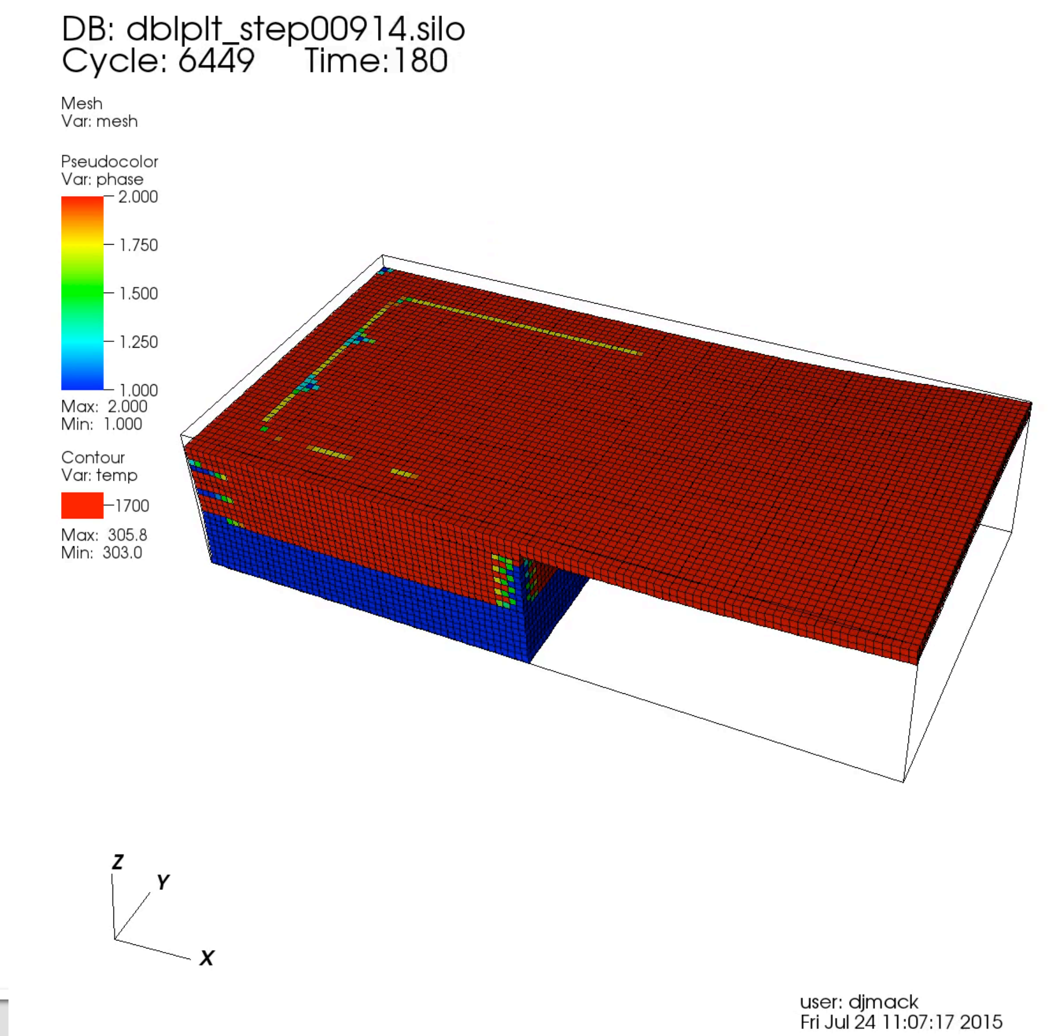




Layer-resolved consolidation

We have successfully modeled effects of melting and solidification and predicted observed defects at overhangs

Example of Diablo simulation

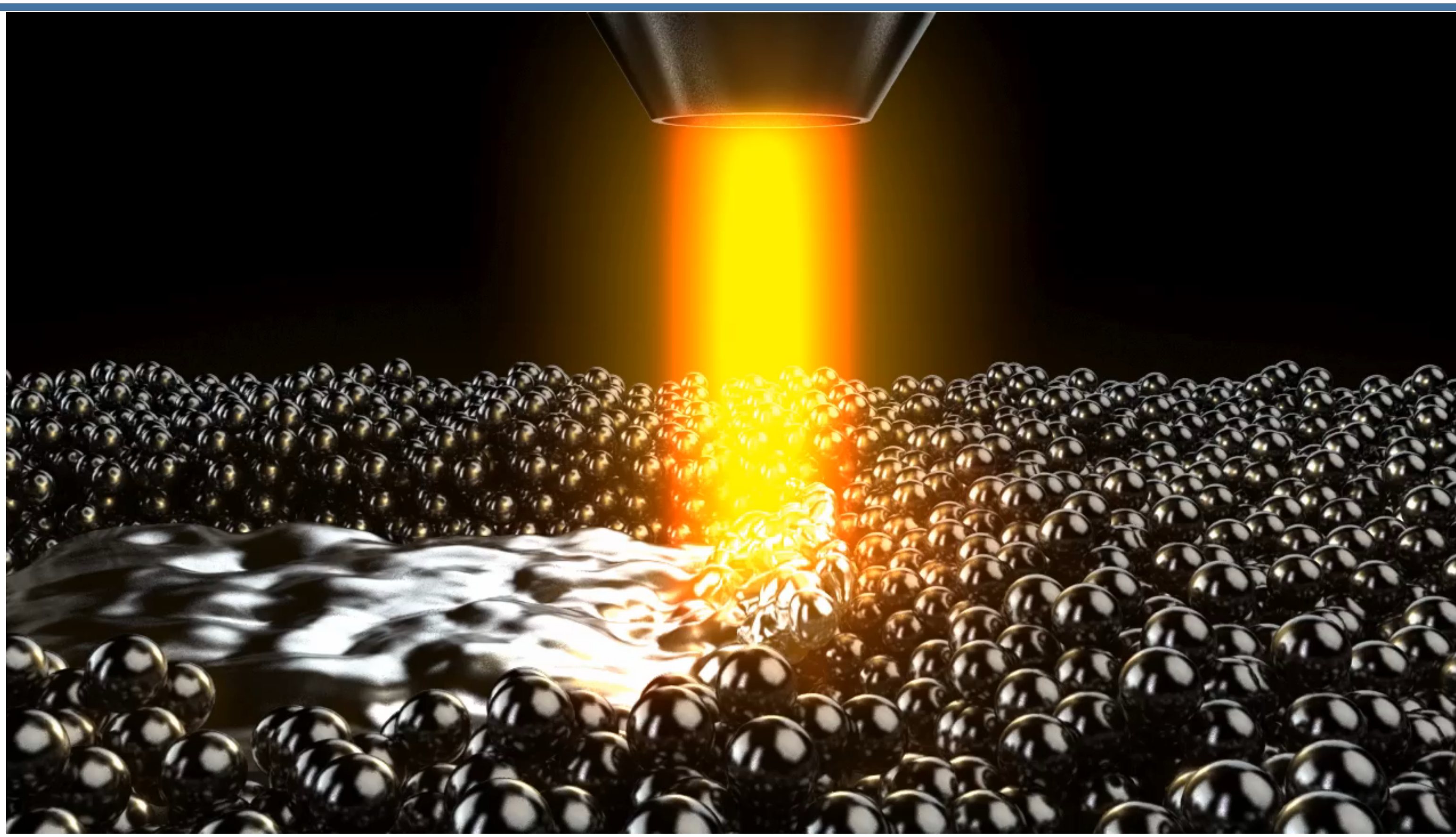


Alternative approaches

- Thermo mechanical models – custom codes
  - Denlinger, E.R., Michaleris, P., 2015. Mitigation of distortion in large additive manufacturing parts. Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture
  - Pal, D., Patil, N., Zeng, K., Stucker, B., 2014. An Integrated Approach to Additive Manufacturing Simulations Using Physics Based, Coupled Multiscale Process Modeling. Journal of Manufacturing Science and Engineering-Transactions of the ASME 136.
  - Neugebauer, F., Keller, N., Ploshikhin, V., Feuerhahn, F., Köhler, H., 2014. Multi Scale FEM Simulation for Distortion Calculation in Additive Manufacturing of Hardening Stainless Steel, International Workshop on Thermal Forming and Welding Distortion. BIAS Verlag, Bremen.
  - Neugebauer, F., Keller, N., Xu, H., Kober, C., Ploshikhin, V., 2014. Simulation of Selective Laser Melting Using Process Specific Layer Based Meshing, DDMC 2014 - Proceedings of the Fraunhofer Direct Digital Manufacturing Conference, Aachen, pp. 297 - 302.

- Thermo mechanical models – commercial codes
  - Schilp, J., Seidel, C., Krauss, H., Weirather, J., 2014. Investigations on Temperature Fields during Laser Beam Melting by Means of Process Monitoring and Multiscale Process Modelling. Advances in Mechanical Engineering.
  - Seidel, C., Zaeh, M.F., Wunderer, M., Weirather, J., Krol, T.A., Ott, M., 2014. Simulation of the Laser Beam Melting Process – Approaches for an Efficient Modelling of the Beam-material Interaction. Procedia CIRP 25, 146-153 DOI..
  - Zaeh, M.F., Branner, G., Krol, T.A., 2010. A three dimensional FE-model for the investigation of transient physical effects in Selective Laser Melting, In: Bartolo, P.J.D., DeLemos, A.C.S., Pereira, A.M.H., Mateus, A.J.D., Mendes, A.L.A., DeMoura, C.S.M., Capela, C.A.B., DaSilva, C.S.G., Domingues, F.A.C., Bartolo, H., Almeida, H.D., Ferreira, I.S.C., Matias, J.M., Alves, N.M.F., Rodrigues, S. (Eds.), Innovative Developments in Design and Manufacturing: Advanced Research in Virtual and Rapid Prototyping. CRC Press-Taylor & Francis Group, Boca Raton, pp. 415-424.

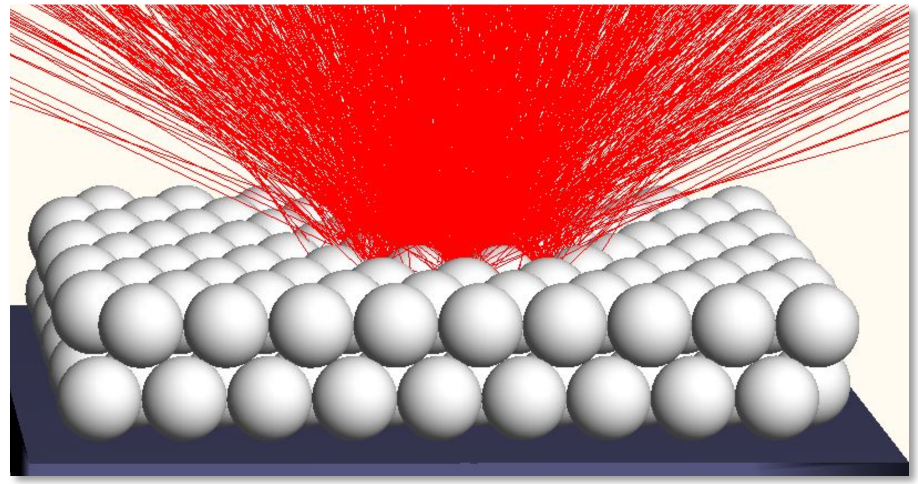
Our powder model represents complex physics at the scale of the metal powder



Using ALE3D (a high performance multi-physics code), we are performing the first full-physics simulations of laser powder bed fusion

First principles calculations are being used to understand the absorptivity of the metal powder

- Powder size (typically tens of microns) is much larger than the laser wavelength (1 µm), so ray tracing can be used
- The refractive index of the metals involved is known or can be measured
- On each reflection, the absorption is determined by Fresnel formulas, which include angular and polarization effects
- Multiple scattering plays an important role
- Commercial code FRED was used for ray tracing. Considerable post-processing was required



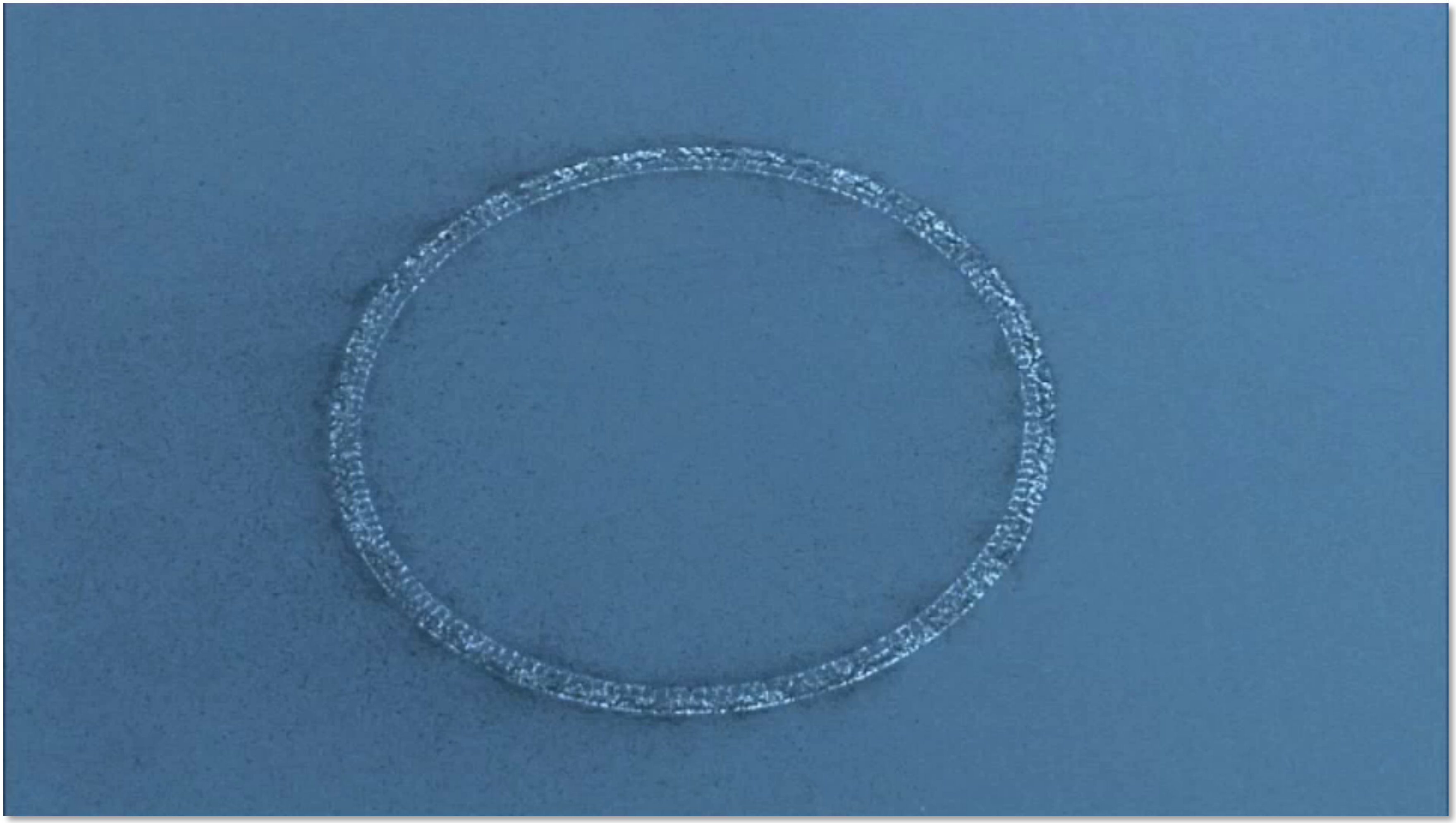
Stainless steel

Power balance

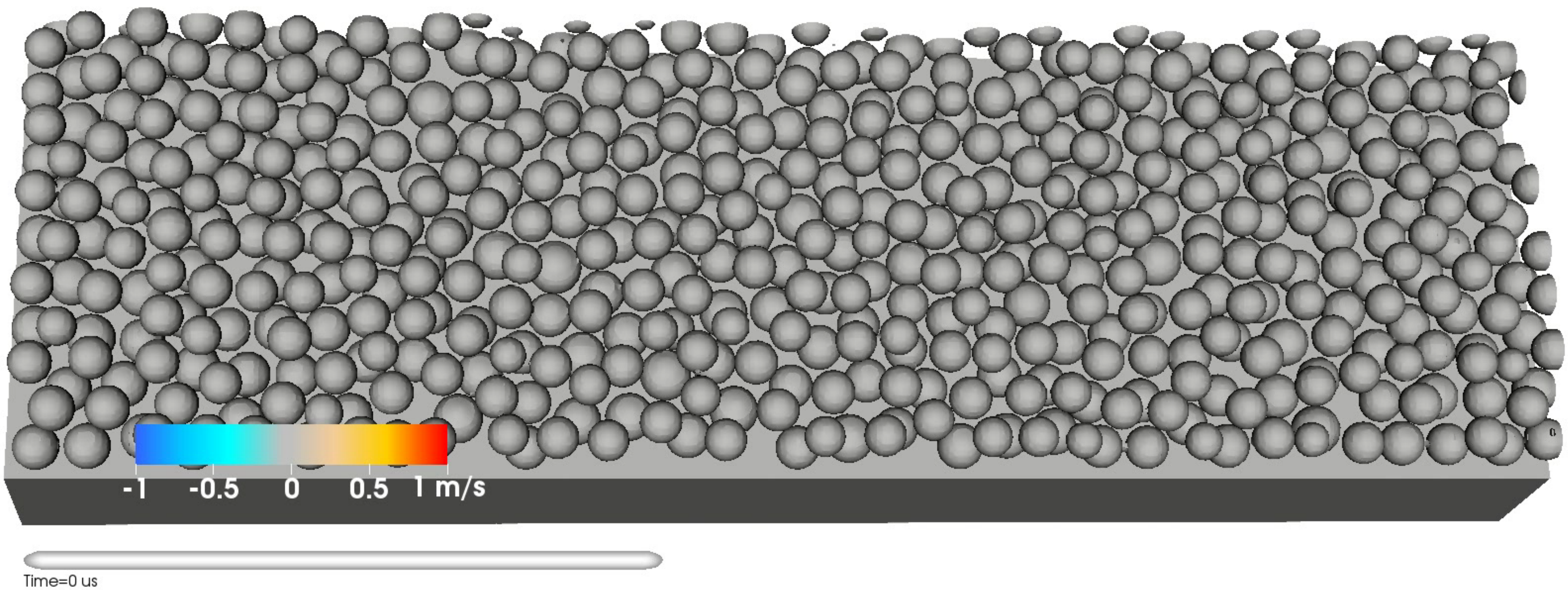
• Absorbed by top layer:	52%
• Absorbed by bottom layer:	6%
• Absorbed by substrate:	2%
• Reflected:	40%

	100%

Metal powder bed fusion-Missing Physics



Mesoscopic 3D simulations provide insight into AM process using ALE3D



Alternative approaches

- Lattice-Boltzmann Methods in 2D
  - Klassen, A., Scharowsky, T., Korner, C., 2014. Evaporation model for beam based additive manufacturing using free surface lattice Boltzmann methods. Journal of Physics D-Applied Physics.
  - Körner, C., Attar, E., Heinl, P., 2011. Mesoscopic simulation of selective beam melting processes. Journal of Materials Processing Technology 211, 978-.
  - Körner, C., Bauereiß, A., Attar, E., 2013. Fundamental consolidation mechanisms during selective beam melting of powders. Model Simul Mater Sc 21, 085011.

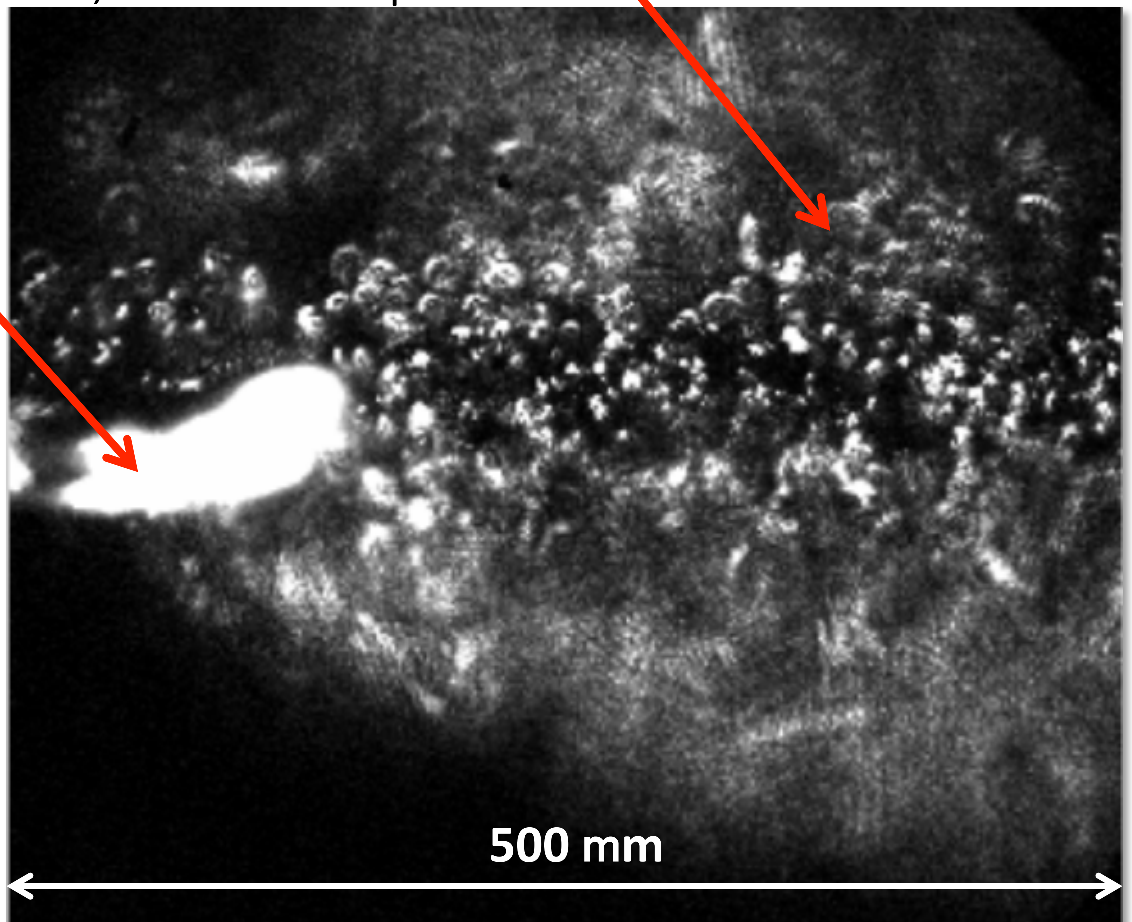
- Open Source Models in 3D
  - Gurtler, F.J., Karg, M., Leitz, K.H., Schmidt, M., 2013. Simulation of laser beam melting of steel powders using the three-dimensional volume of fluid method, In: Emmelmann, C., Zaeh, M.F., Graf, T., Schmidt, M. (Eds.), Lasers in Manufacturing. Elsevier Science Bv, Amsterdam, pp. 874-879.

- Discrete Element Methods in 3D
  - Ganeriwala, R., Zohdi, T.I., 2014. Multiphysics Modeling and Simulation of Selective Laser Sintering Manufacturing Processes. Procedia CIRP 14, 299-304

Experiments reveal Missing Physics

Illuminated, ~60 mm thick powder bed

Thermal emission from melt pool



Out of focus and away from camera

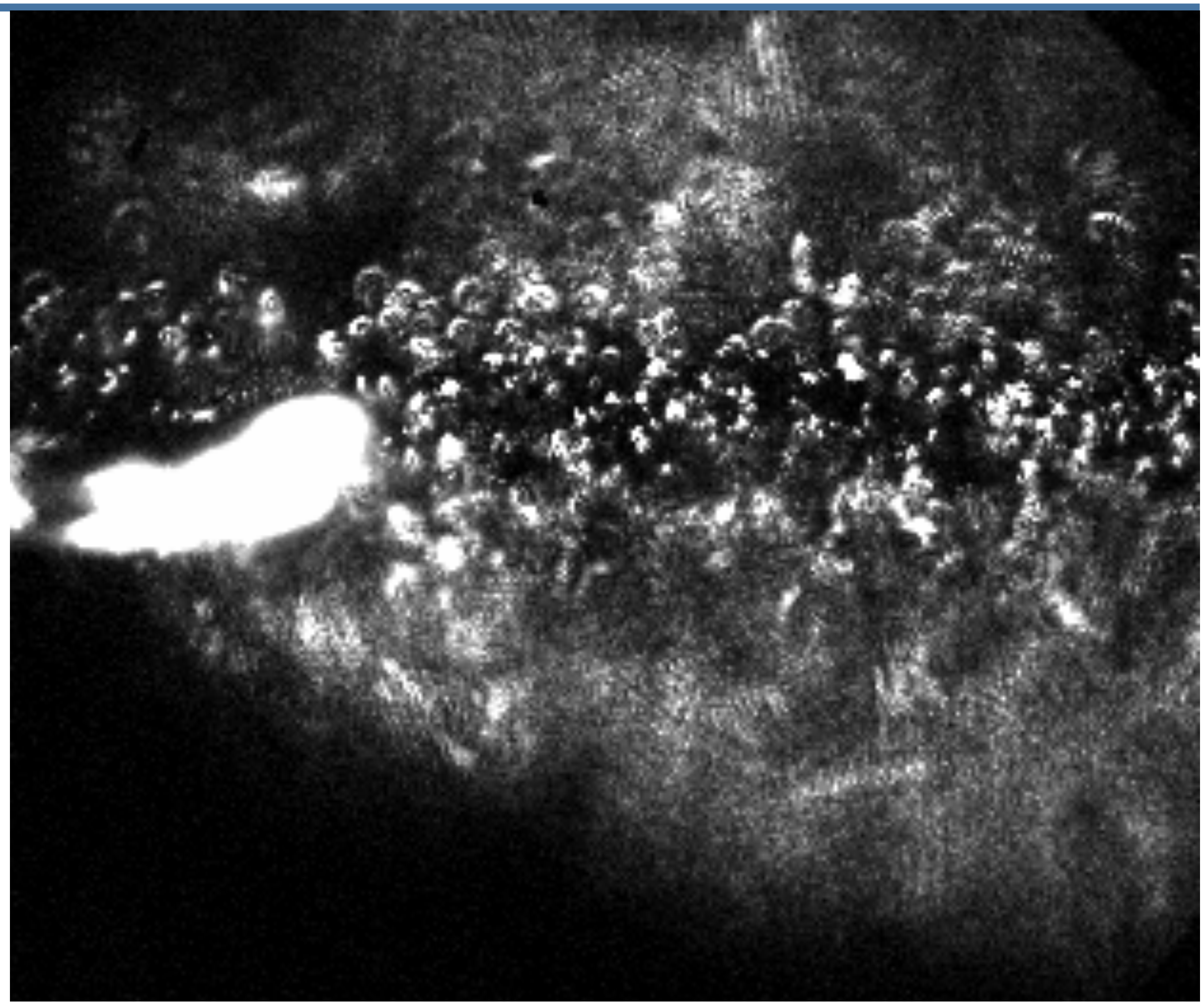
In focus

Out of focus and toward camera

Image capture rate: 500,000 frames/sec

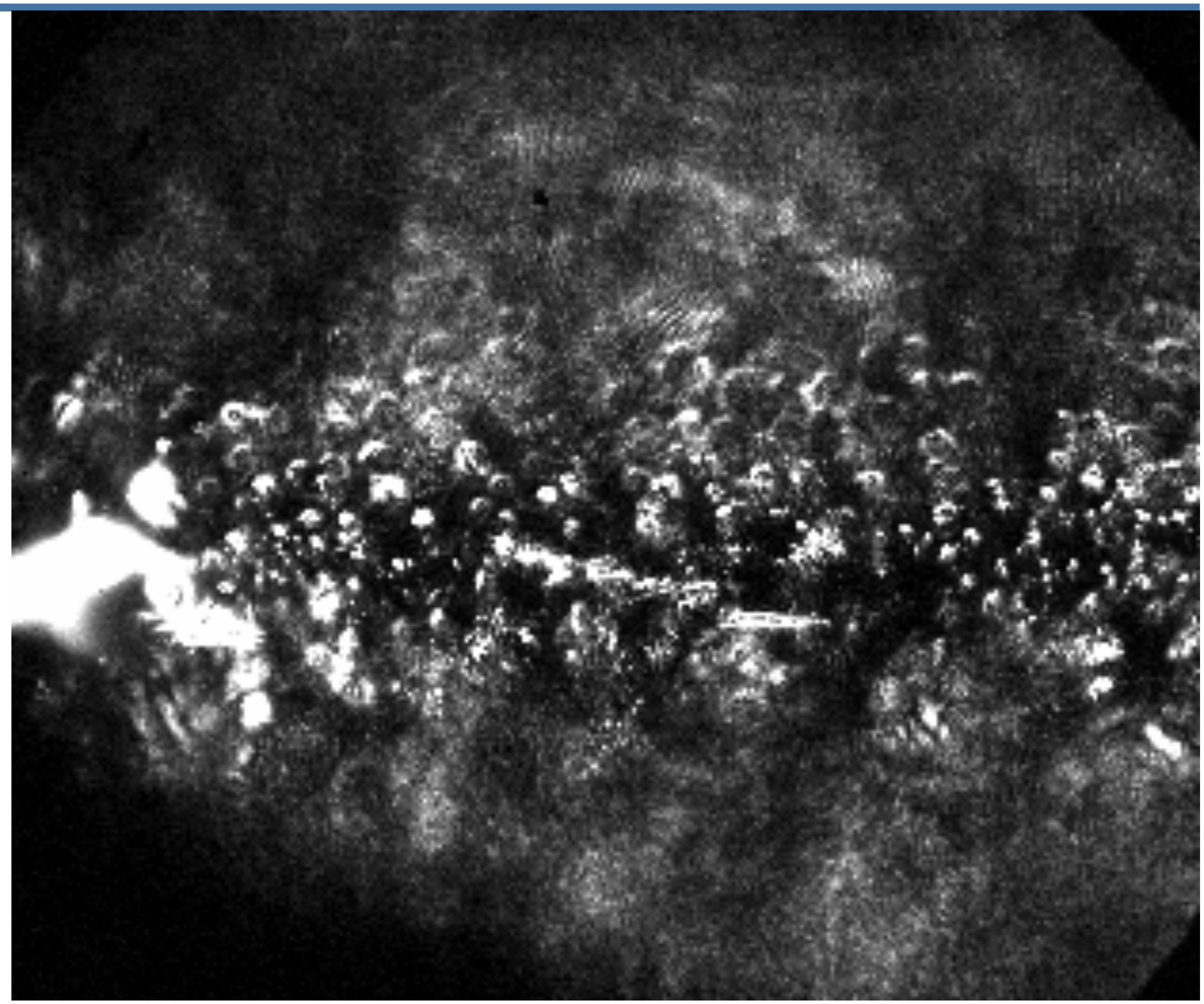
SS316L w/ thermal emission (no band pass filter): 200 W, 1500 mm/s

- Melt pool expansion exerts *forward 'push'* on powder
- Nearby powder is consumed through *capillary forces* into melt pool
- Non-local powder experiences inward force toward melt pool!



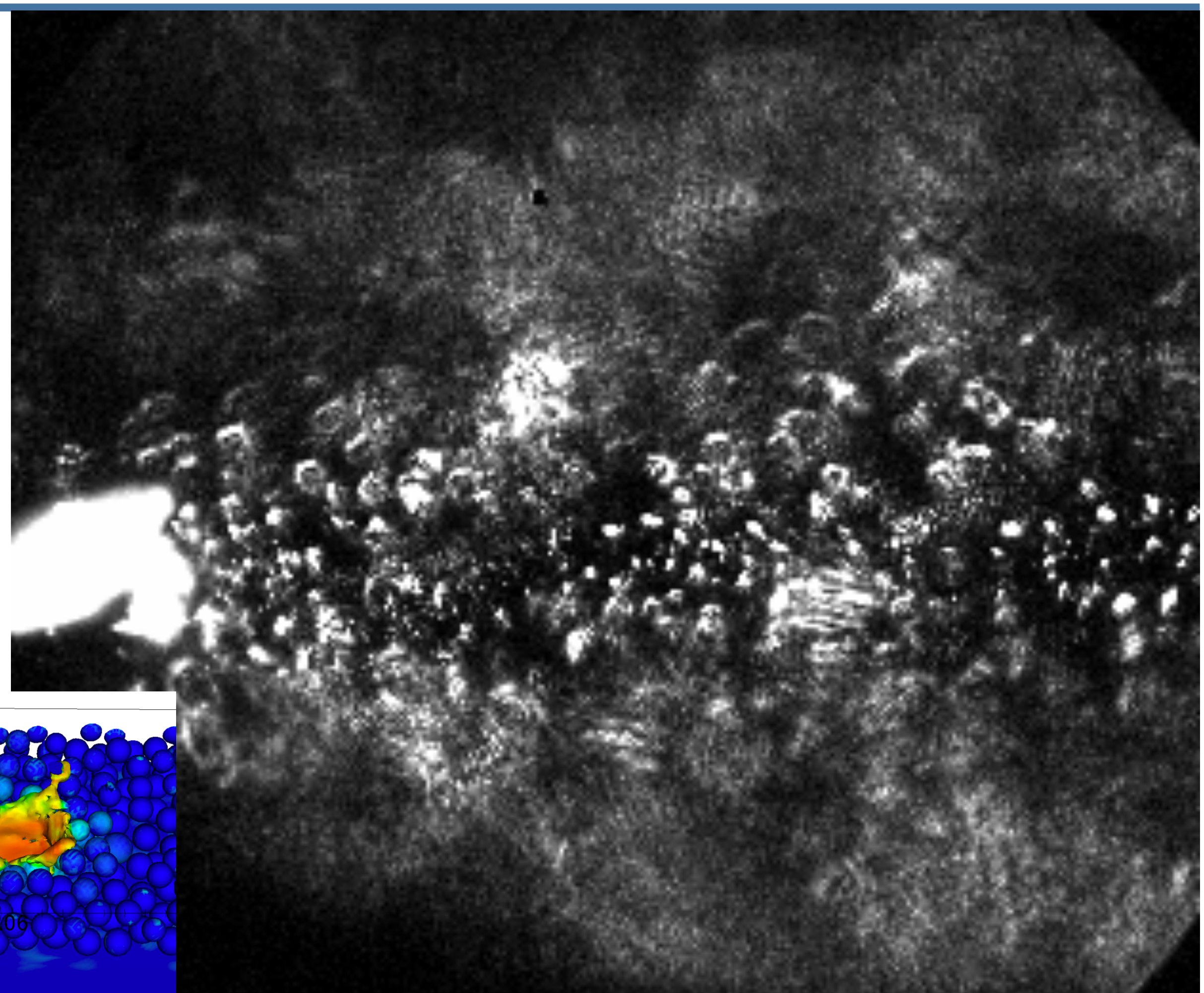
SS316L w/ thermal emission (no band pass filter): 200 W, 1500 mm/s

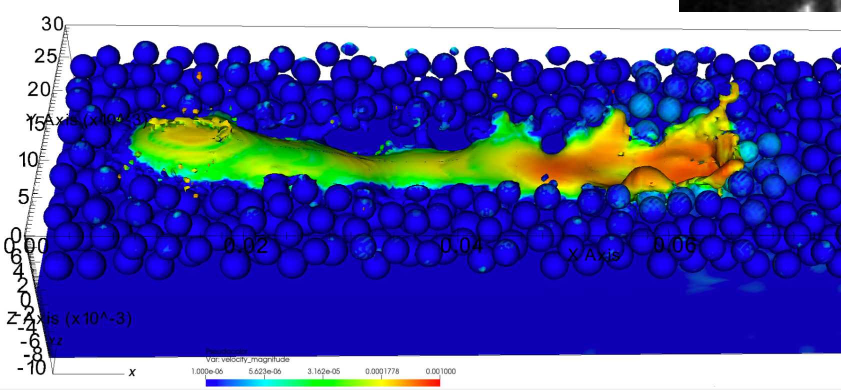
- Unconsumed cold powder is swept *backward and upward (~2–4 m/s)*
- Molten droplets eject in both directions, directly *from melt pool (7–17 m/s)*



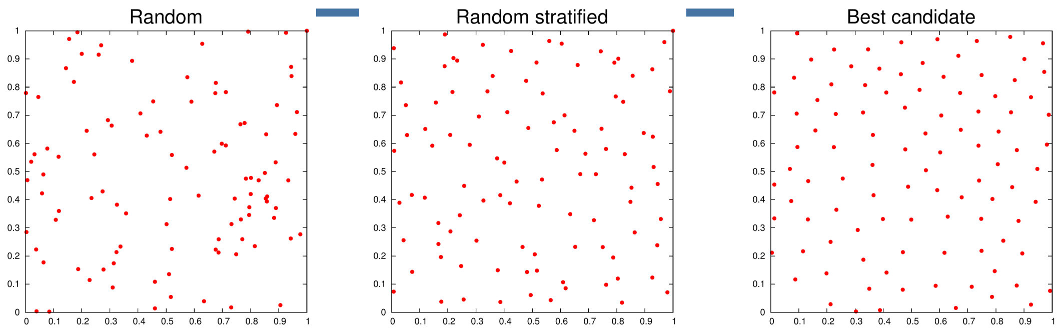
SS316L w/ thermal emission (no band pass filter): 300 W, 2000 mm/s

- At high scan speed and high power, foward 'snowball' ejection is observed *(~2.5 m/s)*
- Faint vapor trail more visible at higher power

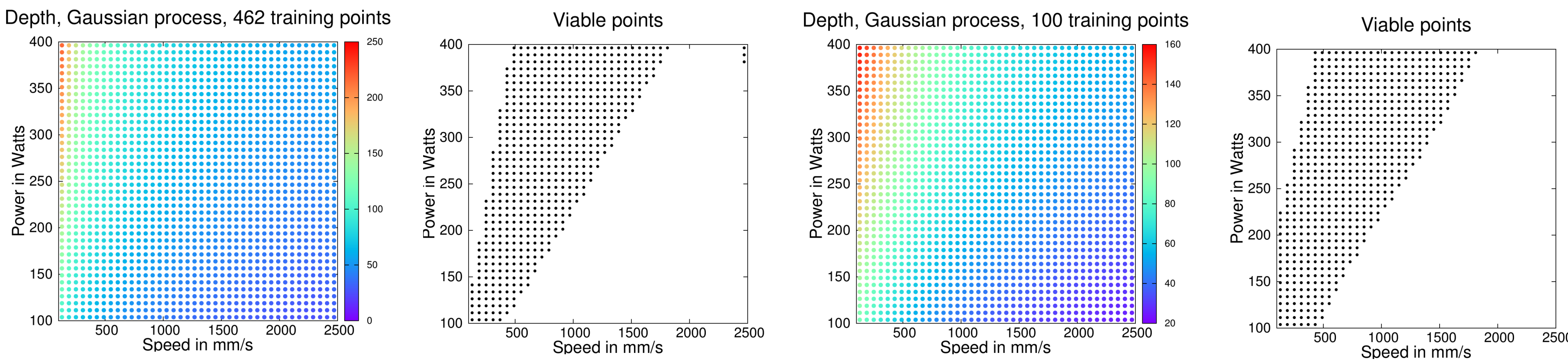




We combine advanced sampling with Gaussian process code surrogate for efficient prediction

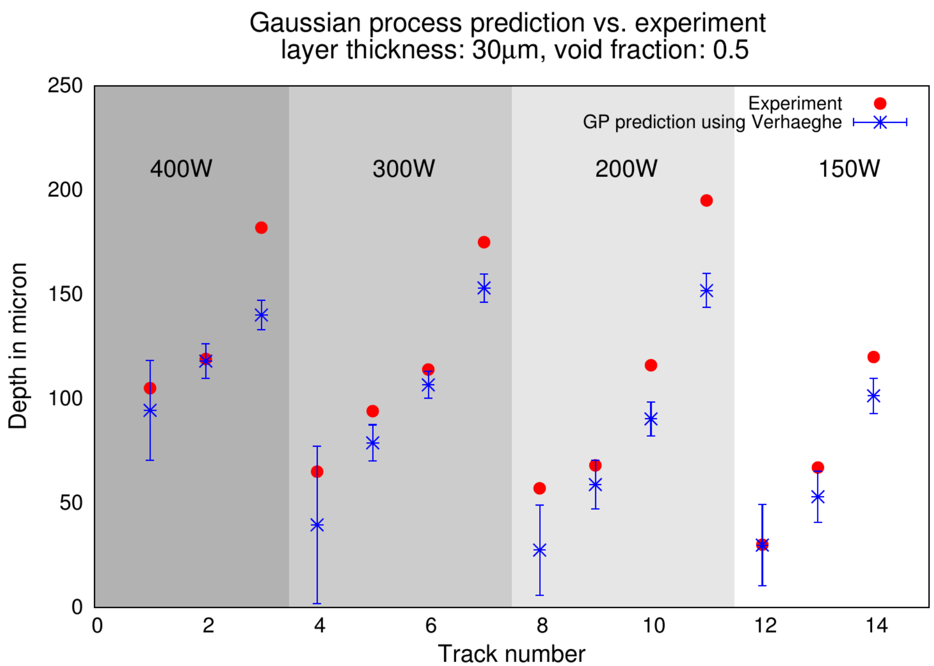


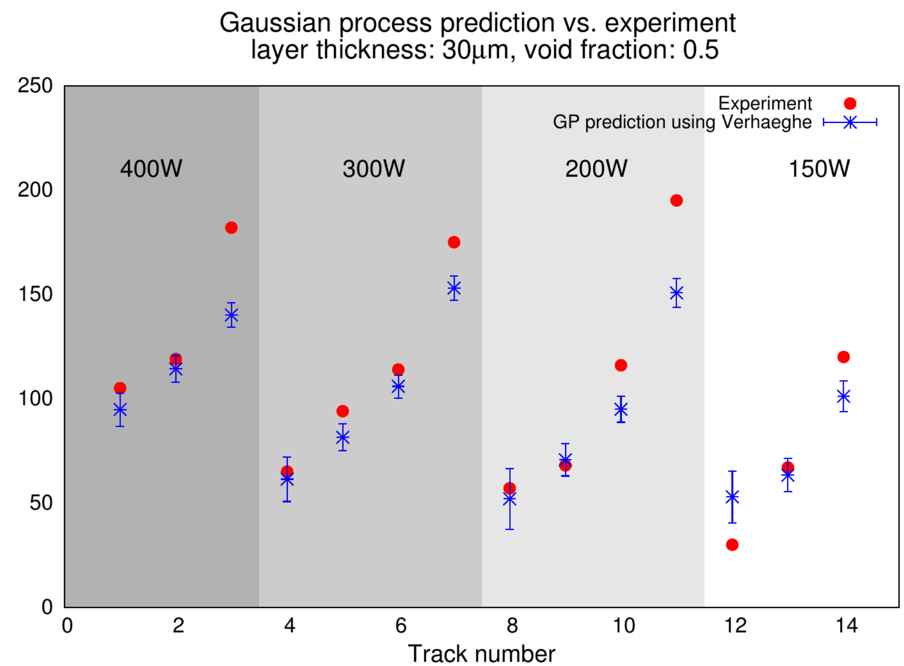
The best-candidate sampling covers the space with few points. It avoids the under- and over-sampling of a random approach and can generate an arbitrary number of samples unlike random stratified sampling..



We build Gaussian process models using the Eagar-Tsai simulation run at 462 stratified random samples (left) and 100 best candidate samples (right). Prediction of depth at 1600 sample points using the model indicates very similar viable regions where depth > 60µm. The GP model runs in seconds and also provides uncertainty estimates.

Using the approach with more complex physical models gives results close to experiments





Approach:

- **Run the more complex Verhaeghe model at select viable points.**
- **Build a Gaussian process model with the results and use to predict depth for single tracks**
- **Left: Prediction using 34 viable points with E-T depth > 60µm. The high error at low depth is due to extrapolation - the maximum speed of samples is 1600 mm/s while the experiments are at 1800mm/s.**
- **Right: Using 41 sample points (depth > 55µm) that include some at higher speeds.**

Issues and Challenges

- Powder model
  - Need better laser absorption model
  - Need to Approximate Some Physics
  - Need thermophysical properties over broad range of temperatures
  - Need for Fine Zoning
  - Explicit Time Marching Limits Time Step
  - Experimental Data Required
  - Including the effects of evaporation
  - Including the effects of the flowing cover gas
- Part-scale model
  - disparate spatial scales of the laser energy source and the overall part geometry
  - disparate time scales of local heating versus overall heat transfer and the actual time of fabrication
  - scant handbook-type property data is available for $T>T_{sol}$

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