Dehao Liu

Personal Information

Job Title: Ph.D. Candidate
Department: George W. Woodruff School of Mechanical Engineering
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Education

Ph.D.   **Georgia Institute of Technology**, Atlanta, GA
Expected December 2020 | Mechanical Engineering
Dissertation Title: *Investigation of process-structure relationship for additive manufacturing with multiphysics simulation and physics-constrained machine learning*
Committee Members: Prof. Yan Wang (Chair), Prof. David L. McDowell (ME), Prof. Shreyes N. Melkote (ME), Prof. Tuo Zhao (ISYE), Prof. Sudarsanam Suresh Babu (ORNL/UT)
Qualification Subjects: Applied Mathematics, Computer-Aided Engineering

B.S.   **Tsinghua University**, Beijing, China
July 2016 | Mechanical Engineering
Senior Design Project: *Molecular dynamics simulation on formation mechanism of grain boundary steps in micro-cutting of polycrystalline copper*

Employment History

Graduate Research Assistant	Georgia Institute of Technology	Aug. 2016–Present
Graduate Intern	Siemens Corporate Technology	May 2019-Aug. 2019
Graduate Intern	Idaho National Laboratory	Jun. 2018-Aug. 2018
Engineering Intern	Sandvik Coromant	Dec. 2015-Jan. 2016

Awards and Honors

- National Encouragement Scholarship (top 5%), 2015
- Outstanding Social Work Scholarship of Tsinghua University (top 10%), 2014
- Academic Excellence Scholarship of Tsinghua University (top 10%), 2013

Research Interests

The overall goal of my research is to establish comprehensive and robust *process-structure-property (P-S-P) relationships* for the systematic *process and materials design* by combining *multiscale multiphysics simulation* and *physics-constrained machine learning*. The main research thrust areas are listed as follows.

- **Multiscale Multiphysics Modeling and Simulation**

  In this research direction, I aim to utilize the *Integrated Computational Materials Engineering (ICME)* approach to establish P-S-P relationships by integrating models at multiple length scales. Specifically, various models, from macro-scale (finite element, finite volume), mesoscale (phase-field method, thermal lattice Boltzmann method, kinetic Monte Carlo), to nano-scale (molecular dynamics, density functional theory), are integrated to make an accurate forward prediction of material properties or behavior. A multiphysics simulation framework called *phase-field and thermal lattice Boltzmann method (PF-TLBM)* has been developed to predict microstructure evolution in metal additive manufacturing, whereas others remain as future work.

- **Physics-Constrained Machine Learning**

  Machine learning (ML) models such as neural networks and deep learning models have been applied successfully in diverse fields. Nevertheless, data sparsity is still the main challenge to apply these models to solve complex scientific and engineering problems. The root cause is the *"curse of dimensionality"* in training these models. Training algorithms need to explore and exploit in a very high dimensional nonlinear parameter space to search the optimal parameters for complex models. This research direction aims to develop novel, robust, and data-efficient physics-constrained machine learning models to alleviate the curse of dimensionality during the construction of P-S-P relationships. A *multi-fidelity physics-constrained neural network (MF-PCNN)* has been developed to be applied in materials modeling. A *physics-constrained neural network with minimax architecture (PCNN-MM)* has been developed to systematically adjust the relative importance of training data and prior knowledge. A new saddle point search method called *Dual-Dimer method* has been developed to search *high-order saddle points* of nonconvex-nonconcave objective functions.

- **Scalable Versatile Bayesian Optimization**

  Once P-S-P relationships are established, the classical Bayesian optimization framework can be used to conduct process and materials design. Since real engineering optimization problems are usually *high-dimensional, constrained, and multi-objective,* some extensions are needed to make the Bayesian optimization framework more versatile. I am also interested in developing a new scalable Bayesian optimization framework using deep neural networks so that the new Bayesian optimization scales linearly with the number of function evaluations. By turning a neural network into a Bayesian framework, the next training data point can be sampling sequentially to reduce the sampling cost. And uncertainties of the prediction of a neural network can be quantified.

Publications and Creative Products

Please see my Google Scholar for a full and updated list of publications.

A. Refereed Book Chapters

1. Sestito J.M.*, **Liu D.**, Lu Y., Song J.-H., Tran A.V., Kempner M.J., Harris T.A.L., Ahn S.-H., and Wang Y. (2020) Multiscale process modeling of shape memory alloy fabrication with directed energy deposition. *Additive Manufacturing for Multifunctional Materials and Structures*, eds. by H. Bruck, Y. Chen, and S.K. Gupta (in press).

2. Tran A.V., **Liu D.**, He L., and Wang Y. (2020) Data-driven acceleration of first-principles saddle point and local minimum search based on scalable Gaussian processes. *Uncertainty Quantification in Multiscale Materials Modeling*, eds. by Y. Wang and D.L. McDowell (Elsevier), Ch.5, pp.119-168.

B. Published and Accepted Journal Articles

1. **Liu D.** and Wang Y. (2020) Multiphysics simulation of nucleation and grain growth in selective laser melting of alloys. *Journal of Computing and Information Science in Engineering*, (in press).

2. **Liu D.** and Wang Y. (2019) Multi-fidelity physics-constrained neural network and its application in materials modeling. *Journal of Mechanical Design*, **141**(12): 121403.

3. Cao L., **Liu D.**, Jiang P., Shao X., Zhou Q., and Wang Y. (2019) Multi-physics simulation of dendritic growth in magnetic field assisted solidification. *International Journal of Heat and Mass Transfer*, **144**: 118673.

4. Tran A.V., **Liu D.**, Tran H., and Wang Y. (2019) Quantifying uncertainty in the process-structure relationship for Al-Cu solidification. *Modelling and Simulation in Materials Science and Engineering*, **27**(6): 064005.

5. **Liu D.** and Wang Y. (2019) Mesoscale multi-physics simulation of rapid solidification of Ti-6Al-4V alloy. *Additive Manufacturing*, **25**: 551-562.

6. Nie Z., Wang G., **Liu D.**, and Rong Y. K. (2018). A statistical model of equivalent grinding heat source based on random distributed grains. *Journal of Manufacturing Science and Engineering*, **140**(5), 051016.

7. **Liu D.**, Wang G., Yu J., and Rong Y. K. (2017). Molecular dynamics simulation on formation mechanism of grain boundary steps in micro-cutting of polycrystalline copper. *Computational Materials Science*, **126**: 418-425.

8. Nie Z., Wang G., Yu J., **Liu D.**, and Rong Y. K. (2016). Phase-based constitutive modeling and experimental study for dynamic mechanical behavior of martensitic stainless steel under high strain rate in a thermal cycle. *Mechanics of Materials*, **101**: 160-169.

9. **Liu D.**, Wang G., Nie Z., and Rong, Y. K. (2016). An in-situ infrared temperature-measurement method with back focusing on surface for creep-feed grinding. *Measurement*, **94**: 645-652.

C. Conference Presentation with Proceedings (Refereed)

1. **Liu D.** and Wang Y. "Simulation of nucleation and grain growth in selective laser melting of Ti-6Al-4V alloy." *Proceedings of 2019 ASME International Design Engineering Technical Conferences & Computers and Information in Engineering Conference (IDETC/CIE2019), August 18-21, 2019, Anaheim, California*, Paper No. DETC2019-97684.

2. **Liu D.** and Wang Y. "Multi-fidelity physics-constrained neural network and its application in materials modeling." *Proceedings of 2019 ASME International Design Engineering Technical*

Conferences & Computers and Information in Engineering Conference (IDETC/CIE2019), August 18-21, 2019, Anaheim, California, Paper No. DETC2019-98115.

3. **Liu D.** and Wang Y. "Mesoscale multi-physics simulation of solidification in selective laser melting process using a phase field and thermal lattice Boltzmann model." *Proceedings of 2017 ASME International Design Engineering Technical Conferences & Computers and Information in Engineering Conference (IDETC/CIE2017), Aug. 6-9, 2017, Cleveland, Ohio*, Paper No. DETC2017-67633.

4. **Liu D.**, Wang, G., Nie, Z., and Rong, Y. K. "Numerical Simulation of the Austenitizing Process in Hypoeutectoid Fe-C Steels." *Proceedings of the ASME 2014 International Manufacturing Science and Engineering Conference (MSEC2014), June 9-13, 2014, Detroit, Michigan*, Paper No. MSEC2014-3948.

D. Journal Articles in Preparation

1. **Liu D.** and Wang Y. A Dual-Dimer Method for Training Physics-Constrained Neural Networks with Minimax Architecture. *Neural Networks* (2020).

2. **Liu D.** and Wang Y. Rapid solidification process optimization for additive manufacturing based on simulation and physics-constrained machine learning. *JOM* (2020).

3. Tran A., Sun J., **Liu D.**, Wildey T., and Wang Y. Stochastic reduced-order model with temporal upscaling for uncertainty propagation in materials modeling. *Computational Materials Science* (2020).

E. Software

1. **Liu D.** and Wang Y., Phase-Filed and Thermal Lattice Boltzmann Method.

2. **Liu D.** and Wang Y., Dual-Dimer method.

F. Patents

1. Mirabella L., Arvanitis E., **Liu D.**, Lammens N., Erdelyi H., and Ludwig C., "System and Method for Fatigue Response Prediction," Filing Number: PCT/US2020/019691. February 25, 2020.

2. Wang G., Nie Z., **Liu D.**, and Rong Y. K., "A Temperature Measurement Device for Grinding Experiments," C.N. Patent No. CN104596646B. December 19, 2017.

3. Wang G., Nie Z., Rong Y. K., **Liu D.**, and Wei S., "System and Method for temperature monitoring and analysis based on LabVIEW and thermocouples," C.N. Patent No. CN103674328B. June 29, 2016.

G. Conference Presentations

G1. Conference Presentations

1. **Liu D.** and Wang Y. **(Invited)** "Mesoscale simulation of nucleation and grain growth of Ti-6Al-4V alloy in selective laser melting," The 2nd International Conference on Simulation for Additive Manufacturing, Sept. 11-13, 2019, Pavia, Italy.

2. Wang Y. and **Liu D. (Plenary Lecture)** "Multi-Fidelity Physics-Constrained Neural Networks for Materials Design," 2018 Design Science Research Workshop on Data Driven Design and Learning, August 23-25, 2018 Montreal, Canada
3. **Liu D.** and Wang Y. "Mesoscale multi-physics simulation of solidification in selective laser melting process," The 4th TMS World Congress on Integrated Computational Materials Engineering (ICME 2017), May 21-25, 2017, Ypsilanti, Michigan.

G2. Invited Seminar Presentations
1. **Liu D.** "Simulation of nucleation and grain growth in selective laser melting of Ti-6Al-4V alloy," Dec. 19, 2019, Southern University of Science and Technology, Shenzhen, China.
2. **Liu D.** "Mesoscale Multi-Physics Simulation of Rapid Solidification of Ti-6Al-4V Alloy," Jan. 28, 2019, Lawrence Livermore National Laboratory, Livermore, California.

Research Experience

Graduate Research Assistant, Georgia Institute of Technology, Atlanta, GA   Aug. 2016-Present
Multi-Scale System Engineering Research Group, Advisor: Prof. Yan Wang
- Investigated Process-Structure relationship for additive manufacturing with multiphysics simulation and physics-constrained machine learning
- Created a multi-fidelity physics-constrained neural network (MF-PCNN) and a physics-constrained neural network with minimax architecture (PCNN-MM) for materials modeling
- Developed a Dual-Dimer method to search high-order saddle points of nonconvex-nonconcave objective functions
- Established a mesoscale multiphysics simulation framework called phase-field and thermal lattice Boltzmann method (PF-TLBM) to predict microstructure evolution
- Applied image processing and feature extraction for cost analytics in cyber manufacturing

Visiting Undergraduate Student, Georgia Institute of Technology, Atlanta, GA   Jul. 2015-Aug. 2015
Multi-Scale System Engineering Research Group, Advisor: Prof. Yan Wang
- Conducted mesoscale simulation of laser cladding using Kinetic Monte Carlo method and Activation Relaxation Technique

Undergraduate Research Assistant, Tsinghua University, Beijing, China   Oct. 2013-Jan. 2014
Institute of Mechatronic Engineering, Advisor: Prof. Chenglong Fu
- Designed an active electrical transfemoral prosthesis

Undergraduate Research Assistant, Tsinghua University, Beijing, China   Sep. 2012-Jul. 2016
Computer-Aided Manufacturing Laboratory, Advisor: Prof. Yiming (Kevin) Rong, Prof. Gang Wang
- Investigated formation mechanism of grain boundary steps in micro-cutting of polycrystalline copper with Molecular Dynamics simulation
- Designed an in-situ infrared measurement device to monitor the temperature of the workpiece in creep-feed grinding
- Simulated solute diffusion during the austenitizing process of steels using finite difference method

Industry Experience

Graduate Intern, Siemens Corporate Technology, Princeton, NJ   May 2019-Aug. 2019
Product Simulation and Modeling Group, Mentor: Dr. Elena Arvanitis, Dr. Lucia Mirabella
- Created a generative machine learning model to generate rough surface profiles for fatigue prediction using conditional Wasserstein Generative Adversarial Networks with Gradient Penalty (WGAN-GP)

Graduate Intern, Idaho National Laboratory, Idaho Falls, ID   Jun. 2018-Aug. 2018
Fuels Modeling and Simulation Department, Mentor: Dr. Larry Aagesen
- Formulated and implemented anisotropic interface energy for a multi-phase multi-order parameter grand potential phase-field model in an open-source finite element framework called Multiphysics Object Oriented Simulation Environment (MOOSE)

Engineering Intern, Sandvik Coromant, Beijing, China   Dec. 2015-Jan. 2016
- Designed a new micro-scale adjustable boring cutter using Solidworks and ANSYS

Teaching Experience

Guest Lecturer, Computer-Aided Design (ME 6104)   Spring 2020
Graduate Class, Number of Students: 67
- **Conducted teaching practicum to deliver two lectures**
- Designed and prepared a lecture to introduce python programming and common numeric libraries
- Delivered a lecture to teach implicit surface modeling

Graduate Teaching Assistant, Computer-Aided Design (ME 6104)   Spring 2018-2020
Graduate Class, Number of Students: 56 (Spring 2018), 54 (Spring 2019), 67 (Spring 2020)
- Held office hours to help students understand the course-related material and answered questions
- Led discussions, answered questions, and clarified materials on the online course forum
- Prepared and compiled resources for learning python programming language
- Instructed students to debug and identify problems in their codes
- Graded homework and provided feedbacks

Mentorship for Undergraduate Students

1. Alizay Shah (Summer 2017)
   Research Project: *Process monitoring and data analytics for cyber manufacturing*
2. Yufeng Wang (Spring 2017)
   Research Project: *Big data analytics for cyber manufacturing*
3. Pranav Pusarla (Spring 2020)
   Research Project: *A physics-constrained long short-term memory (LSTM) neural network for materials modeling*

Service

A. Symposium/Event Organized

Committee Member   2020 ASME Computers and Information in Engineering (CIE) Student Hackathon: Identifying, Extracting, Analyzing of Value from Large Unstructured Data Sets in Mechanical Engineering
https://asmehackathon2020.github.io/

B. Journal/Conference Proceedings Review

Guest Reviewer   Additive Manufacturing (Impact Factor: 7.173)

Guest Reviewer   Computational Materials Science (Impact Factor: 2.644)

Guest Reviewer   Materials Research Express (Impact Factor: 1.449)

Guest Reviewer   Modelling and Simulation in Materials Science and Engineering (Impact Factor: 1.826)

Guest Reviewer   ASME International Design Engineering Technical Conference & Computers and Information in Engineering Conference (IDETC/CIE), 2017-2020

C. Academic Program Development

Guest Lecturer   International Summer Exchange Program, Georgia Tech Manufacturing Institute, Summer 2017

D. Professional Associations

Student Member   The American Society of Mechanical Engineers (ASME), 2015-2020

Student Member   The Minerals, Metals & Materials Society (TMS), 2017