

# DEHAO LIU

Ph.D. Candidate

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## EDUCATION

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**Georgia Institute of Technology**

Atlanta, GA

**Ph.D., Mechanical Engineering**

Expected May 2021

Dissertation: *Investigation of process-structure relationship for additive manufacturing with multiphysics simulation and physics-constrained machine learning*

Committee: 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

**Tsinghua University**

Beijing, China

**B.S., Mechanical Engineering**

July 2016

Senior Design Project: *Molecular dynamics simulation on formation mechanism of grain boundary steps in micro-cutting of polycrystalline copper*

## RESEARCH EXPERIENCE

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**Graduate Research Assistant, Georgia Institute of Technology**

Atlanta, GA

Multi-Scale System Engineering Research Group

Aug. 2016-Present

Advisor: Prof. Yan Wang

- 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 in additive manufacturing
- Applied image processing and machine learning for cost analytics in cyber manufacturing

**Visiting Undergraduate Student, Georgia Institute of Technology**

Atlanta, GA

Multi-Scale System Engineering Research Group

Jul. 2015-Aug. 2015

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

Institute of Mechatronic Engineering

Oct. 2013-Jan. 2014

Advisor: Prof. Chenglong Fu

- Designed an active electrical transfemoral prosthesis

**Undergraduate Research Assistant, Tsinghua University**

Computer-Aided Manufacturing Laboratory

Advisor: Prof. Yiming (Kevin) Rong, Prof. Gang Wang

Beijing, China

Sep. 2012-Jul. 2016

- 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**

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**Graduate Intern, Siemens Corporate Technology**

Product Simulation and Modeling Group

Mentor: Dr. Elena Arvanitis, Dr. Lucia Mirabella

Princeton, NJ

May 2019-Aug. 2019

- 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 (INL)**

Fuels Modeling and Simulation Department

Mentor: Dr. Larry Aagesen

Idaho Falls, ID

Jun. 2018-Aug. 2018

- 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

**RESEARCH INTERESTS**

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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 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.

## AWARDS AND HONORS

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- 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

## PUBLICATIONS AND CREATIVE PRODUCTS

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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. Refereed Journal Articles**

1. **Liu D.** and Wang Y. (2021) A Dual-Dimer method for training physics-constrained neural networks with minimax architecture. *Neural Networks*, **136**: 112-125.
2. **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*, **20**(5).
3. **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.
4. 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.
5. 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.
6. **Liu D.** and Wang Y. (2019) Mesoscale multi-physics simulation of rapid solidification of Ti-6Al-4V alloy. *Additive Manufacturing*, **25**: 551-562.
7. 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.
8. **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.
9. 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.
10. **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. Refereed Conference Proceedings**

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. Submitted Manuscripts**

1. **Liu D.** and Wang Y. Physics-constrained neural networks to predict dendritic growth in metal additive manufacturing. *JOM* (2020).
2. 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. Presentations**

##### **G1. Conference Presentations**

1. **Liu D.** and Wang Y. “Optimizing metallic materials for additive manufacturing based on physics-constrained machine learning and Bayesian optimization,” 2020 ASME International Design Engineering Technical Conferences & Computers and Information in Engineering Conference (IDETC/CIE2020), August 16-19, 2020, St. Louis, Missouri
2. **Liu D.** and Wang Y. (**Invited**) “Mesoscale simulation of nucleation and grain growth of Ti-6Al-4V alloy in selective laser melting,” The 2<sup>nd</sup> International Conference on Simulation for Additive Manufacturing, Sept. 11-13, 2019, Pavia, Italy.
3. 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
4. **Liu D.** and Wang Y. “Mesoscale multi-physics simulation of solidification in selective laser melting process,” The 4<sup>th</sup> 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.

## **TEACHING EXPERIENCE**

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### **Guest Lecturer, Georgia Institute of Technology**

Spring 2020

Graduate Course: Computer-Aided Design, 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, Georgia Institute of Technology**

Spring 2018-2020

Graduate Course: Computer-Aided Design, 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 feedback

## **PROPOSAL WRITING EXPERIENCE**

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- Wrote a white paper for ONR FOA Announcement #N00014-20-S-F002 with Prof. Yan Wang on “*Investigation of Process-Structure-Property Relationship for Additive Manufacturing with Multiphysics Simulation and Physics-Constrained Machine Learning.*” (March 2020)
- Contributed to a proposal for DARPA-SN-18-65 disruption opportunity called “The Physics of Artificial Intelligence (PAI)” with Prof. Yan Wang on “*Physics Constrained Machine Learning.*” (July 2018)
- Contributed to a proposal for SAMSUNG GRO program called “Material Informatics-Data-Driven Materials Property/Structure Prediction” with Prof. Yan Wang on “*Physics-Based Data-Driven Process-Structure-Property Relationship Exploration.*” (June 2017)

## **MENTORSHIP FOR UNDERGRADUATE STUDENTS**

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1. Pranav Pusarla (Spring 2020-Present)  
Research Project: *Multi-fidelity physics-constrained neural networks with minimax architecture for materials modeling*
2. Alizay Shah (Summer 2017)  
Research Project: *Process monitoring and data analytics for cyber manufacturing*
3. Yufeng Wang (Spring 2017)

## SERVICE

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### 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  
Guest Reviewer Computational Materials Science  
Guest Reviewer Materials Research Express  
Guest Reviewer Modelling and Simulation in Materials Science and Engineering  
Guest Reviewer Journal of Thermal Science  
Guest Reviewer Journal of Computing and Information Science in Engineering  
Guest Reviewer ASME International Design Engineering Technical Conference &  
Computers and Information in Engineering Conference  
(IDETC/CIE), 2017-2020

### C. Proposals Review

Reviewer Georgia Tech President's Undergraduate Research Awards, June 19,  
2020

### D. Academic Program Development

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

### E. Professional Memberships

Student Member The American Society of Mechanical Engineers (ASME), 2015-  
2020  
Student Member The Minerals, Metals & Materials Society (TMS), 2017

## REFERENCES

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- Prof. Yan Wang  
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- Dr. Larry Aagesen

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Fuels Modeling and Simulation Department  
Idaho National Laboratory, Idaho Falls, ID  
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(847)560-0376  
<https://bios.inl.gov/Lists/Researcher/DisplayOverrideForm.aspx?ID=459>

- Dr. Elena Arvanitis (Preferred contact via phone)  
Senior Project Manager  
Product Modeling and Simulation Group  
Siemens Corporate Technology, Princeton, NJ  
[elena.arvanitis@siemens.com](mailto:elena.arvanitis@siemens.com)  
(609)865-9578  
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