DEHAO LIU

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EDUCATION

Georgia Institute of Technology Atlanta, GA
Ph.D., Mechanical Engineering Aug. 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

Georgia Institute of Technology Atlanta, GA
M.S., Mechanical Engineering Dec. 2020

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

Postdoctoral Researcher, Texas A&M University College Station, TX
Computational Materials Science Lab, Scientific Machine Learning Lab Sep. 2021-Present
Advisor: Prof. Raymundo Arroyave, Prof. Ulisses Braga-Neto

Graduate Research Assistant, Georgia Institute of Technology Atlanta, GA
Multi-Scale System Engineering Research Group Aug. 2016-Aug. 2021
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 Beijing, China
Computer-Aided Manufacturing Laboratory Sep. 2012-Jul. 2016
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
Product Simulation and Modeling Group May 2019-Aug. 2019
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 (INL) Idaho Falls, ID
Fuels Modeling and Simulation Department Jun. 2018-Aug. 2018
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

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 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

- 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

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. *Manufacturing in the Era of 4th Industrial Revolution: A World Scientific Reference Volume 1: Recent Advances in Additive Manufacturing,* eds. by H. Bruck, Y. Chen, and S.K. Gupta (World Scientific), pp. 41-76.
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. 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* (2021).
2. Biswas S., **Liu D.**, Aagesen, L. K., and Jiang W. Solidification and grain formation in alloys: A grand-potential-based phase-field study. *Computational Materials Science* (2021).

E. Under Preparation Journal Papers

1. **Liu D.**, Pusarla P., and Wang Y. Multi-fidelity physics-constrained neural networks with minimax architecture.
2. **Liu D.** and Wang Y. Physics-constrained neural networks with minimax architecture for multiphysics problems.
3. **Liu D.** and Wang Y. Rapid solidification process optimization for metal additive manufacturing based on multi-objective Bayesian optimization.
4. **Liu D.** and Wang Y. Predicting state of health for batteries based on physics-constrained neural networks.

F. Software

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

G. 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.

H. 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.

TEACHING EXPERIENCE

Guest Lecturer, Georgia Institute of Technology Spring 2020

Graduate Course: Computer-Aided Design, Number of Students: 67

- Conducted teaching practicum to deliver two 75-minute 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 2018-2021

Graduate Course: Computer-Aided Design, Number of Students: 56 (Spring 2018), 54 (Spring 2019), 67 (Spring 2020), 76 (Spring 2021)

- 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

- 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

1. Rohan Sundeep Punamiya (Summer 2021)
   Research Project: *Physics-constrained neural networks for battery life prediction*
2. Yash Patel (Fall 2020-Spring 2021)
   Research Project: *Physics-constrained neural networks for battery life prediction*
3. Pranav Pusarla (Spring 2020-Spring 2021)
   Research Project: *Multi-fidelity physics-constrained neural networks with minimax architecture for materials modeling*
4. Alizay Shah (Summer 2017)
   Research Project: *Process monitoring and data analytics for cyber manufacturing*
5. Yufeng Wang (Spring 2017)
   Research Project: *Big data analytics for cyber manufacturing*

SERVICE

A. Symposium/Event Organized

Committee Member	ASME Computers and Information in Engineering (CIE) Student Hackathon, 2020-2021 https://asmehackathon.github.io/

B. Journal/Conference Proceedings Review

Guest Reviewer	Additive Manufacturing
Guest Reviewer	Computational Materials Science
Guest Reviewer	Expert Systems with Applications
Guest Reviewer	Journal of Computing and Information Science in Engineering
Guest Reviewer	Journal of Thermal Science
Guest Reviewer	Materials Research Express
Guest Reviewer	Modelling and Simulation in Materials Science and Engineering
Guest Reviewer	ASME International Design Engineering Technical Conference & Computers and Information in Engineering Conference (IDETC/CIE), 2017-2021

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), 2015-2021
Student Member	The Minerals, Metals & Materials Society (TMS), 2017