Lu Lu

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Department of Chemical and Biomolecular Engineering, University of Pennsylvania

Education

Brown University 8/2014–5/2020

- **Ph.D.** in Applied Mathematics
- **M.Sc.** in Computer Science
- **M.Sc.** in Applied Mathematics
- **M.Sc.** in Engineering
- Advisor: George Em Karniadakis

Tsinghua University, Beijing, China 8/2009–7/2013

- **B.Eng.** in Energy, Power System and Automation
- **B.Ec.** in Economics
- **Minor** in Computer Technology and Application

Research Experience

Assistant Professor, Department of Chemical and Biomolecular Engineering, University of Pennsylvania 8/2021–present

Applied Mathematics Instructor, Department of Mathematics, Massachusetts Institute of Technology 9/2020–5/2021

- **Deep learning**
  - **Theory**: Proved that deep neural networks will converge to erroneous mean states of the target function with high probability. Quantified the generalization error of neural networks for classification problems in terms of data distribution and neural network smoothness.
  - **Algorithms & applications**: Developed physics-informed neural networks (PINNs) to solve forward and inverse partial differential equations (PDEs), fractional PDEs, and stochastic PDEs, and topology optimization, with applications to nano-optics, metamaterials, and systems biology. Developed multifidelity networks to predict mechanical properties of solid materials. Developed deep operator networks (DeepONets) to learn nonlinear operators based on the universal approximation theorem of operators, and DeepM&Mnet to solve the multiphysics and multiscale problems of electroconvection, hypersonics, and bubble growth dynamics.
  - **Software**: Developed DeepXDE[1], a deep learning library for solving differential equations. (>100,000 downloads on PyPI and Anaconda, >500 GitHub Stars)
- **Computational biophysics**
  - **Molecular biomechanics**: Developed a multiscale coarse-grained particle model of sickle hemoglobin (HbS) to probe the polymerization process, mechanical and structural properties of HbS fibers in sickle cell disease (SCD). Developed coarse-grained models to simulate the self-assembly of amyloids.
  - **Cellular biomechanics**: Simulated the dynamics of red blood cells (RBCs) traversing the interendothelial slit in the human spleen, which reveals that the spleen senses and clears RBCs with abnormal shapes and deformability.
  - **Kinetics**: Developed a kinetic model of erythrocyte sickling to examine the effectiveness of potential anti-sickling drug candidates.
  - **Software**: Developed OpenRBC[2], a fast simulator of red blood cells at protein resolution. (Third Prize, IBM OpenPOWER Developer Challenge contest, 2016)

Publications

- Google Scholar

[1] https://github.com/lululxvi/deepxde
[2] https://devpost.com/software/openrbc, https://github.com/yhtang/OpenRBC

- All the papers, presentations, and talks are available at https://lululxvi.github.io
- *Contributed equally

Preprints

1. P. Clark Di Leoni, **L. Lu**, C. Meneveau, G. E. Karniadakis, & T. A. Zaki. DeepONet prediction of linear instability waves in high-speed boundary layers. *arXiv preprint arXiv:2105.08697*, 2021.
2. B. Deng, Y. Shin, **L. Lu**, Z. Zhang, & G. E. Karniadakis. Convergence rate of DeepONets for learning operators arising from advection-diffusion equations. *arXiv preprint arXiv:2102.10621*, 2021.
3. **L. Lu**, R. Pestourie, W. Yao, Z. Wang, F. Verdugo, & S. G. Johnson. Physics-informed neural networks with hard constraints for inverse design. *arXiv preprint arXiv:2102.04626*, 2021.
4. Z. Mao, **L. Lu**, O. Marxen, T. A. Zaki, & G. E. Karniadakis. DeepM&Mnet for hypersonics: Predicting the coupled flow and finite-rate chemistry behind a normal shock using neural-network approximation of operators. *arXiv preprint arXiv:2011.03349*, 2020.

Journal Papers

1. Y. Deng*, **L. Lu***, L. Aponte, A. M. Angelidi, V. Novak, G. E. Karniadakis, & C. S. Mantzoros. Deep transfer learning and data augmentation improve glucose levels prediction in type 2 diabetes patients. *npj Digital Medicine*, 4, 109, 2021.
2. G. E. Karniadakis*, I. G. Kevrekidis*, **L. Lu***, P. Perdikaris*, S. Wang*, & L. Yang*. Physics-informed machine learning. *Nature Reviews Physics*, 3(6), 422–440, 2021.
3. S. Cai, Z. Wang, **L. Lu**, T. A. Zaki, & G. E. Karniadakis. DeepM&Mnet: Inferring the electroconvection multiphysics fields based on operator approximation by neural networks. *Journal of Computational Physics*, 436, 110296, 2021.
4. **L. Lu**, P. Jin, G. Pang, Z. Zhang, & G. E. Karniadakis. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. *Nature Machine Intelligence*, 3, 218–229, 2021. (**Highlighted on *Nature Machine Intelligence*, 3, 192–193, 2021**)
5. C. Lin, Z. Li, **L. Lu**, S. Cai, M. Maxey, & G. E. Karniadakis. Operator learning for predicting multiscale bubble growth dynamics. *The Journal of Chemical Physics*, 154(10), 104118, 2021.
6. **L. Lu**, X. Meng, Z. Mao, & G. E. Karniadakis. DeepXDE: A deep learning library for solving differential equations. *SIAM Review*, 63(1), 208–228, 2021.
7. A. Yazdani*, **L. Lu***, M. Raissi, & G. E. Karniadakis. Systems biology informed deep learning for inferring parameters and hidden dynamics. *PLoS Computational Biology*, 16(11), e1007575, 2020. (**Highlighted on *Nature Computational Science*, 1, 16, 2021**)
8. **L. Lu***, Y. Shin*, Y. Su, & G. E. Karniadakis. Dying ReLU and initialization: Theory and numerical examples. *Communications in Computational Physics*, 28(5), 1671–1706, 2020.
9. P. Jin*, **L. Lu***, Y. Tang, & G. E. Karniadakis. Quantifying the generalization error in deep learning in terms of data distribution and neural network smoothness. *Neural Networks*, 130, 85–99, 2020.
10. Y. Chen, **L. Lu**, G. E. Karniadakis, & L. D. Negro. Physics-informed neural networks for inverse problems in nano-optics and metamaterials. *Optics Express*, 28(8), 11618–11633, 2020.
11. **L. Lu***, M. Dao*, P. Kumar, U. Ramamurty, G. E. Karniadakis, & S. Suresh. Extraction of mechanical properties of materials through deep learning from instrumented indentation. *Proceedings of the National Academy of Sciences*, 117(13), 7052–7062, 2020.
12. G. Pang*, **L. Lu***, & G. E. Karniadakis. fPINNs: Fractional physics-informed neural networks. *SIAM Journal on Scientific Computing*, 41(4), A2603–A2626, 2019.
13. **L. Lu***, Z. Li*, H. Li*, X. Li, P. G. Vekilov, & G. E. Karniadakis. Quantitative prediction of erythrocyte sickling for the development of advanced sickle cell therapies. *Science Advances*, 5(8), eaax3905, 2019. (**Highlighted on *Science Advances* homepage**)
14. D. Zhang, **L. Lu**, L. Guo, & G. E. Karniadakis. Quantifying total uncertainty in physics-informed neural networks for solving forward and inverse stochastic problems. *Journal of Computational Physics*, 397, 108850, 2019.
15. H. Li*, **L. Lu***, X. Li, P. A. Buffet, M. Dao, G. E. Karniadakis, & S. Suresh. Mechanics of diseased red blood cells in human spleen and consequences for hereditary blood disorders. *Proceedings of the National Academy of Sciences*, 115(38), 9574–9579, 2018.
16. H. Li, D. Papageorgiou, H. Y. Chang, **L. Lu**, J. Yang, & Y. Deng. Synergistic integration of laboratory and numerical approaches in studies of the biomechanics of diseased red blood cells. *Biosensors*, 8(3), 76, 2018.
17. **L. Lu***, Y. Deng*, X. Li, H. Li, & G. E. Karniadakis. Understanding the twisted structure of amyloid fibrils via molecular simulations. *The Journal of Physical Chemistry B*, 122(49), 11302–11310, 2018.

18. H. Li, J. Yang, T. T. Chu, R. Naidu, **L. Lu**, R. Chandramohanadas, M. Dao & G. E. Karniadakis. Cytoskeleton remodeling induces membrane stiffness and stability changes of maturing reticulocytes. *Biophysical Journal*, 114(8), 2014–2023, 2018. (**Highlighted on *Biophysical Journal* homepage**)
19. H. Li, H. Y. Chang, J. Yang, **L. Lu**, Y. H. Tang, & G. Lykotrafitis. Modeling biomembranes and red blood cells by coarse-grained particle methods. *Applied Mathematics and Mechanics*, 39(1), 3–20, 2018.
20. **L. Lu**, H. Li, X. Bian, X. Li, & G. E. Karniadakis. Mesoscopic adaptive resolution scheme toward understanding of interactions between sickle cell fibers. *Biophysical Journal*, 113(1), 48–59, 2017. (**Cover Article**)
21. Y. H. Tang*, **L. Lu***, H. Li, C. Evangelinos, L. Grinberg, V. Sachdeva, & G. E. Karniadakis. OpenRBC: A fast simulator of red blood cells at protein resolution. *Biophysical Journal*, 112(10), 2030–2037, 2017. (**Highlighted on *Biophysical Journal* homepage**)
22. **L. Lu**, X. Li, P. G. Vekilov, & G. E. Karniadakis. Probing the twisted structure of sickle hemoglobin fibers via particle simulations. *Biophysical Journal*, 110(9), 2085–2093, 2016. (**Highlighted on *Biophysical Journal* homepage**)
23. **L. Lu**, X. Zhang, Y. Yan, J. M. Li, & X. Zhao. Theoretical analysis of natural-gas leakage in urban medium-pressure pipelines. *Journal of Environment and Human*, 1(2), 71–86, 2014.

Conference Papers

1. **L. Lu**, H. He, P. Kasimbeg, R. Ranade, & J. Pathak. One-shot learning for solution operators of partial differential equations. *ICLR Workshop on Deep Learning for Simulation*, 2021.

Patents

1. S. Suresh, **L. Lu**, G. E. Karniadakis, & M. Dao. Machine learning techniques for estimating mechanical properties of materials. *US Application* No. 62/865,670, *PCT Application* No. PCT/US2020/021401, *Taiwan Application* No. 109121601, filed on June 24, 2019.
2. X. Dong, J. M. Li, Y. Yan, H. Zhang, **L. Lu**, J. Wang, & H. Xiao. A test device and method for simulating natural gas leakage in soil. *China Invention Patent* CN103712755A, filed on June 14, 2013, and issued on April 9, 2014.

Awards and Honors

- SIAM Early Career Travel Award, SIAM Conference on Applications of Dynamical Systems, 2021.
- SIAM Early Career Travel Award, SIAM Conference on Computational Science and Engineering, 2021.
- Chinese Government Award for Outstanding Self-financed Students Abroad, 2020. (500 Ph.D. students each year all over the world)
- Joukowsky Family Foundation Outstanding Dissertation Award, Brown University, 2020. (the most prestigious Ph.D. award at Brown; 4 students per year)
- David Gottlieb Memorial Award, Division of Applied Mathematics, Brown University, 2020. (1 student in the division)
- Full Member, Sigma Xi, 2020.
- SIAM Student Travel Award, SIAM Conference on Mathematics of Data Science, 2020.
- Luis W. Alvarez Fellowship, Lawrence Berkeley National Laboratory, 2020. (declined)
- Lawrence Fellowship, Lawrence Livermore National Laboratory, 2020. (declined)
- Stephen Timoshenko Fellowship, Stanford University, 2020. (declined)
- Eugene P. Wigner Fellowship, Oak Ridge National Laboratory, 2020. (declined)
- J. H. Wilkinson Fellowship, Argonne National Laboratory, 2020. (declined)
- Conference Travel Fund, Brown University, 2020.
- Travel Grant, Physics Informed Machine Learning Workshop, 2020.
- J. Robert Oppenheimer Fellowship, Los Alamos National Laboratory, 2019. (declined)
- Travel Support Award, Machine Learning and the Physical Sciences workshop (NeurIPS), 2019.
- Open Graduate Education Travel Award, Brown University, 2019.
- International Conference Travel Fund, Brown University, 2019.
- Associate Member, Sigma Xi, 2018.
- George Irving Hopkins Fellowship, Brown University, 2017.
- Open Graduate Education Program, Brown University, 2017. (10 Brown doctoral students selected per year to pursue a master's degree in a secondary field)
- Third Prize, IBM OpenPOWER Developer Challenge contest, 2016. (top 6 of more than 350 teams around the world)

- Fellowship for graduate students, Brown University, 2015.
- Provincial Outstanding Graduates, Beijing, China, 2013. (top 5% of graduating students)
- Provincial Merit Student, Beijing, China, 2013. (top 1 student in every department)
- Outstanding Graduates, Tsinghua University, 2013. (top 2% of graduating students)
- Outstanding Undergraduate Graduation Thesis, Tsinghua University, 2013. (top 5% of graduating students)
- Excellent Student Cadre, Tsinghua University, 2013. (top 3 students in every department)
- December Ninth Scholarship, Tsinghua University, 2012. (top 1 student in every department)
- Summer Research Scholarship, Chinese Undergraduate Visiting Research Program, Stanford University, 2012. (18 students selected in China)
- Outstanding Volunteer, Tsinghua University learning center, 2012.
- Member of "Spark" Innovative Talent Cultivation Program, Tsinghua University, 2011. (top 36 of 3300 students)
- Tsinghua Friend–Kai Feng Fellowship, Tsinghua University, 2011. (top 10 students in every grade)
- Best Paper Award, 10th National Symposium on Refrigerators, Air Conditioners and Compressors, Shandong, China, 2011. (the only undergraduate student received the award)
- Third Prize, 29th "Challenge Cup" Tsinghua University Students' Extracurricular Academic Science and Technology Works Contest, 2011.
- Three-star Volunteer, Tsinghua University, 2011. (entitled to those who devoted more than 100 hours to voluntary work)
- Tsinghua Friend–Kai Feng Fellowship, Tsinghua University, 2010. (top 10 students in every grade)
- First Prize, 27th Annual National Physics Contest for College Students, Beijing, China, 2010.
- Second Prize, 4th Intelligent Car Competition, Tsinghua University, 2010.
- First Prize, Chinese Physics Olympiad, Jiangsu, China, 2008.
- First Prize, Chinese Mathematical Olympiad, Jiangsu, China, 2008.
- Third Prize, Chinese Chemistry Olympiad, Jiangsu, China, 2008.
- Second Prize, Chinese Physics Olympiad, Jiangsu, China, 2007.

Talks and Presentations

Invited Talks

1. Physics-informed deep learning. *Synced*, Aug. 2021.
2. DeepONet: Learning nonlinear operators. *University of Iowa, Department of Mathematics*, May 2021.
3. Integrating machine learning & multiscale modeling. *Purdue University, Department of Mathematics*, Feb. 2021.
4. Integrating machine learning & multiscale modeling in biomedicine. *Queen's University, Department of Mechanical and Material Engineering*, Feb. 2021.
5. Integrating machine learning & multiscale modeling in biomedicine. *University of Pennsylvania, Department of Chemical and Biomolecular Engineering*, Feb. 2021.
6. Physics-informed deep learning. *Emory University, Scientific Computing Group*, Apr. 2020.
7. Scientific machine learning. *Lawrence Berkeley National Laboratory, Computing Sciences*, Mar. 2020.
8. Scientific machine learning. *Lawrence Livermore National Laboratory*, Feb. 2020.
9. Scientific machine learning. *Worcester Polytechnic Institute, Mathematical Sciences Department*, Feb. 2020.
10. Scientific machine learning. *Oak Ridge National Laboratory*, Jan. 2020.
11. Scientific machine learning. *Argonne National Laboratory, Mathematics and Computer Science Division*, Jan. 2020.
12. Scientific machine learning. *University of Pittsburgh, Department of Mechanical Engineering and Materials Science*, Nov. 2019.
13. Scientific machine learning. *University of North Carolina at Charlotte, Department of Mathematics and Statistics*, Nov. 2019.
14. Collapse of deep and narrow neural nets. *ICERM Scientific Machine Learning*, Providence, RI, Jan. 2019.

Conference Presentations

1. DeepONet: Learning nonlinear operators. *Conference on the Numerical Solution of Differential and Differential-Algebraic Equations*, Martin Luther University Halle-Wittenberg, Germany, Sept. 2021.
2. DeepONet: Learning nonlinear operators. *SIAM Conference on Applications of Dynamical Systems*, Virtually, May 2021.
3. One-shot learning for solution operators of partial differential equations. *ICLR Workshop on Deep Learning for Simulation*, Virtually, May 2021.

4. DeepONet: Learning nonlinear operators based on the universal approximation theorem of operators. *SIAM Conference on Computational Science and Engineering*, Virtually, Mar. 2021.
5. DeepXDE: A deep learning library for solving differential equations. *Workshop on Mathematical Machine Learning and Application*, Pennsylvania State University, Virtually, Dec. 2020.
6. DeepONet: Learning nonlinear operators based on the universal approximation theorem of operators. *SIAM Conference on Mathematics of Data Science*, Virtually, June 2020.
7. DeepXDE: A deep learning library for solving differential equations. *SIAM Conference on Mathematics of Data Science*, Virtually, June 2020.
8. DeepXDE: A deep learning library for solving differential equations. *AAAI Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physical Sciences*, Stanford, CA, Mar. 2020.
9. DeepONet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators. *Joint Mathematics Meetings*, Denver, CO, Jan. 2020.
10. DeepXDE: A deep learning library for solving forward and inverse differential equations. *3rd Physics Informed Machine Learning Workshop*, Santa Fe, NM, Jan. 2020.
11. DeepXDE: A deep learning library for solving differential equations. *Conference on Neural Information Processing Systems Workshop on Machine Learning and the Physical Sciences*, Vancouver, Canada, Dec. 2019.
12. DeepXDE: A deep learning library for solving differential equations. *Deep Learning for Science School*, Berkeley, CA, July 2019.
13. Quantitative prediction of erythrocyte sickling for anti-polymerization activities in sickle cell disease. *60th Annual Red Cell Meeting*, New Haven, CT, Oct. 2018.
14. OpenRBC: A fast simulator of red blood cells at protein resolution. *SIAM Annual Meeting*, Pittsburgh, PA, July 2017.
15. Probing the twisted structure of sickle hemoglobin fibers via particle simulations. *20th Biennial Hemoglobin Switching Conference*, Pacific Grove, CA, Sept. 2016.
16. Shock tube ignition delay time study of RP-1/oxygen/argon mixtures. *Stanford Undergraduate Visiting Research Symposium*, Stanford, CA, Aug. 2012.
17. The feasibility analysis of small-sized commercial ice-storage air-conditioning system. *10th National Symposium on Refrigerators, Air Conditioners and Compressors*, Qingdao, Shandong, Aug. 2011.

Professional Services

- Minisymposium Organizer: SIAM Conference on Computational Science and Engineering – Machine Learning for Physical Systems (2021), SIAM Conference on Mathematics of Data Science – Machine Learning for Physical Systems (2020)
- Journal Reviewer: Nature Computational Science, Nature Communications, IEEE Transactions on Neural Networks and Learning Systems, Computer Methods in Applied Mechanics and Engineering, Computers & Mathematics with Applications, SIAM Journal on Scientific Computing, Neural Networks, Journal of Scientific Computing, Multiscale Modeling & Simulation, Neurocomputing, Journal of Computational Physics, Computers in Biology and Medicine, PLoS ONE, European Journal of Applied Mathematics, Journal of Materials Research, Computation, Journal of Eye Study and Treatment, International Journal of Blood Research and Disorders
- Conference Reviewer: Conference on Neural Information Processing Systems, International Conference on Machine Learning, International Conference on Learning Representations, Mathematical and Scientific Machine Learning

Teaching Experience

Massachusetts Institute of Technology

- Instructor, 18.085 Computational Science and Engineering I — Spring 2021
- Recitation Instructor, 18.02 Multivariable Calculus — Fall 2020

Brown University

- Teaching Assistant, APMA 2550 Numerical Solution of Partial Differential Equations I — Fall 2017, Fall 2018
- Teaching Assistant, APMA 1200 Operations Research: Probability Models — Spring 2018
- Teaching Assistant, APMA 1690 Computational Probability and Statistics — Fall 2017
- Teaching Assistant, ENGN 1860 Advanced Fluid Mechanics — Spring 2015

Tsinghua University

- Instructor, Tsinghua University National Students' Innovation Camp (instructed 24 senior high school students to complete 8 innovation projects in one week) 8/2011
- Instructor, Tsinghua University learning center (taught freshmen mathematics and physics) 3/2010–12/2011

Last updated: September 7, 2021