

Ellen D. Zhong

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Academic Experience

- Princeton University** 2022 - Present
Assistant Professor, Department of Computer Science
- Massachusetts Institute of Technology** 2017 - 2022
Ph.D., Computational and Systems Biology, Computer Science and Artificial Intelligence Lab
Advisors: Bonnie Berger, Joey Davis
Thesis: Machine learning for reconstructing dynamic protein structure from cryo-EM data
- University of Virginia** 2010 - 2014
B.S. Chemical Engineering with highest distinction
Advisor: Michael R. Shirts
Thesis: Thermodynamics of protein folding with Hamiltonian Monte Carlo simulations

Industry Experience

- Flatiron Institute**, New York, NY 2022 - Present
Visiting Research Scholar
- Google DeepMind**, London, UK Summer 2021
Research Scientist Intern - Science team
Deep learning for protein structure prediction. Hosted by John Jumper and the AlphaFold team
- D. E. Shaw Research**, New York, NY 2014 - 2017
Scientific Associate and Scientific Programmer
Algorithms and production-scale infrastructure for estimating protein-drug binding free energy calculations from molecular dynamics simulation on Anton supercomputers. Automated tools for ligand forcefield fitting via *ab initio* quantum mechanical calculations.
- D. E. Shaw Research**, New York, NY Summer 2013
Scientific Programmer Intern
- NASA/Johns Hopkins University Applied Physics Lab**, Laurel, Maryland Summer 2011
MESSENGER Imaging Team

Publications and Preprints

- Amortized inference for heterogeneous reconstruction in cryo-EM.
Levy A, Wetzstein G, Martel J, Poitevin F, **Zhong ED**.
Neural Information Processing Systems (NeurIPS), 2022.
- Latent Space Diffusion Models of Cryo-EM Structures
Kreis K, Dockhorn T, Li Z, **Zhong ED**.
NeurIPS Machine Learning in Structural Biology (MLSB) Workshop, 2022. **Oral presentation.**
- Deep Generative Modeling for Volume Reconstruction in Cryo-Electron Microscopy.
Donnat C, Levy A, Poitevin F, **Zhong ED**, Miolane N.
Journal of Structural Biology, 2022.

- Uncovering structural ensembles from single particle cryo-EM data using cryoDRGN.
Kinman LF+, Powell BM+, **Zhong ED***+, Berger B*, Davis JH*.
(*Corresponding, +Equal contribution)
Nature Protocols, 2022.
- Conformational landscape of the yeast SAGA complex as revealed by cryo-EM.
Vasyliuk D, Felt J, **Zhong ED**, Berger B, Davis JH, Yip CK.
Scientific Reports, 2022.
- Cryo-EM structure of the plant 26S proteasome.
Kandolf S, Grishkovskaya I, Belai K, Bolhuis DL, Amann S, Foster B, Imre R, Mechtler K,
Schleiffer A, Tagare HD, **Zhong ED**, Meinhart A, Brown NG, Haselbach D.
Plant Communications, 2022.
- CryoDRGN2: *Ab initio* neural reconstruction of 3D protein structures from real cryo-EM images.
Zhong ED, Lerer A, Davis JH, Berger B.
International Conference on Computer Vision (ICCV), 2021.
- CryoDRGN: Reconstruction of heterogeneous cryo-EM structures using neural networks.
Zhong ED, Bepler T, Berger B, Davis JH.
Nature Methods, 2021. doi:10.1038/s41592-020-01049-4.
- Learning the language of viral evolution and escape.
Hie B, **Zhong ED**, Berger B, Bryson B.
Science, 2021. doi:10.1126/science.abd7331.
- Exploring generative atomic models in cryo-EM reconstruction.
Zhong ED, Lerer A, Davis JH, Berger B.
NeurIPS Machine Learning in Structural Biology (MLSB) Workshop, 2020.
- Learning mutational semantics.
Hie B, **Zhong ED**, Bryson B, Berger B.
Neural Information Processing Systems (NeurIPS) 2020.
- RNA timestamps identify the age of single molecules in RNA sequencing.
Rodrigues SG, Chen LM, Liu S, **Zhong ED**, Scherrer JR, Boyden ES, Chen F.
Nature Biotechnology, 2020. doi:10.1038/s41587-020-0704-z.
- Structures of radial spokes and associated complexes important for ciliary motility.
Gui M, Ma M, Sze-Tu E, Wang X, Koh F, **Zhong ED**, Berger B, Davis JH, Dutcher S, Zhang R,
Brown A.
Nature Structural and Molecular Biology, 2020. <https://doi.org/10.1038/s41594-020-00530-0>.
- Reconstructing continuous distributions of 3D protein structure from cryo-EM images.
Zhong ED, Bepler T, Davis JH, Berger B.
International Conference on Learning Representations (ICLR) 2020. **Spotlight presentation.**
* Machine Learning in Computational Biology (MLCB), 2019. **Oral presentation.**
* NeurIPS Learning Meaningful Representations of Life (LMRL) workshop, 2019.
- Explicitly disentangling image content from translation and rotation with spatial-VAE.
Bepler T, **Zhong ED**, Kelley K, Brignole E, Berger B.
Neural Information Processing Systems (NeurIPS) 2019.
- Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset.
Shirts MR, Klein C, Swails JM, Yin J, Gilson MK, Mobley DL, Case DA, **Zhong ED**.
J. Comput. Aided. Mol. Des. 2016. doi:10.1007/s10822-016-9977-1.
- Thermodynamics of Coupled Protein Adsorption and Stability using Hybrid Monte Carlo simulations.
Zhong ED, Shirts MR.
Langmuir 2014. doi:10.1021/la500511p
- Areas of permanent shadow in Mercurys south polar region ascertained by MESSENGER orbital imaging.
Chabot NL, Ernst CM, Denevi BW, ... **Zhong ED**.
Geophys. Res. Lett. 2012. doi:10.1029/2012GL051526.

Selected Presentations

Upcoming

- International Congress on Industrial and Applied Mathematics, Tokyo, Japan, Aug, 2023
- ICLR Neural Fields Across Fields Workshop, Kigali, Rwanda, May, 2023
- University of Pennsylvania Structural Biology Symposium, Philadelphia, PA, May, 2023
- Caltech, AI4Science seminar series, Apr, 2023
- Stanford, SCIEN seminar series, Apr, 2023
- Centre International de Rencontres Mathématiques, Marseille, France, March, 2023
- University of Washington Institute of Protein Design, Seattle, WA, March, 2023
- Columbia Physiology and Cellular Biophysics, New York, NY, March 2023
- Biophysical Society Annual Meeting, San Diego, CA, February, 2023
- Brigham Young University Department of Chemistry and Biochemistry, Provo, UT, January, 2023

2022

- Guest lecture, MIT 6.S980 Machine Learning for Inverse Graphics, December, 2022
- Institute of Pure and Applied Mathematics (IPAM) workshop, ULCA, November 2022
- Cold Springs Harbor Laboratory, Course on Cryo-EM, November, 2022
- Chan Zuckerberg Imaging Institute, Frontiers in cryo-electron tomography, San Francisco, CA, November, 2022
- Yale Department of Statistics and Data Science, New Haven, CT, October, 2022
- Keynote, MIT Molecule Machine Learning Conference, Cambridge, MA, October, 2022
- Purdue Computer Science, Virtual, October, 2022
- Rutgers Institute for Quantitative Biomedicine and RCSB Protein Data Bank, Virtual, October, 2022
- Nature Conferences, Frontiers in Electron Microscopy for Physical and Life Sciences, Princeton, NJ, September, 2022
- Van Andel Institute, Virtual, September, 2022
- Microscopy & Microanalysis, Portland, OR, August, 2022
- CVPR, Tutorial on neural fields in computer vision, New Orleans, LA, June, 2022
- ICLR Deep Generative Models for Highly Structured Data Workshop, Virtual, April, 2022
- VIB-VUB Center of Structural Biology, Virtual, April, 2022
- CCP-EM/CCPBioSim Cryo-EM Dynamics Discussion Meeting, Virtual, April, 2022
- Vienna Biocenter IMBA/IMP Young Investigator Symposium, Virtual, March, 2022
- Society for Industrial and Applied Mathematics (SIAM) Conference on Imaging Science, Cryo-EM Mini-symposium, Virtual, March, 2022
- SLAC/Stanford University, March, 2022
- John Hopkins University Cryo-EM Seminar Series, Virtual, March, 2022

- Brookhaven National Lab Applied Mathematics Seminar Series, Virtual, March, 2022
- Selected talk: International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, March, 2022
- OpenEye CUP, Santa Fe, NM, March, 2022
- Princeton Department of Computer Science, Princeton, NJ, February, 2022
- Columbia Department of Computer Science, Virtual, February, 2022

2021

Machine learning for solving protein structures and dynamics.

- The MRC Laboratory of Molecular Biology, Cambridge, UK, November, 2021
- The Francis Crick Institute, London, UK, November, 2021

Cryo-EM and AlphaFold in translational research

- Introductory remarks and discussion leader: Gordon Research Conference, Visualizing Biological Complexity Across Scales, October, 2021

Advances in heterogeneous reconstruction with cryoDRGN

- Microsoft Research New England, November, 2021
- Scientific Computing in Structural Biology Workshop, Stanford SLAC Users Meeting, September, 2021
- RosettaCon, August, 2021
- American Crystallographic Association Annual Meeting, August, 2021
- CCP-EM Spring Symposium, Oxfordshire, UK, April, 2021
- GlaxoSmithKline (GSK) Data Forum seminar series, London, UK, April, 2021
- Princeton University Applied Mathematics IDeAS Seminar, Princeton, NJ, Feb, 2021
- UIUC Coordinated Science Laboratory Student Conference (CSLSC), Champaign, IL, Feb, 2021

2020 and earlier

CryoDRGN: Reconstructing continuous distributions of protein structure from cryo-EM images.

- Vienna BioCenter, Research Institute of Molecular Pathology (IMP) Seminar Series, Vienna, Austria, Nov, 2020
- (Cancelled) Machine Learning in Cryo-EM workshop, Institute of Mathematical Sciences, Singapore, Oct, 2020
- SciLifeLab Advanced Cryo-EM Seminar Series, Stockholm, Sweden, Sept, 2020
- Microscopy & Microanalysis, Milwaukee, WI, August, 2020
- (Cancelled) SIAM Conference on Imaging Science Cryo-EM Mini-symposium, Toronto, ON, July, 2020
- SBGrid Annual Symposium, Boston, MA, May, 2020
- (Cancelled) International Conference on Image Analysis in Three-dimensional Cryo-EM, Lake Tahoe, CA, March, 2020
- Relay therapeutics, Boston, MA, Feb, 2020

- Oral presentation (top 8% of submissions): Machine learning in Computational Biology (MLCB) meeting, Vancouver, BC, Dec 2019
- Poster: NeurIPS Learning Meaningful Representations of Life (LMRL) workshop, Vancouver, BC, Dec 2019
- Harvard Cryo-EM Club, Cambridge, MA, Dec 2019
- Poster: Janelia Women in Computational Biology Meeting, Ashburn, VA, Nov 2019
- New England CryoEM symposium, Worcester, MA, October 2019
- Poster: Flatiron Institute Computational Cryo-EM Workshop, New York, NY, August 2019
- Poster: MIT Biology Departmental Retreat, Cape Cod, MA, June 2019

Testing the limits of modern heterogeneous reconstruction algorithms: The autophagy initiation complex.

- Poster: Purdue Cryo-EM Symposium, Lafayette, IN, Nov 7, 2018

From silicon to medicine: Core challenges of using molecular dynamics for early-stage drug discovery.

- Talk: Out in STEM National Conference, Pittsburgh, PA, Nov.14, 2015.

Optimizing molecular visualization for drug discovery.

- Talk: Grace Hopper Annual Conference, Houston, TX, Oct. 14 2015

Efficient simulation of protein stability on surfaces using a Hamiltonian Monte Carlo approach.

- Talk: AIChE Annual Meeting, San Francisco, CA, Nov. 6, 2013

Academic Service

Reviewer:

- Nature Methods
- Neural Information Processing Systems (NeurIPS)
- International Conference on Learning Representations (ICLR)
- International Conference on Machine Learning (ICML)
- Machine Learning in Computational Biology Workshop (MLCB)
- Machine Learning in Structural Biology Workshop (MLSB)
- IEEE Transactions on Computational Biology and Bioinformatics
- IEEE Transactions on Computational Imaging
- Biophysical Journal
- Journal of Physical Chemistry Letters
- Scientific Reports

Meetings:

- Co-organizer, Machine Learning in Structural Biology Workshop at NeurIPS 2022, 2021, 2020
- Co-organizer, MIT Biology career seminar series 2018-2019

Teaching

COS597N: Advanced Topics in Computer Science: Machine Learning for Structural Biology Fall 2022
7.57 Graduate Quantitative Biology TA with Prof. Joey Davis Spring 2019
ChE 2216 Modeling and Simulation TA with Prof. Michael Shirts Spring 2013

Grants and Fellowships

2018 MIT J Clinic for Machine Learning and Health. *Deep Generative Models for Cryo-EM Reconstruction of Heterogeneous Biomolecular Structures* (to Prof. B. Berger and Prof. J. Davis)
2017 NSF Graduate Research Fellowship Award
2014 NSF Graduate Research Fellowship Award (Declined)

Awards

2021 American Crystallographic Association Etter Student Lecturer Award
2019 Best paper award at Machine Learning in Computational Biology
2019 Teaching Award from MIT Biology Department
2019 Best poster award at MIT Biology Department Retreat
2014 Louis T. Rader Chemical Engineering Prize: Awarded from UVA Dept. of ChemE
2014 American Institute of Chemists Award: Awarded from UVA Dept. of ChemE
2013 Barry M. Goldwater Scholarship
2012, 2013 Astronaut Scholarship