

# DAVID H. BROOKES

(240) 499-4647 ◊ david.brookes@berkeley.edu ◊ Berkeley, CA  
dhbrookes.github.io

## EDUCATION

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### **Ph.D., Biophysics Graduate Group**

August 2016 - May 2021

*Berkeley AI Research Lab*

University of California, Berkeley

### **B.S., Bioengineering**

August 2011 - May 2015

*Concentration in Computational Biology*

University of California, Berkeley

*Relevant coursework:* Graduate Statistical Mechanics I & II, Graduate Quantum Mechanics I (audit), Introduction to Machine Learning, Efficient Algorithms and Intractable Problems, Numerical Analysis, Introduction to Artificial Intelligence.

## PROFESSIONAL EXPERIENCE

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### **AI Resident, Google X**

May 2019 - August 2019

- Combined machine learning expertise with software engineering skills to bolster an early-stage confidential project, as well as shape the project's future direction.
- Effectively communicated advanced modeling ideas to a team of people with vastly different expertise.

## RESEARCH EXPERIENCE

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### **Graduate Student Researcher, Berkeley AI Research Lab**

February 2018 - Present

Supervisor: Prof. Jennifer Listgarten

- Developed probabilistic modeling approaches for biological sequence design. Specifically, a rigorous probabilistic framework for sampling sequences that satisfy desired properties using joint supervised and generative modeling approaches ([2] and [3], below).
- Used insights from the above practical work to derive a novel connection between Estimation of Distribution algorithms and Expectation Maximization ([1], below).
- In ongoing work, we are applying our design methods in conjunction with novel modeling strategies to design a library of viral capsid sequences to be used in a downstream Directed Evolution experiment run by collaborators.

### **Student Researcher, UC Berkeley College of Chemistry**

October 2014 - February 2018

Supervisor: Prof. Teresa Head-Gordon

- Developed a Bayesian inference procedure for determining likely ensembles of intrinsically disordered protein structures given a set of experimental data ([6]).
- Lead developer of software suite to solve for electrostatic interactions on the surface of biological macromolecules. ([4] and [5], below, with code available at [github.com/dhbrookes/pbsolvers](https://github.com/dhbrookes/pbsolvers))
- Solved a linear model of physically relevant basis functions to find the distribution of possible structures of liquid water that satisfy a set of experimental data ([7]).

**Papers**

- [1] **D. H. Brookes**, A. Busia, C. Fannjiang, K. Murphy, and J. Listgarten. A view of Estimation of Distribution Algorithms through the lens of Expectation Maximization. *Proceedings of The Genetic and Evolutionary Computation Conference*, 2020.
- [2] **D. H. Brookes**, H. Park, and J. Listgarten. Conditioning by adaptive sampling for robust design. *Proceedings of ICML*, 2019. **Selected for a 20 minute oral presentation (< 5% of submissions)**.
- [3] **D. H. Brookes** and J. Listgarten. Design by adaptive sampling. *NeurIPS Workshop on Machine Learning for Molecules and Materials*, 2018.
- [4] E. Jurrus, D. Engel, K. Star, K. Monson, J. Brandi, L. E. Felberg, **D. H. Brookes**, L. Wilson, J. Chen, K. Liles, M. Chun, P. Li, T. Dolinsky, R. Konecny, D. Koes, J. E. Nielsen, T. Head-Gordon, W. Geng, R. Krasny, M. Gunner, G.-W. Wei, M. J. Holst, J. A. McCammon, N. A. Baker. Improvements to the APBS biomolecular solvation software suite. *Protein Sci.* 27 (1), pp. 112-128, 2018.
- [5] L. E. Felberg, **D. H. Brookes**, E. Jurrus, N. Baker, and T. Head-Gordon. PB-AM: An open-source, fully analytical linear Poisson-Boltzmann solver. *J. Comp. Chem.* 38 (15), pp. 1275-1282, 2017.
- [6] **D. H. Brookes** and T. Head-Gordon. Experimental inferential structure determination of ensembles for intrinsically disordered proteins *J. Am. Chem. Soc.* 138 (13), pp. 4530-4538, 2016.
- [7] **D. H. Brookes** and T. Head-Gordon. The family of oxygen-oxygen radial distribution functions for water. *J. Phys. Chem. Lett.* 6 (15), pp. 2938-2943, 2015
- [8] L. E. Felberg, **D. H. Brookes**, J. E. Rice, T. Head-Gordon, and W. Swope. Role of hydrophilicity and length of diblock arms for determining star polymer physical properties. *J. Phys. Chem. B.* 119 (3), pp. 944-957, 2015.

**Invited talks and posters**

- 1. A view of Estimation of Distribution Algorithms through the lens of Expectation Maximization *The Genetic and Evolutionary Computation Conference*, Jul. 2020.
- 2. Conditioning by adaptive sampling for robust design. *ICML*, Jun. 2019.
- 3. Design by Adaptive Sampling. *Google AI, Mountain View*, Jan. 2019.
- 4. Design by Adaptive Sampling. *NeurIPS Workshop on Machine Learning for Molecules and Materials*, Dec. 2018.
- 5. Sequence Design by Adaptive Sampling. *Berkeley Center for Computational Biology Retreat*, Nov. 2018.