Derek Jones

Education

Sept. 2020 – present
Ph.D, *University of California - San Diego*, La Jolla, CA, 3.0.
Major: Computer Science
Advisor(s): Dr. Tajana S. Rosing & Dr. Niema Moshiri

Aug. 2016 - May. 2018
M.Sc., *University of Kentucky*, Lexington, KY, 3.7.
Major: Computer Science
Advisor(s): Dr. Nathan Jacobs & Dr. Sally R. Ellingson

Aug. 2011 - May. 2016
B.S., *University of Kentucky*, Lexington, KY, 3.1.
Major: Computer Science & Mathematical Economics
Advisor(s): Dr. Judy Goldsmith

Experience

May 2023 - Pres.
Principal Investigator, *University of California Office of the President*, Oakland, CA.
Leading the UC Lab Fees project "Molecular Simulation to Enable Novel Target Generalization of Structure-Based Deep Learning Models". Responsible for definition and execution of project tasks, communication with project stakeholders regarding progress. Supervised by Dr. Tajana S. Rosing and Dr. Jonathan E. Allen

Jan. 2023 - Mar. 2023
Grad. Teaching Assistant, *University of California - San Diego*, La Jolla, CA.
Assisted Dr. Miles Jones with the delivery of "Theory of Computation" for advanced undergraduate students. Responsibilities included grading of assignments, responding to student feedback, providing general information on Piazza, and holding office hours.

Sept. 2020 - Pres.
Grad. Research Assistant, *University of California - San Diego*, La Jolla, CA.
Researching the application of hardware accelerators and machine learning to enable accurate long-time scale molecular simulation of biological systems.

Sept. 2018 - Pres.
Data Scientist, *ATOM Consortium*, San Francisco, CA.
Contributing machine learning and generative modeling expertise on behalf on Lawrence Livermore National Laboratory to develop an open source framework for automated, data-driven, chemical design of disease therapeutics. Specifically developing models and software to enable scalable training and analysis for massive chemical libraries.

Sept. 2018 - Pres.
Research Data Scientist, *Lawrence Livermore National Laboratory*, Livermore, CA.
Working as part of an inter-disciplinary team to develop structure based deep learning models to augment physics-based simulation pipelines to drive more effective exploration of protein-ligand binding dynamics.

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Jun. 2018 - Sept. 2018 **Intern**, *Lawrence Livermore National Laboratory*, Livermore, CA.
Developed spatial graph deep learning technique to model protein-ligand interactions, presenting a poster covering a series of transfer learning experiments. Supervised by Dr. Jonathan E. Allen.

Jun. 2017 - Aug. 2017 **Intern**, *Lawrence Berkeley National Laboratory*, Berkeley, CA.
Conducted research with the Computational Chemistry, Materials, and Climate group in the Computational Research Division of LBNL. Applied machine learning and HPC resources to process high dimensional biochemical data for drug discovery and develop a novel random-forest based feature selection algorithm. Supervised by Dr. Bert de Jong.

Jan. 2017 - May. 2018 **Grad. Research Assistant**, *University of Kentucky - Markey Cancer Center*, Lexington, KY.
Worked as part of an interdisciplinary team to study the prediction of potential off-target effects of candidate cancer therapeutics. Developed data processing pipeline and feature selection algorithms to aid in the understanding of important properties of selectivity in the kinase class of proteins.

Aug. 2016 - May. 2017 **Grad. Teaching Assistant**, *University of Kentucky - Department of Computer Science*, Lexington, KY.
Lab instructor for "Introduction to Programming Design and Abstraction" course, taught in C++. Led 90 minute lab sessions, held office hours to consult with students outside of class, and graded lab assignments, programming assignments, and exams.

Industry Knowledge

○ Deep Learning ○ Molecular Dynamics ○ ○ High-Performance Computing (HPC) ○ Statistical Data Analysis ○ Large Language Models (LLMs) ○ Generative Models ○ Variational Autoencoders ○ Sequence Modeling ○ Message Passing Neural Networks (MPNNs) ○ Graph Convolution Neural Networks (GCNNs) ○ Convolutional Neural Networks (CNNs) ○ Mathematics ○ Research Projects ○ Bioinformatics ○ Computational Biology ○ Drug Discovery ○ Computer Science ○ Programming ○ Statistical Modeling ○ Machine Learning ○ Data Analysis ○ Statistics ○ Data Visualization

Tools & Technologies

○ Python ○ C++ ○ C ○ Matlab ○ R ○ STATA ○ Linux ○ PyTorch ○ Keras ○ Tensorflow ○ Numpy ○ Pandas ○ Matplotlib ○ Scipy ○ Git ○ LaTeX ○ MySQL ○ SLURM ○ LSF ○ POWER architecture ○ Microsoft Office

Soft Skills

○ Inter-personal communication ○ Inter-disciplinary collaboration ○ Teamwork ○ Leadership ○ Public speaking on technical subjects ○ Presentation of complex analysis for general audiences

Publications

Journals

Garrett A Stevenson, Dan Kirshner, Brian J Bennion, Yue Yang, Xiaohua Zhang, Adam Zemla, Marisa W Torres, Aidan Epstein, Derek Jones, Hyojin Kim, W F Drew Bennett, Sergio E Wong, Jonathan E Allen, and Felice C Lightstone. Clustering protein binding pockets and identifying potential drug interactions: A novel Ligand-Based featurization method. *J. Chem. Inf. Model.*, 63(21):6655–6666, November 2023.

Derek Jones, Jonathan E Allen, Yue Yang, William F Drew Bennett, Maya Gokhale, Niema

Moshiri, and Tajana S Rosing. Accelerators for classical molecular dynamics simulations of biomolecules. *J. Chem. Theory Comput.*, 18(7):4047–4069, July 2022.

Edmond Y Lau, Oscar A Negrete, W F Drew Bennett, Brian J Bennion, Monica Borucki, Feliza Bourguet, Aidan Epstein, Magdalena Franco, Brooke Harmon, Stewart He, Derek Jones, Hyojin Kim, Daniel Kirshner, Victoria Lao, Jacky Lo, Kevin McLoughlin, Richard Mosesso, Deepa K Murugesh, Edwin A Saada, Brent Segelke, Maxwell A Stefan, Garrett A Stevenson, Marisa W Torres, Dina R Weilhammer, Sergio Wong, Yue Yang, Adam Zemla, Xiaohua Zhang, Fangqiang Zhu, Jonathan E Allen, and Felice C Lightstone. Discovery of Small-Molecule inhibitors of SARS-CoV-2 proteins using a computational and experimental pipeline. *Front Mol Biosci*, 8:678701, July 2021.

Sam Ade Jacobs, Tim Moon, Kevin McLoughlin, Derek Jones, David Hysom, Dong H. Ahn, John Gyllenhaal, Pythagoras Watson, Felice C. Lightstone, Jonathan E. Allen, Ian Karlin, and Brian Van Essen. Enabling rapid covid-19 small molecule drug design through scalable deep learning of generative models. *International Journal of High Performance Computing Applications*, March 2021.

Derek Jones, Hyojin Kim, Xiaohua Zhang, Adam Zemla, Garrett Stevenson, William D Bennett, Dan Kirshner, Sergio Wong, Felice Lightstone, and Jonathan E Allen. Improved protein-ligand binding affinity prediction with Structure-Based deep fusion inference. *J. Chem. Inf. Model.*, March 2021.

W F Drew Bennett, Stewart He, Camille L Bilodeau, Derek Jones, Delin Sun, Hyojin Kim, Jonathan E Allen, Felice C Lightstone, and Helgi I Ingólfsson. Predicting small molecule transfer free energies by combining molecular dynamics simulations and deep learning. *J. Chem. Inf. Model.*, September 2020.

Fangqiang Zhu, Xiaohua Zhang, Jonathan E Allen, Derek Jones, and Felice C Lightstone. Binding affinity prediction by pairwise function based on neural network. *J. Chem. Inf. Model.*, 60(6):2766–2772, June 2020.

Conference Proceedings

Derek Jones, Jonathan E Allen, Xiaohua Zhang, Behnam Khaleghi, Jaeyoung Kang, Weihong Xu, Niema Moshiri, and Tajana S Rosing. HD-Bind: Encoding of molecular structure with low precision, hyperdimensional binary representations. In *(in progress)*, March 2023.

Garrett A Stevenson, Derek Jones, Hyojin Kim, W F Drew Bennett, Brian J Bennion, Monica Borucki, Feliza Bourguet, Aidan Epstein, Magdalena Franco, Brooke Harmon, Stewart He, Max P Katz, Daniel Kirshner, Victoria Lao, Edmond Y Lau, Jacky Lo, Kevin McLoughlin, Richard Mosesso, Deepa K Murugesh, Oscar A Negrete, Edwin A Saada, Brent Segelke, Maxwell Stefan, Marisa W Torres, Dina Weilhammer, Sergio Wong, Yue Yang, Adam Zemla, Xiaohua Zhang, Fangqiang Zhu, Felice C Lightstone, and Jonathan E Allen. High-Throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. In *Supercomputing (SC) 21*, 2021.

Derek Jones, Jeevith Bopaiah, Fatemah Alghamedy, Nathan Jacobs, Heidi L Weiss, W A de Jong, and Sally R Ellingson. Polypharmacology within the full kinome: a machine learning approach. In *AMIA 2018 Informatics Summit*, 2018.

Fatemah Alghamedy, Jeevith Bopaiah, Derek Jones, Xiaofei Zhang, Heidi L Weiss, and Sally R Ellingson. Incorporating protein dynamics through ensemble docking in machine learning models to predict drug binding. In *AMIA 2018 Informatics Summit*, 2018.

Preprints

Garrett A Stevenson, Derek Jones, Hyojin Kim, W F Drew Bennett, Brian J Bennion, Monica Borucki, Feliza Bourguet, Aidan Epstein, Magdalena Franco, Brooke Harmon, Stewart He,

Max P Katz, Daniel Kirshner, Victoria Lao, Edmond Y Lau, Jacky Lo, Kevin McLoughlin, Richard Mosesso, Deepa K Murugesh, Oscar A Negrete, Edwin A Saada, Brent Segelke, Maxwell Stefan, Marisa W Torres, Dina Weilhammer, Sergio Wong, Yue Yang, Adam Zemla, Xiaohua Zhang, Fangqiang Zhu, Felice C Lightstone, and Jonathan E Allen. High-Throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. April 2021.

Derek Jones, Hyojin Kim, Xiaohua Zhang, Adam Zemla, Garrett Stevenson, William D Bennett, Dan Kirshner, Sergio Wong, Felice Lightstone, and Jonathan E Allen. Improved protein-ligand binding affinity prediction with Structure-Based deep fusion inference. May 2020.

Poster Sessions

Derek Jones, Nathan Jacobs, and Sally Ellingson. Learning deep feature representations for kinase polypharmacology. In *ACM Richard Tapia Celebration of Diversity in Computing*, 2018.

Derek Jones, Sally R Ellingson, and W A de Jong. How low can you go? feature selection for drug discovery. In *Commonwealth Computational Summit*, 2017.

Talks

Derek Jones. Informing deep learning methodologies for drug discovery with biophysical simulation. Deep Learning For Chemistry: Resilience of Methods Workflows at ACS Fall Meeting 2021, 2021.

Derek Jones. Accelerators for classical molecular dynamics simulations of biomolecules. LLNL Biosecurity Center Seminar, 2021.

Derek Jones. Fusion of structure based deep learning to accelerate molecular docking predictions. 5th Computational Approaches for Cancer Workshop at SC19, 2019.

Derek Jones. Leveraging large scale molecular dynamics simulations and deep learning for binding activity models. SIAM 2019 Conference on Computational Science and Engineering, 2019.

Theses

Derek Jones. Scalable feature selection and extraction with applications in kinase polypharmacology. Master's thesis, University of Kentucky, 2018.

Panels

Derek Jones. Panel discussion on diversity and inclusion for careers in cse: Challenges and best practices. SIAM 2021 Conference on Computational Science and Engineering, 2021.

Derek Jones. Broader engagement (be): Mentoring panel and networking session. SIAM 2021 Conference on Computational Science and Engineering, 2021.

Refereed Journals

2023 IEEE/ACM Transactions on Computational Biology and Bioinformatics

2023 Physical Chemistry Chemical Physics (PCCP), Royal Society of Chemistry

2021 Journal of Chemical Information and Modeling, American Chemical Society

2021 Journal of Computer-Aided Molecular Design, Springer Nature

Grants and Awards

2023 Best Poster - Semiconductor Research Corporation (SRC) PRISM Center Annual Review

2023 UC National Laboratory Fees Research Program Fellow

2022 Lawrence Livermore National Laboratory Director's Award - Science and Technology
2021 Lawrence Livermore National Laboratory Director's Award - Science and Technology
2021 ACM Gordon Bell Award Finalist
2020 Lawrence Livermore Physical and Life Sciences Summer Directorate Award
2020 Lawrence Livermore Computing Directorate Noteworthy Achievement Award
2020 Alfred P. Sloan Foundation Graduate Fellowship
2018 ACM Student Research Competition (SRC) Travel Award
2018 ACM Richard Tapia 2018 Travel Scholarship
2018 UK CS Departmental travel grant
2017 Supercomputing (SC) 2017 Student Volunteer Travel Award
2017 CRA Computing Sciences Research Pathways Fellowship (LBNL)
2017 Lyman T. Johnson Fellowship
2017 AAAI 2017 Scholarship
2017 AAAI 2017 Diversity Workshop travel award
2017 UK CS Departmental travel grant

Mentoring

2024 Yash Ravipati - UCSD
2022 Kay Krachenfels, LLNL - Data Science Summer Institute (DSSI)
2021 Andrei Rekesh (co-advised with Stewart He), LLNL - Data Science Summer Institute (DSSI)
2019 Eric M. Coleman (co-advised with Sam A. Jacobs), LLNL - Consortium Enabling Cybersecurity Opportunities and Research (CECOR)

Volunteering Experience

2020 UCSD CSE PhD Information Session
2017 Supercomputing (SC) 2017 Student Volunteer
2017 AAAI 2017 Student Volunteer

Organizations

2016-present Association for Computing Machinery (ACM)
2022-present American Chemical Society (ACS)