Karl Lundquist, Ph.D.

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EXECUTIVE SUMMARY

Dedicated and innovative Data Scientist with a PhD in Physics, specializing in machine learning models and visualization of biological data. Proven expertise in developing tools and algorithms to solve complex problems in bioinformatics and data science. Strong background in statistical modeling, protein simulations, and cloud computing.

CAREER HIGHLIGHTS

- Developed proprietary application that provides an ordered list of human gene targets with high probability of clinical success based on training ML models on aggregate data from PubMed, clinical trials, and patent databases.
- Developed first-ever application that took data from plant metabolism database and converted into easy-to-use system that identified shortest path signaling pathways based on compound of interest.
- Elucidated mechanism of gram-negative outer surface protein assembly using molecular dynamic simulations, which enabled cryo-EM images to validate the predictions. (Published in Nature Communications 2021)
- Identified new target for development of therapeutic modalities for antimicrobial resistance, by performing molecular dynamics simulations and empirical laboratory validation, resulting in the identification of specific amino acid mutations that contribute to antimicrobial resistance. (Published in PNAS 2018)

CORE COMPETENCIES

- ✓ Machine Learning
- ✓ Computational Biology
- ✓ Molecular Dynamics
- ✓ Protein modeling
- ✓ Software Development
- ✓ Scientific communication
- ✓ Cloud Computing
- ✓ Collaboration

RELEVANT EXPERIENCE

Metapages (Astera Institute), Berkeley, CA — Oct 2024 – present

Scientific Consultant (contract)

- Developed interactive computational biology platform using React and Python, enabling browser-based scientific workflows and data visualization for research applications
- Implemented containerized data processing pipelines combining Python, R, and Docker to scale from browser computation to high-performance processing
- Created competition platform driving community engagement in computational biology challenges, resulting in novel solutions for protein design and RNA analysis

EMD Serono (Merck group), Rockland, MA — May 2023 - Nov 2023

Bioinformatics Scientist (contract)

- Developed algorithm resulting in unique metric to identify high-interest genes by leveraging ML models and NLP data from over 30 million publications, clinical trials, and patents to improve drug target prioritization pipeline for immune disorders.
- Consolidated inconsistent clinical identifiers into single comprehensive database by using public data from Drugbank, MeSH, DOID, GO, MedDRA, SNOMED, and ICD-10 for optimization of machine learning models to include disease specificity.
- Optimized ML model by testing RNN (GRU, LSTM), regression, and tree-based methods to prototype analysis of human gene annotations using TensorFlow (python) and Tidymodels (R) to optimize sensitivity and specificity
- Final deliverable of project included deployment and maintenance of custom web app for visualization of data and gene trendiness scores to enable time-saving drug-target prioritization output.
- Identified additional, proprietary use-case for custom web app that enabled derisked recommendations for IP licensing opportunities, based on predicted probability of clinical trial success.

Calyxt (now Cibus), Minneapolis, MN — May 2022 - Nov 2022

Data Scientist (contract)

- Used ML and DL models to develop systematized, scalable, plasmid design pipeline to optimize rare compound production for pharmaceutical manufacturing
- Proposed and implemented DOE (JMP) to reduce experimental turnaround time and identify key variables for optimization in rare compound biosynthesis
- Designed and deployed a Dash web app with built-in Agile framework (CI/CD) to enable immediate identification and visualization of optimal biosynthesis pathways

Purdue University, West Lafayette, IN — Sep 2019 - Sep 2021

Postdoctoral Research Associate

- Developed molecular dynamic simulations to produce the first-ever image of protein assembly for a unique bacterial membrane protein, validated empirically by cryo-EM
- Developed methodology to identify mechanism of chaperone-mediated enzyme assembly using high throughput screening of naturally occurring peptides
- Performed standard laboratory molecular techniques including cloning, primer design, PCR, cell culture, and FPLC

Georgia Institute of Technology, Atlanta, GA — Aug 2012 - May 2019

Graduate Research Associate

- Utilized optical tweezer laser methods to characterize rheological properties (viscosity, elasticity) of the joint-tissue extracellular matrix, providing modeling framework for wound healing and tissue remodeling in fibrotic diseases.

- *In silico* molecular modeling and chemical property predictions of bacterial and human membrane protein complexes, to reveal protonation states and atomic geometries for downstream molecular dynamics simulations.
- Performed benchmarking, wrote Bash scripts, and utilized SLURM to manage and optimize job submissions on cloud-based HPCC platforms, enhancing computational efficiency and resource utilization for high-performance scientific computing tasks.
- Designed and executed molecular dynamics simulations to explore the folding process of bacterial membrane proteins and analyzed binding site energetics using free energy methods, aiding in antibiotic development and therapeutic strategies for antimicrobial resistance.
- Molecular dynamics simulations of IL2RB mutations to determine changes in protein secondary structure for therapeutic target development/validation in novel immune disease (Published in J.Ex.Med 2019)

SELECTED PROJECTS

Bits to Binders 2024 Protein Design Competition

- Developed computational pipeline to design protein binders targeting CD20 using RFDiffusion, ProteinMPNN, Rosetta FastRelax, AlphaFold2, and MD simulation
- Created custom scoring function including interaction free energy, enthalpy, and topological factors to rank and select binders

TECHNICAL SKILLS

Computational	Python (numpy, pandas, scikit-learn, pytorch, tensorflow, biopython, dash, plotly), R (DESeq2, Bioconductor, rshiny, dplyr, tidyr, ggplot2), SQL, Bash, AI/ML (NLP, Diffusion models, Graph Neural Networks, Statistical modeling), Cloud Computing (Azure, AWS, GCP, Docker)
Molecular	Protein modeling (VMD, PyMol), MD simulations (NAMD, Amber), homology modeling, sequence alignment, RNAseq, NGS
Laboratory	Bacterial cell culture, protein expression/purification, gel electrophoresis, PCR, CryoEM

SELECTED PUBLICATIONS

Runrun Wu, Jeremy W Bakelar, Karl Lundquist, Zijian Zhang, Katie M Kuo, David Ryoo, Yui Tik Pang, Chen Sun, Tommi White, Thomas Klose, others (2021). Plasticity within the barrel domain of BamA mediates a hybrid-barrel mechanism by BAM. *Nature Communications*.

Karl Lundquist, Jeremy Bakelar, Nicholas Noinaj, James C Gumbart (2018). C-terminal kink formation is required for lateral gating in BamA. *Proceedings of the National Academy of Sciences*.

See full list of publications

EDUCATION

2012 – 2019	PhD, Physics	Georgia Institute of Technology, Atlanta, Georgia
2012 – 2019	BS, Physics	University of Michigan, Ann Arbor, Michigan