

Michelle Lynn Gill, PhD

Applied Research Manager, NVIDIA Virtual Cell Team

GitHub | LinkedIn | Personal Website

Overview

I am an Applied Research Manager on NVIDIA's Virtual Cell team. Our team uses data, deep learning, and HPC to develop models that simulate cellular states. My focus is on the benchmarks and development of supporting tools that help evaluate and improve these models.

Previously I was a Senior Machine Learning Engineer and Data Scientist at BenevolentAI and a member of Arthur Palmer's research group where I developed and applied nuclear magnetic resonance (NMR) spin relaxation experiments to understand how enzyme dynamics are critical to biological function.

Education

Ph.D., Molecular Biophysics & Biochemistry 2003–2006

Yale University, New Haven, CT

Thesis: Development of ^{205}Tl NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids

Advisors: J. Patrick Loria and Scott Strobel

M.Phil., Molecular Biophysics & Biochemistry 2001–2003

Yale University, New Haven, CT

B.S., Biochemistry 1997–2001

University of Kansas, Lawrence, KS

Highest Distinction and Honors (Summa Cum Laude)

Experience

Applied Research Manager, NVIDIA, Virtual Cell Team 2022–Present

Lead benchmarking efforts for virtual cell models, including internal and external collaborations

Developed benchmarking framework and tooling for model assessment and reproducibility

Collaboration with Chan Zuckerberg Initiative on cz-benchmarks for evaluating virtual cell models

Scientific Lead, BioNeMo, NVIDIA 2019–2023

R&D Manager and Scientific Lead for Clara Discovery, NVIDIA's platform for accelerating drug discovery

Developed BioNeMo for pre-training and fine tuning of large language models for cheminformatics and proteomics

Senior AI and Deep Learning Scientist, NVIDIA 2019–2023

Focused on proteomics including deep learning models to predict peptide spectral matches with >95% F1

Led team using GCNNs to predict molecular properties

Senior Data Scientist and Machine Learning Engineer,

2018-2019

BenevolentAI

Matrix factorization and GCNNs for drug mechanism importance in knowledge graphs

3D CNNs for ligand pose and affinity prediction

Senior Deep Learning Consultant, NVIDIA

2017-2018

Assisted clients in pharmaceutical and materials science in utilizing deep learning

Scientist, National Cancer Institute, NIH

2014-2016

Developed parallelized, compressed sensing methods for NMR data reconstruction

Postdoctoral Research Fellow, Columbia University, Department of Biochemistry and Molecular Biophysics

2008-2014

Demonstrated conformational selection in DNA methyltransferase AlkB

Developed multiple quantum NMR spin relaxation experiments

Advisor: Professor Arthur G. Palmer, III

Publications

S. Dicks, L. Heumos, S. Jimenez, P. Angerer, I. Gold, I. Virshup, F. Fischer, L. May, C. J. Nolet, M. Gill, M. Boerries, and F. Theis **"Accelerating single-cell analysis with GPU-enabled RAPIDS-singlecell"** In preparation (2025).

E. Sevgen, J. Moller, A. Lange, J. Parker, S. Quigley, J. Mayer, P. Srivastava, S. Gayatri, D. Hosfield, M. Korshunova, M. Livne, M. Gill, R. Ranganathan, A.B. Costa, and A.L. Ferguson **"ProT-VAE: Protein transformer variational autoencoder for functional protein design"** *Proceedings of the National Academy of Sciences* (2025).

P. St. John, D. Lin, P. Binder, M. Greaves, V. Shah, J. St. John, A. Lange, P. Hsu, R. Illango, A. Ramanathan, A. Anandkumar, D.H. Brookes, A. Busia, A. Mahajan, S. Malina, N. Prasad, S. Sinai, L. Edwards, T. Gaudet, C. Regep, M. Steinegger, B. Rost, A. Brace, K. Hippe, L. Naef, K. Kamata, G. Armstrong, K. Boyd, Z. Cao, H.Y. Chou, S. Chu, A. Santos Costa, S. Darabi, E. Dawson, K. Didi, C. Fu, M. Geiger, M. Gill, D.J. Hsu, G. Kaushik, M. Korshunova, S. Kothan-Hill, Y. Lee, M. Liu, M. Livne, Z. McClure, J. Mitchell, A. Moradzadeh, O. Mosafi, Y. Nashed, S. Paliwal, Y. Peng, S. Rabhi, F. Ramezanghorbani, D. Reidenbach, C. Ricketts, B.C. Roland, K. Shah, T. Shimko, H. Sirelkhatim, S. Srinivasan, A.C. Stern, D. Toczydlowska, S.P. Veccham, N.A.E. Venanzi, A. Vorontsov, J. Wilber, I. Wilkinson, W.J. Wong, E. Xue, C. Ye, X. Yu, Y. Zhang, G. Zhou, B. Zandstein, A. Chacon, P. Sohani, M. Stadler, C. Hundt, F. Zhu, C. Dallago, B. Trentini, E. Kucukbenli, T. Rvachov, E. Calleja, J. Israeli, H. Clifford, R. Haukioja, N. Haemel, K. Tretina, N. Tadimeti, and A.B. Costa

"BioNeMo Framework: a modular, high-performance library for AI model development in drug discovery" [arXiv](#) (2024).

M.T. Strauss, I. Bludau, W.F. Zeng, E. Voytik, C. Ammar, J. Schessner, R. Illango, [M.L. Gill](#), F. Meier, S. Willems, and M. Mann **"AlphaPept, a modern and open framework for MS-based proteomics"** [Nature Communications](#) (2024).

D. Reidenbach, M. Livne, R.K. Illango, [M.L. Gill](#), and J.I. Israeli **"Improving small molecule generation using mutual information machine"** [arXiv](#) (2022).

[M.L. Gill](#), A. Hsu, and A.G. Palmer **"Detection of chemical exchange in methyl groups of macromolecules"** [Journal of Biomolecular NMR](#) (2019).

[M.L. Gill](#), R.A. Byrd, and A.G. Palmer **"Dynamics of GCN4 facilitate DNA interaction: a model-free analysis of an intrinsically disordered region"** [Physical Chemistry and Chemical Physics](#) (2016).

S. Sun, [M.L. Gill](#), Y. Li, M. Huang, and R.A. Byrd **"Efficient and generalized processing of multidimensional NUS NMR data: the NESTA algorithm and comparison of regularization terms"** [Journal of Biomolecular NMR](#) (2015).

B. Ergel, [M.L. Gill](#), L. Brown, B. Yu, A.G. Palmer, and J.F. Hunt **"Protein dynamics control the progression and efficiency of the catalytic reaction cycle of AlkB"** [Journal of Biological Chemistry](#) (2014).

[M.L. Gill](#), and A.G. Palmer **"Local isotropic diffusion approximation for coupled internal and overall molecular motions in NMR spin relaxation"** [Journal of Physical Chemistry B](#) (2014).

[M.L. Gill](#), and A.G. Palmer **"Multiplet-filtered and gradient-selected zero-quantum TROSY experiments for $^{13}\text{C}^1\text{H}_3$ methyl groups in proteins"** [Journal of Biomolecular NMR](#) (2011).

Patents	Automated FEP Path Generation and Optimization by Molecule Foundation Models and Generative AI	2025
	Peng, Y., Kucukbenli, E., Zhou, G., Gill, M.L. , Livne, M., Korshunova, M., Rvachov, T., Israeli, Y. US Patent Application No. 19/208,119; Filing Date: 2025/05/14	
	Extraction of Informative Embeddings from Encoder-Decoder Models	2024
	Livne, M., Gill, M.L. US Patent Application No. 18/957,301; Filing Date: 2024/11/22	
	Contrastive Framework for Unified Generative and Discriminative Representation Learning	2024
	Livne, M., Gill, M.L. US Patent Application No. 18/957,294; Filing Date: 2024/11/22	
	Efficient Data Loading for Deep Learning Workloads	2024

Darabi, S., Korshunova, M., Grewal, J., [Gill, M.L.](#), Morkisz, P.
US Patent Application No. 18/885,428; Filing Date: 2024/09/13

Guardrails for Molecular Generation 2024

Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., [Gill, M.L.](#), Kucukbenli, E., Israeli, Y.
US Patent Application No. 18/807,805; Filing Date: 2024/08/16

End to End Deep Learning Workflow for In Silico Molecule Design 2024

Stern, A., [Gill, M.L.](#), Stepniewska-Dziubinska, M., Grzegorzec, T., Nowaczynski, A.,
Toczydlowska, D., Israeli, Y., Ribalta Lorenzo, P.
US Patent Application No. 18/412,168; Filing Date: 2024/01/12

Small Molecule Generation Using Machine Learning Models 2023

Livne, M., Reidenbach, D., [Gill, M.L.](#), Ilango, R., Israeli, Y.
US Patent Application No. 18/450,745; Filing Date: 2023/08/16

Presentations

Scientific Discovery: From the Lab Bench to the GPU, Andy Byrd 2024
Retirement Symposium

Invited Keynote, April 19, 2024, Institute for Bioscience & Biotechnology Research,
University of Maryland, NIST, Bethesda, MD
[Slides](#) · [Program](#)

Scientific Discovery: From the Lab Bench to the GPU, PyData NYC 2023
Invited Keynote, November 2, 2023, New York, NY
[Slides](#) · [Video](#) · [Abstract](#)

NVIDIA BioNeMo: A framework and service for development and use of generative AI in drug discovery, 6th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry Conference 2023
Invited Keynote, September 5, 2023, Cambridge, UK
[Slides](#) · [Program](#)

Exploring Molecular Space and Accelerating Drug Discovery on the GPU with Clara Discovery, Gates Foundation Grand Challenges: Applications of Artificial Intelligence in Machine Learning 2021
Invited Talk, November 10, 2021, Virtual

Accelerating Drug Discovery with Clara Discovery and MegaMolBART, 4th RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry 2021
Invited Talk, September 27, 2021, Virtual
[Slides](#)

Real Time, GPU-Accelerated Analysis and Visualization in the Life Sciences, Ken Kennedy Institute Data Science Conference 2020
[Michelle Gill](#) and Avantika Lal
Invited Keynote, October 26-27, 2020, Virtual
[Slides](#) · [Abstract](#) · [Program](#)

Artificial intelligence driven drug discovery , NYC R Conference	2019
Invited Presentation, May 10, 2019, New York, NY	
Slides	
Machine learning for target identification and lead optimization in drug discovery , New York Area Group for Informatics and Modeling	2019
Alix Lacoste and Michelle Gill	
Invited Presentation, February 26, 2019, New York, NY	
Abstract	
Accelerating the journey from data to medicine , NeurIPS	2018
Amir Saffari, Dan Neil, Alix Lacoste, and Michelle Gill	
Expo Talk, 2018, Montreal, Canada	
Abstract	
Artificial intelligence as a catalyst for scientific discovery , JupyterCon	2018
Invited Keynote, 2018, New York, NY	
Slides · Video · Abstract	
From structural biology to AI: a holistic approach to studying molecular machines , Brookhaven National Laboratory	2018
Invited Presentation, 2018, Upton, NY	
Slides	
Efficient image search and identification: the making of Wine-O.AI , SciPy Conference	2017
Selected Presentation, 2017, Austin, TX	
Slides · Video · Code	
Development of ^{205}Tl NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids , Ph.D. Thesis Defense, Yale University	2006
Thesis Defense, 2006, New Haven, CT	
Slides · Thesis	

Awards	NIH Postdoctoral Research Fellowship (F32 GM089047)	2009-2012
	Global BCG Strategy Olympics, Winning Team	2007
	NSF Graduate Research Fellowship	2002-2006
	Barry M. Goldwater Scholar	2000-2001
	Outstanding Undergraduate Honors Research Thesis	2001
	Kansas Board of Regents Full Tuition Merit Scholarship	1997-2001

Service

Judge, Preliminary and Final Rounds , NYC STEM Fair, New York, NY Evaluated submissions in the biochemistry track	2022
Program Chair , PyData NYC, New York, NY Responsible for conference content, proposal review, speaker selection, and scheduling	2018
Machine Learning Symposium Co-Chair , SciPy Conference, Austin, TX Co-chair of machine learning / deep learning symposium	2018