Michelle Lynn Gill

R&D Manager, NVIDIA Virtual Cell Team

GitHub | LinkedIn | Personal Website

Currently

I am an R&D 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 205Tl 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, BenevolentAI 2018-2019
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

Senior Data Scientist, Metis 2016-2017
Co-instructed 12-week data science bootcamps
Developed 12-week machine learning course for F100 company

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

Consultant, The Boston Consulting Group 2006-2007
Worked with clients in finance and pharmaceutical sectors
Part of winning team for 2007 Global BCG Strategy Olympics

Publications

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

Sevgen, E., Moller, J., Lange, A., Parker, J., Quigley, S., Mayer, J., Srivastava, P., Gayatri, S., Hosfield, D., Korshunova, M., Livne, M., Gill, M., Ranganathan, R., Costa, A.B., Ferguson, A.L.. "ProT-VAE: Protein transformer variational autoencoder for functional protein design." **Proceedings of the National Academy of Sciences** 122 (2025), doi: 10.1073/pnas.2408737122.

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

"BioNeMo Framework: a modular, high-performance library for AI model development in drug discovery." **arXiv** (2024), doi: 10.48550/arXiv.2411.10548.

Strauss, M.T., Bludau, I., Zeng, W.F., Voytik, E., Ammar, C., Schessner, J., Illango, R., Gill, M.L., Meier, F., Willems, S., Mann, M.. "AlphaPept, a modern and open framework for MS-based proteomics." **Nature Communications** 15 (2024), doi: 10.1038/s41467-024-46485-4.

Gill, M.L.. "The rise of the machines in chemistry." **Magnetic Resonance in Chemistry** 60, 1044–1051 (2022), doi: 10.1002/mrc.5304.

Reidenbach, D., Livne, M., Illango, R.K., Gill, M.L., Israeli, J.I.. "Improving small molecule generation using mutual information machine." **arXiv** (2022), doi: 10.48550/arXiv.2208.09016.

Gill, M.L., Hsu, A., Palmer, A.G.. "Detection of chemical exchange in methyl groups of macromolecules." **Journal of Biomolecular NMR** 73, 443–450 (2019), doi: 10.1007/s10858-019-00240-w.

Tong, M., Pelton, J., Gill, M.L., Zhang, W., Picart, F., Seeliger, M.. "Survey of solution dynamics in Src kinase reveals cross talk between the ligand binding and regulatory sites." **Nature Communications** 8, 2160 (2017), doi: 10.1038/s41467-017-02240-6.

Gill, M.L., Byrd, R.A., Palmer, A.G.. "Dynamics of GCN4 facilitate DNA interaction: a model-free analysis of an intrinsically disordered region." **Physical Chemistry and Chemical Physics** 18, 5839–5849 (2016), doi: 10.1039/c5cp06197k.

Sun, S., Gill, M.L., Li, Y., Huang, M., Byrd, R.A.. "Efficient and generalized processing of multidimensional NUS NMR data: the NESTA algorithm and comparison of regularization terms." **Journal of Biomolecular NMR** 62, 105–117 (2015), doi: 10.1007/s10858-015-9923-x.

Gill, M.L., Palmer, A.G.. "Local isotropic diffusion approximation for coupled internal and overall molecular motions in NMR spin relaxation." **Journal of Physical Chemistry B** 118, 11120–11128 (2014), doi: 10.1021/jp506580c.

Gill, M.L., Byrd, R.A.. "Dynamic activation of apoptosis: conformational ensembles of cIAP1 are linked to a spring-loaded mechanism." **Nature Structural Molecular Biology** 21, 1022–1023 (2014), doi: 10.1038/nsmb.2925.

Ergel, B., Gill, M.L., Brown, L., Yu, B., Palmer, A.G., Hunt, J.F.. "Protein dynamics control the progression and efficiency of the catalytic reaction cycle of AlkB." **Journal of Biological Chemistry** 289, 29584–29601 (2014), doi: 10.1074/jbc.M114.575647.

Gill, M.L., Palmer, A.G.. "Multiplet-filtered and gradient-selected zero-quantum TROSY experiments for 13C1H3 methyl groups in proteins." **Journal of Biomolecular NMR** 51, 245–251 (2011), doi: 10.1007/s10858-011-9533-1.

Ramsey, J.D., Gill, M.L., Kamerzell, T.J., Price, E.S., Joshi, S.B., Bishop, S.M., Oliver, C.N., Middaugh, C.R.. "Using empirical phase diagrams to understand the role of intramolecular dynamics in immunoglobulin

G stability." **Journal of Pharmaceutical Sciences** 98, 2432–2447 (2009), doi: 10.1002/jps.21619.

Gill, M.L., Strobel, S.A., Loria, J.P.. "Crystallization and characterization of the thallium form of the Oxytricha nova G-quadruplex." **Nucleic Acids Research** 34, 4506–4514 (2006), doi: 10.1093/nar/gkl616.

Beach, H., Cole, R., Gill, M.L., Loria, J.P.. "Conservation of μs-ms enzyme motions in the apo- and substrate-mimicked state." **Journal of the American Chemical Society** 127, 9167–9176 (2005), doi: 10.1021/ja0514949.

Gill, M.L., Strobel, S.A., Loria, J.P.. "205Tl NMR methods for the study of monovalent metal binding sites in nucleic acids." **Journal of the American Chemical Society** 127, 16723–16732 (2005), doi: 10.1021/ja055358f.

Adams, P.L., Stahley, M.R., Gill, M.L., Kosek, A.B., Wang, J., Strobel, S.A.. "Crystal structure of a group I intron splicing intermediate." **RNA** 12, 1867–1887 (2004), doi: 10.1038/nature02642.

Wiethoff, C.M., Gill, M.L., Koe, G.S., Koe, J.G., Middaugh, C.R.. "A fluorescence study of the structure and accessibility of plasmid DNA condensed with cationic gene delivery vehicles." **Journal of Pharmaceutical Sciences** 92, 1272–1285 (2003), doi: 10.1002/jps.10391.

Wiethoff, C.M., Gill, M.L., Koe, G.S., Koe, J.G., Middaugh, C.R.. "The structural organization of cationic lipid-DNA complexes." **Journal of Biological Chemistry** 277, 44980–44987 (2002), doi: 10.1074/jbc.M207758200.

Silchenko, S., Sippel, M.L., Kuchment, O., Benson, D.R., Mauk, A.G., Altuve, A., Rivera, M.. "Hemin is kinetically trapped in cytochrome b5 from rat outer mitochondrial membrane." **Biochemical and Biophysical Research Communications** 273, 467–472 (2000), doi: 10.1006/bbrc.2000.2968.

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

Guardrails for Conditional Molecular Generation 2024

Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y.
US Patent Application No. 18/807,808; Filing Date: 2024/08/16

Training-Time Guardrails for Molecular Generation 2024

Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y.
US Patent Application No. 18/807,811; Filing Date: 2024/08/16

Guardrails for Instruction-Tuned Molecular Generation 2024

Korshunova, M., Peng, Y., Zhou, G., Rvachov, T., Gill, M.L., Kucukbenli, E., Israeli, Y.
US Patent Application No. 18/807,814; 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., Grzegorzek, 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 Retirement Symposium 2024

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

Panel: Careers in data science, Tri-Institutional Career Symposium — 2019
April 9, 2019, Memorial Sloan Kettering Cancer Center, The Rockefeller University and Weill Cornell Medicine, New York, NY
Program

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 205Tl NMR methods for the direct study of monovalent metal ions and ligands in nucleic acids, Ph.D. Thesis Defense, Yale University — 2006
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 2022
Evaluated submissions in the biochemistry track

Program Chair, PyData NYC, New York, NY 2018
Responsible for conference content, proposal review, speaker selection, and scheduling

Machine Learning Symposium Co-Chair, SciPy Conference, Austin, TX 2018
Co-chair of machine learning / deep learning symposium

Proposal Reviewer, JupyterCon 2018

Reviewer, Journal of Open Source Software (JOSS) 2018-2019