ALEX MOREHEAD

Machine Learning & Computational Biology Researcher

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"Machine Learning & Computational Biology Researcher with over 5 years of experience developing cutting-edge deep learning algorithms for geometric (e.g., structural biology) data. Track record of bringing new ideas to life and implementing them using AI-standard programming languages/frameworks. Experienced leading research teams, fostering collaborations, and presenting research findings at top conferences."

SKILLS

Python | PyTorch | PyG | PyTorch Lightning | W&B | Hydra | Slurm | Git | LaTeX | Pandas | Java

Geometric deep learning | Generative modeling | Graph neural networks | AI4Science | CompBio/Chem

EXPERIENCE

Hopper Postdoctoral Fellow (Supervisor: Dr. Wahid Bhimji)

Lawrence Berkeley National Laboratory | NERSC

Jun 2025 – Ongoing | California, USA

Awarded Berkeley Lab's **2025 Hopper Postdoctoral Fellowship** in computing sciences, courtesy of NERSC.

- Research and develop deep generative models **for science**.
- Conduct **large-scale** deep learning HPC experiments and make contributions to **open-source code** along the way.

Deep learning | Generative models | AI4Science | CompBio/Chem

Graduate Research Assistant (Supervisor: Dr. Jianlin Cheng)

University of Missouri | Bioinformatics & Machine Learning Lab

Aug 2020 – May 2025 | Missouri, USA

Awarded two competitive first-year PhD fellowships and the **outstanding PhD** awards for EECS/CS graduate studies.

- Researched geometric and generative modeling methods for bioinformatics, yielding **20+ academic works**.
- Developed two state-of-the-art protein representation learning methods along with the first diffusion model to successfully generate valid large 3D molecules and flow model for blind protein-ligand docking. Published results at top-tier machine learning conferences (**ICLR**) and scientific venues (**ISMB** / **Bioinformatics**, **CASP16**, & **Nature Communications Chemistry**).
- Introduced the first deep learning benchmark for **broadly applicable** protein-ligand docking.
- Orchestrated several **large-scale** deep learning HPC experiments and contributed to **open-source code**.

Deep learning | Geometric & graph representation learning | Generative models | Structural bioinformatics

Research Intern (Supervisor: Dr. Jeffrey Ruffolo)

Profluent Bio | AI Research Lab

May 2023 – Aug 2023 | California, USA

- Created **MMDiff**, the first SE(3) diffusion model for joint sequence-structure generation of DNA, RNA, and proteins, which achieved a **9% nucleic acid design success rate**. Presented at NeurIPS 2023 MLSB. **Paper** and **Code**.

Diffusion models | Structure generation | Sequence generation | Differential geometry | Google Cloud

Research Intern (Supervisor: Joshua Meier)

Absci | AI Research Lab

Jun 2022 – Apr 2023 | New York, USA

- Collaboratively attained a **0.1%** *de novo* antibody binder design success rate using deep learning, **a first-of-its-kind result**. **Paper** and **Data**.

Protein design | Generative AI | Data science | Model prototyping & benchmarking | Kubernetes

MY LIFE PHILOSOPHY

"The cure to boredom is curiosity.
There is no cure for curiosity." - Dorothy Parker

ACHIEVEMENTS

Berkeley Lab's 2025 Hopper Postdoctoral Fellow
• Won a *competitive* postdoctoral fellowship for recent PhD graduates in computing sciences.

LoG Top-10 Reviewer
• Awarded large monetary prize for being a *top-3%* reviewer for the 2023 Learning on Graphs (LoG) conference.

Dean's Engineering Excellence & O'Neill Graduate Fellowships and Top-Ranked EECS/CS PhD Student Awards
• Won *two* competitive graduate fellowships for first-year PhD students and the *outstanding EECS & CS PhD student* awards.

Public outreach
• Research featured in *two* public-facing venues including HPCwire and Marktechpost.

INVITED TALKS

- FlowDock: Geometric Flow Matching for Protein-Ligand Docking and Affinity Prediction, 3DSIG @ ISMB, Jul 2025, Liverpool, UK
- Geometric Deep Learning and Generative Models For Protein-Ligand Docking, Computational modeling of molecular structures course @ MU, Nov 2024, Columbia, Missouri, USA
- RNA-FrameFlow for *de novo* 3D RNA backbone design, SPIGM @ ICML, Jul 2024, Vienna, AT
- A Gated Graph Transformer for Protein Complex Structure Quality Assessment, 3DSIG @ ISMB, Jul 2023, Lyon, FR
- Geometry-Complete Perceptron Networks for 3D Molecular Graphs, AI2ASE @ AAAI, Feb 2023, Washington D.C., USA
- Neural Diffusion Models: Next-Generation Generative Deep Learning, Advanced topics in deep learning course @ MU, Nov 2022, Columbia, Missouri, USA

EDUCATION

M.S. & Ph.D. in Machine Learning & Computational Biology

University of Missouri | O'Neill and College of Engineering Dean's Graduate Fellow

Aug 2020 - May 2025

PhD Topic:
- Geometric Deep Learning & Generative Modeling of 3D Biomolecules

Collaborations:
- University of Cambridge, Research Labs of Prof. Pietro Lió & Prof. Sir Tom Blundell

Coursework:
- Highest distinction (GPA=4.0/4.0)

B.S. in Computer Science

Missouri Western State University | General Studies and Outstanding Graduate Honors

Aug 2016 - May 2020

- Graduated **top of class** among all 2020 graduates in computer science, mathematics, and physics (GPA=4.0/4.0)

REFERENCES

Dr. Jianlin Cheng
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Dr. Dong Xu
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Dr. Xiaoqin Zou
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REVIEWING

- **Conferences**:
  - Neural Information Processing Systems (NeurIPS), also AI4Sci, AI4D3, GenBio, & MLSB workshops **[2021-…]**
  - International Conference on Learning Representations (ICLR), also GEM, AI4NA, and FPI workshops **[2024-…]**
  - International Conference on Machine Learning (ICML), also AI4Sci, CB, AccMLBio, & SPIGM workshops **[2024-…]**
    - Also served on the ICML 2024 ML4LMS workshop's organizing committee **[2024]**
  - Association for the Advancement of Artificial Intelligence (AAAI) **[2025]**
  - Learning on Graphs Conference (LoG) of PMLR **[2024-…]**, organizing comittee **[2024-2025]**
  - ACM Conference on Bioinformatics, Computational Biology, & Health Informatics (ACM BCB) **[2024-…]**
- **Journals:**
  - Nature Machine Intelligence & Nature Methods **[2023-…]**
  - Bioinformatics, Briefings in Bioinformatics, BMC Bioinformatics, JCIM, and CSB Journal **[2024-…]**
  - IEEE Trans. on Neural Nets. & Learning Systems (TNNLS) & Emerging Topics in Comp. Intell. (TETCI) **[2023-…]**

PUBLICATIONS

Conference Proceedings

[1] C. K. Joshi et al., "GRNAde: Geometric deep learning for 3d RNA inverse design," in *Thirteenth International Conference on Learning Representations (ICLR)*, Selected as an ICLR 2025 *spotlight*, 2025.

[2] **A. Morehead** and J. Cheng, "Flowdock: Geometric flow matching for generative protein-ligand docking and affinity prediction," in *Intelligent Systems for Molecular Biology (ISMB)*, Presented as a CASP16 top-5 method, 2025.

[3] A. R. Jamasb* et al., "Evaluating representation learning on the protein structure universe," in *Twelth International Conference on Learning Representations (ICLR)*, also presented at NeurIPS 2023 MLSB (poster), 2024.

[4] **A. Morehead**, N. Giri, J. Liu, and J. Cheng, "Deep learning for protein-ligand docking: Are we there yet?" In *ICML AI4Science Workshop*, presented as a *spotlight*, top 20% - 30/159, 2024.

[5] X. Chen*, **A. Morehead***, J. Liu, and J. Cheng, "A gated graph transformer for protein complex structure quality assessment and its performance in casp15," in *Intelligent Systems for Molecular Biology (ISMB)*, 2023.

[6] **A. Morehead**, A. Bhatnagar, J. A. Ruffolo, and A. Madani, "Towards joint sequence-structure generation of nucleic acid and protein complexes," in *NeurIPS Machine Learning in Structural Biology (MLSB) Workshop*, 2023.

[7] **A. Morehead**, W. Chantapakul, and J. Cheng, "Semi-supervised graph learning meets dimensionality reduction," in *IEEE International Conference on Machine Learning and Applications*, 2023.

[8] E. Soltanikazemi, R. S. Roy, F. Quadir, N. Giri, **A. Morehead**, and J. Cheng, "Drlcomplex: Reconstruction of protein quaternary structures using deep reinforcement learning," in *International Conference on Intelligent Biology and Medicine*, 2023.

[9] **A. Morehead**, C. Chen, and J. Cheng, "Geometric transformers for protein interface contact prediction," in *Tenth International Conference on Learning Representations (ICLR)*, 2022.

[10] M. Shoman, A. Aboah, **A. Morehead**, Y. Duan, A. Daud, and Y. Adu-Gyamfi, "A region-based deep learning approach to automated retail checkout," in *Proceedings of the IEEE/CVF CVPR Workshops*, 2022.

[11] M. Gao et al., "High-performance deep learning toolbox for genome-scale prediction of protein structure and function," in *IEEE/ACM Machine Learning with Graphs in High Performance Computing Environments (MLHPC) Workshop*, 2021.

[12] **A. Morehead**, L. Ogden, G. Magee, R. Hosler, B. White, and G. Mohler, "Low cost gunshot detection using deep learning on the raspberry pi," in *IEEE International Conference on Big Data*, 2019.

Journal Articles

[13] R. Anand* et al., "Rna-frameflow for de novo 3d rna backbone design," *Transactions on Machine Learning Research*, 2025, presented at ICML 2024 SPIGM (*oral*) and AI4Science (*spotlight*) workshops.

[14] A. A. Elhag, A. Raja, **A. Morehead**, S. M. Blau, G. M. Morris, and M. M. Bronstein, "Learning inter-atomic potentials without explicit equivariance," *arXiv*, 2025.

[15] H. La, A. Gupta, **A. Morehead**, J. Cheng, and M. Zhang, "Megafold: System-level optimizations for accelerating protein structure prediction models," *arXiv*, 2025.

[16] **A. Morehead**, "Geometric deep learning and generative modeling of 3d biomolecules," *University of Missouri-Columbia*, 2025, Ph.D. dissertation.

[17] **A. Morehead**, J. Liu, P. Neupane, N. Giri, and J. Cheng, "Protein-ligand structure and affinity prediction in casp16 using a geometric deep learning ensemble and flow matching," *Proteins: Structure, Function, and Bioinformatics*, 2025, Presented as a CASP16 top-5 method.

[18] **A. Morehead** et al., "How to go with the flow: Flow matching in bioinformatics and computational biology," *Authorea Preprints*, 2025.

[19] M. Pourmirzaei, **A. Morehead**, F. Esmaili, J. Ren, M. Pourmirzaei, and D. Xu, "Gcp-vqvae: A geometry-complete language for protein 3d structure," *bioRxiv*, pp. 2025–10, 2025.

[20] Z. Wang, A. Jamasb, M. Hajij, **A. Morehead**, L. Braithwaite, and P. Liò, "Topotein: Topological deep learning for protein representation learning," *arXiv*, 2025.

[21] **A. Morehead** and J. Cheng, "Geometry-complete diffusion for 3d molecule generation," *Nature Communications Chemistry*, 2024, also presented at ICLR 2023 MLDD (poster).

[22] **A. Morehead** and J. Cheng, "Geometry-complete perceptron networks for 3d molecular graphs," *Bioinformatics*, 2024, also presented at AAAI 2023 DLG (poster) and AI2ASE (*oral*).

[23] C. Chen, X. Chen, **A. Morehead**, T. Wu, and J. Cheng, "3d-equivariant graph neural networks for protein model quality assessment," *Bioinformatics*, 2023.

[24] M. F. Lensink et al., "Impact of alphafold on structure prediction of protein complexes: The casp15-capri experiment," *Proteins: Structure, Function, and Bioinformatics*, 2023.

[25] S. Mahmud, **A. Morehead**, and J. Cheng, "Accurate prediction of protein tertiary structural changes induced by single-site mutations with equivariant graph neural networks," *bioRxiv*, 2023.

[26] **A. Morehead**, C. Chen, A. Sedova, and J. Cheng, "Dips-plus: The enhanced database of interacting protein structures for interface prediction," *Nature Scientific Data*, 2023.

[27] **A. Morehead** and J. Cheng, "Protein structure accuracy estimation using geometry-complete perceptron networks," *Protein Science*, 2023.

[28] A. Shanehsazzadeh et al., "Unlocking de novo antibody design with generative artificial intelligence," *bioRxiv*, 2023, follow-up work presented at NeurIPS 2023 MLSB (poster).

[29] **A. Morehead**, X. Chen, T. Wu, J. Liu, and J. Cheng, "Egr: Equivariant graph refinement and assessment of 3d protein complex structures," *arXiv*, 2022.

[30] O. Kouckya et al., "Synthetic biology bicistronic designs support gene expression equally well in vitro and in vivo," *AJUR*, 2020.