Austin Clyde

Data Science and Learning Division
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 240
Lemont, IL 60439
Phone: (630) 252-3738
aclyde@anl.gov

Chicago, IL 60657
Phone: (585) 406-9146
aclyde11@gmail.com
austinclyde.com

RESEARCH INTERESTS

AI for science, high-performance computing, large language models, science and technology studies (STS).

EMPLOYMENT

Assistant Computational Scientist, Argonne National Laboratory   2022 to present
Research Assistant, Argonne National Laboratory   2019 to 2022
Desk Developer, Cryptocurrencies, XR Trading,   2018 to 2019

EDUCATION

University of Chicago

Ph.D. Computer Science   Expected December 2022
Thesis: *Artificial Intelligence and High-Performance Computing for Accelerating Structure-Based Drug Discovery*

M.S. Computer Science   June 2019

B.A. Mathematics   June 2019

FELLOWSHIPS

Visiting Research Fellow, Science, Technology, and Society, Harvard Kennedy School   2021 to 2022

AWARDS AND RECOGNITION

- **Pozen Family Center for Human Rights Graduate Lectureship** '22
  The Pozen Center awards up to three lectureships per academic year to advanced doctoral students, each of whom teaches one undergraduate Human Rights course of their design.
- **Special recognition in Department of Energy Secretary's Honor Award** for COVID-19 Research '21.
  Annual award recognizing DOE employees and contractors for their service and contributions to the Department's mission and the benefit of the Nation.
- **ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research** '20 and finalist '21.
  Gordon Bell Prize, commonly referred to as the 'Nobel Prize' of supercomputing, is awarded each year to recognize outstanding achievement in high-performance computing.
- **Impact Argonne Award** for Discovery '20 and for Innovation '20.
  Internal Argonne Award for the first sighting of new knowledge which appears to lead the way to finding more knowledge (development of drug screening pipeline), and for the initial development of a new concept (reinforcement learning for drug discovery).

GRANTS

Active Grants (PI)

9/22 – 5/24
Title: "Finding Ligands Targeting the Conserved RNA Binding Site of SARS-CoV-2 NSP13"
Principal Investigator: **Austin Clyde**
Funder: CACHE (Critical Assessment of Computational Hit-finding Experiments) Challenge 2
Total Direct Costs: $31,500

12/21 – 10/23
Title: "Predict Hits for the WDR Domain of LRRK2"
Principal Investigator: **Austin Clyde**
Funder: CACHE (Critical Assessment of Computational Hit-finding Experiments) Challenge 1
Total Direct Costs: $31,500

Active Grants *(Non-PI)*

1/22 – 12/25	*Title:* "IMPROVE: Innovative Methodologies and New Data for Predictive Oncology Model Evaluation"
	Principal Investigators: Rick Stevens
	Funder: National Cancer Institute
	Total Annual Direct Costs: $2,400,00
	Role: Key personnel, author of milestones

4/22 – 9/23   *Title:* "Autonomous Discovery for Science"
Principal Investigators: Thomas Brettin
Funder: Argonne National Laboratory Directed Research and Development
Total Annual Direct Costs: $1,700,000
Role: Key personnel, author of milestones

6/20 – 6/23   *Title:* "AI-driven Data Integration, Inference and Multi-scale Modeling Approaches to Low-dose Radiation Effects Understanding (RadBio-AI-3)"
Principal Investigators: Rick Stevens (Argonne), Anuj Kapadia (Oak Ridge), Francis Alexander (Brookhaven)
Funder: Office of Science, Department of Energy
Total Annual Direct Costs: $5,000,000, Argonne: $2,000,000
Role: Key personnel, author of Argonne milestones

9/18 – 9/24   *Title:* "Virtual Drug Response Prediction"
Principal Investigator: Rick Stevens
Funder: Argonne Leadership Computing Facility, Department of Energy
Total Annual Direct Costs: Computing time
Role: Key personnel, author of Argonne milestones

PUBLICATIONS

In Preparation

5. **Protein-Ligand Docking Surrogate Models: A SARS-CoV-2 Benchmark for Deep Learning Accelerated Virtual Screening**
Austin Clyde, et al.

4. **The Black Box Civic Epistemology: AI Senselessness and Democratic Participation**
Austin Clyde.

3. **Uncertainty Calibrated Cancer Drug-Response Prediction**
Austin Clyde, et al.

2. **Accelerating COVID-19 Drug Discovery with High-Performance Computing**
Austin Clyde, to appear in *High Performance Computing (HPC) for Drug Discovery and Biomedicine* (ed. Heifetz).

1. **Human Rights and AI for Science**
Austin Clyde.

Peer-reviewed Journals

9. **Scaffold-Induced Molecular Graph (SIMG): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery**
Austin Clyde, et al.
BMC Bioinformatics.

8. **Intelligent Resolution: Integrating Cryo-EM with AI-driven Multi-resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action**
Anda Trifan, Defne Gorgun, Zongyi Li, Alexander Brace, Maxim Zvyagin, Heng Ma, **Austin Clyde**, et al.
The International Journal of High Performance Computing (to appear); Finalist for Gordon Bell Special Prize for HPC-Based COVID-19 Research '21.

7. **#COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol**
Abigail Dommer, Lorenzo Casalino, Fiona Kearns, Mia Rosenfeld, Nicholas Wauer, Surl-Hee Ahn, John Russo, Sofia Oliveira, Clare Morris, Anthony Bogetti, Anda Trifan, Alexander Brace, Terra Sztain, **Austin Clyde**, et al.
The International Journal of High Performance Computing (to appear); Finalist for Gordon Bell Special Prize for HPC-Based COVID-19 Research '21.

6. **High Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Non-Covalent Inhibitor**
Austin Clyde, et al.
Journal of Chemical Informatics 2022 (front cover).

5. **Structural, electronic and electrostatic determinants for inhibitor binding to subsites S1 and S2 in SARS-CoV-2 main protease**
Daniel Kneller, Hui Li, Stephanie Galanie, Gwyndalyn Phillips, Audrey Labbe, Kevin Weiss, Qiu Zhang, Mark Arnould, **Austin Clyde**, et al.
Journal of Medicinal Chemistry 2021 (appeared as supplemental cover).

4. **A cross-study analysis of drug response predictions in cancer cell lines**
Fangfang Xia, Jonathan Allen, Prasanna Balaprakash, Thomas Brettin, Cristina Garcia-Cardona, **Austin Clyde**, et al.
Briefings in Bioinformatics 2021.

3. **Pandemic Drugs at Pandemic Speed: Accelerating COVID-19 Drug Discovery with Hybrid Machine Learning-and Physics-based Simulations on High Performance Computers**
Agastya Bhati, Shunzhou Wan, Dario Alfè, **Austin Clyde**, et al.
Interface Focus 2021.

2. **AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics.**
Lorenzo Casalino, Abigail C Dommer, Zied Gaieb, Emilia P Barros, Terra Sztain, Surl-Hee Ahn, Anda Trifan, Alexander Brace, Anthony T Bogetti, **Austin Clyde**, et al.
The International Journal of High-Performance Computing Applications, Gordon Bell Special Prize for HPC-Based COVID-19 Research '20.

1. **Learning Curves for Drug Response Prediction in Cancer Cell Lines**
Alexander Partin, Thomas Brettin, Yvonne A Evrard, Yitan Zhu, Hyunseung Yoo, Fangfang Xia, Songhao Jiang, **Austin Clyde**, et al.
BMC Bioinformatics 2021.

Conference Proceedings

8. **Spatial Graph Attention and Curiosity-driven Policy for Antiviral Drug Discovery**
Yulun Wu, Nicholas Choma, Andrew Chen, Mikaela Cashman, Érica T Prates, Manesh Shah, Verónica G Melesse Vergara, **Austin Clyde**, et al.
The 10th International Conference on Learning Representations (ICLR) 2022.

7. **Autodock on Enamine Hit Locator Library and Drugbank**
Hubertus van Dam, Martin Purschke, Dean Hidas, Oleg Tchoubar, Maksim Rakitin, Xiaohui Qu, **Austin Clyde**, et al.
IEEE Healthcare Summit Data Hackathon 2021.

6. **IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads**
Aymen Al Saadi, **Austin Clyde**, et al.
50th International Conference on Parallel Processing (ICPP 21).

5. **Stream-AI-MD: Streaming AI-driven Adaptive Molecular Simulations for Heterogeneous Computing Platforms**

Alexander Brace, Michael Salim, Vishal Subbiah, Heng Ma, Murali Emani, Anda Trifan, **Austin Clyde**, et al.
Platform for Advanced Scientific Computing (PASC '21).

4. **Scalable HPC and AI Infrastructure for COVID-19 Therapeutics" in the Platform for Advanced Scientific Computing**
Hyungro Lee, Andre Merzky, Li Tan, Mikhail Titov, Matteo Turilli, Dario Alfe, Agastya Bhati, Alex Brace, **Austin Clyde**, et al.
Platform for Advanced Scientific Computing (PASC '21).

3. **Targeting SARS-CoV-2 with AI-and HPC-enabled lead generation: a first data release**
Yadu Babuji, Ben Blaiszik, Tom Brettin, Kyle Chard, Ryan Chard, Austin Clyde, et al.
Platform for Advanced Scientific Computing (PASC '21).

2. **Benchmarking Machine Learning Workloads in Structural Bioinformatics Applications**
Heng Ma, **Austin Clyde**, et al.
First International Workshop on Benchmarking Machine Learning Workloads on Emerging Hardware '20.

1. **Virtual screening with deep learning using cancer cell line dose-response data**
Austin Clyde, et al.
American Association for Cancer Research '20.

Workshops

5. **Scaffold embeddings: Learning the structure spanned by chemical fragments, scaffolds and compounds**
Austin Clyde, et al.
NeurIPS Workshop on Learning Meaningful Representation of Life '21.

4. **Created in our Likeness: Is Open-Source AI at Odds with Animal Rights?**
Austin Clyde
MANCEPT Workshop on Politics, Animals, and Technology '21.

3. **Scaffold-Induced Molecular Graph (SIMG): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery**
Austin Clyde, et al.
Sixth Computational Approaches to Cancer Workshop at Supercomputing '20.

2. **Integrating High-Performance Simulations and Learning toward Improved Cancer Therapy**
Austin Clyde, et al.
Fifth Computational Approaches to Cancer Workshop at Supercomputing '19.

1. **Combining molecular simulation and machine learning to INSPIRE improved cancer therapy**
David Wright, Adrian Devitt-Lee, **Austin Clyde**, et al.
CompBioMed Conference '19.

Book Chapters

2. **Large Language Models for Science**
Austin Clyde, Arvind Ramanathan, Rick Stevens
Forthcoming in *AI for Science.*

1. **Ultrahigh Throughput Protein–Ligand Docking with Deep Learning**
Austin Clyde
Artificial Intelligence in Drug Design, Methods in Molecular Biology. Springer, New York, NY, 2022.

Inventions and Patents

1. **RLMM: Reinforcement Learning for Molecular Mechanics**
Austin Clyde, Arvind Ramanathan, Rick Stevens
ANL-IN-20-123, patent filed.

Pre-prints

4. **Open Science Discovery of Oral Non-Covalent SARS-CoV-2 Main Protease Inhibitor Therapeutics**
   COVID Moonshot Consortium.

3. **COVID Moonshot: Open Science Discovery of SARS-CoV-2 Main Protease Inhibitors by Combining Crowdsourcing, High-Throughput Experiments, Computational Simulations, and Machine Learning**
   COVID Moonshot Consortium.

2. **Regression enrichment surfaces: a simple analysis technique for virtual drug screening models.**
   Austin Clyde, et al.

1. **A Systematic Approach to Featurization for Cancer Drug Sensitivity Predictions with Deep Learning**
   Austin Clyde, et al.

Public Opinion Pieces

3. **Algorithmic Systems Designed to Reduce Polarization Could Hurt Democracy, Not Help It**
   Tech Policy Press '22.

2. **AI for science and global citizens**
   Patterns, Cell Press '22.

1. **Human-in-the-Loop Systems Are No Panacea for AI Accountability**
   Tech Policy Press '21.

Short Stories

1. **MyMuse**
   Future Humans: An Anthology

Presentations and Invited Talks

23. **AI for Science: Drug Design**
    ALCF Intro to AI-Driven Science Training, Chicago, 2022.

22. **Safeguarding Information Integrity**
    Harvard Data Science Institute Trust in Science Workshop, Boston, 2022.

21. **Realigning Deep Learning with Virtual Ligand Screening**
    AI-Driven Drug Discovery Summit, Boston, 2022.

20. **AI and Biology: A 100 Year History & AI-Driven Drug Discovery as an Emerging Technology**
    Non-Proliferation Emerging Technology Seminar Series, Depts. of Commence and Energy, 2022.

19. **The Boundaries of AI Ethics in American Undergraduate Computer Science Education**
    Science and Democracy Network, Harvard Kennedy School, Boston, 2022.

18. **Sharing What's Possible, Not Just What's Done**
    Democratizing HPC for Science, Platform for Advanced Scientific Computing, Basel, 2022.

17. **End-to-End Computational Drug Design for COVID-19: From Screening to Series and Back Again**
    CompBioMed2 Workshop, Rome, 2022.

16. **Automating Biological Discoveries at Scale**
    ISC High Performance, Hamburg, 2022

15. **The Demos and the Expert: On Techniques of Self-Rule**
    Night of Ideas, French Embassy and Harvard University, 2022.

14. **Throwing Away the Mirror: Why Algorithmic Disgorgement is an Epistemic Rights Violation**
    A Right to Truth? Information, Communication, and Democracy in the 21st Century, HKS, 2022.

13. **How Does AI Change the Ethics of Synthetic Biology?**
    Convergence of SynBio and Data Science: *Prospects, Promise and Perils*, Northwestern University, 2022.

12. **AI and Democracy**
    University of Chicago Department of Computer Science Student Seminar 2021.

11. **The Human-in-the-Loop Learning Fallacy**
    Harvard Kennedy School STS Fellows 2021.

10. **Virtual Screening with Deep Learning: Understanding Speed and Accuracy in Context**
    Frontline Genomics Webinar 2021.

9. **AI for Drug Discovery**
   ATOM Consortium, June 2021.

8. **Panelist**
   Intellectual Property Management: A Seminar Series, Argonne National Laboratory 2021.

7. **Ensemble Models and Consensus Scoring for Computational Docking**
   National Virtual Biotechnology Laboratory Seminar 2021.

6. **Integrating Simulations and Learning Towards Improved Cancer Therapy**
   CompBioMed Webinar 2020.

5. **Tiered BFE Estimation Workflow**
   CompBioMed Conference 2020.

4. **Accelerating Virtual Docking Screens with Deep Learning**
   Janssen Pharmaceuticals Seminar 2020.

3. **Virtual Drug Screening with Deep Learning**
   NIH.AI Workshop on Applications of Machine Learning for NGS and Drug Data 2019.

2. **Computational Drug Discovery at Scale**
   ComBioMed Kick-off meeting 2019.

1. **Molecule Generation, Search, and Optimization**
   ATOM Technical Meeting 2019.

TEACHING

1. **AI, Algorithms, and Human Rights** (HMRT 23450, CMSC 10450, MAAD 13450)
   Instructor, Fall 2022
   Awarded Pozen Family Center for Human Rights Graduate Lectureship, University of Chicago
   Cross-listed in Computer Science and Media Arts and Design.

2. **Introduction to Computer Science II** (C/C++) (CMSC 15200)
   Instructor, Summer 2021
   Department of Computer Science, University of Chicago.

3. **Reinforcement Learning for Drug Discovery Practicum** (MPCS 57010)
   Instructor, Spring 2020
   University of Chicago Master's Program in Computer Science.

4. **Computational Thinking** (CAAP)
   Instructor, Summer 2022, 2021 & 2020
   University of Chicago Academic Achievement Program.

5. **Machine Learning in Biology and Medicine** (CMSC 35440)
   Graduate Teaching Assistant, Fall 2019
   University of Chicago.

TRAINING, MENTORING, AND ADVISING

1. Max Zvyagin, post-bac student at ANL, deep learning for discovery.

2. Ryien Hosseini, master's student, deep learning for discovery.
3. Bharat Kale, Ph.D. student, chemical informatics, and visualization.

SERVICE AND OUTREACH

- Organizer for South by Southwest Panel on the Future Faces of AI, on DEI and equity in AI.
- Organizer of AI and human rights workshop series between University of Chicago's Pozen Family Center for Human Rights and Harvard Kennedy School's Program on Science, Technology, and Society.
- Advisor, SEED AI.
- Organizer, panel, AI Across America with first-generation low-income students along with members of the congressional AI Caucus and technology company executives.
- Co-host of Science Technology and Society Podcast for New Books Network
- Organizer, minisymposium titled "Democratizing AI" at Platform for Advanced Scientific Computing (PASC '22).
- Reviewer for Cell Patterns (2021, 2022), NeurIPS workshop on Machine Learning and the Physical Sciences (2021, 2022), NeurIPS dataset and benchmark track (2022), ICML (2022)
- Volunteer, Hour of Code, December 2018.
- Panelist, Socioeconomic Diversity Summit, University of Chicago, 2018.
- Member, Association for Computing Machinery (ACM).