Austin Clyde

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RESEARCH INTERESTS
Intersection of AI and "Science," drug discovery, representation learning, democracy and science

EDUCATION
PhD in Computer Science (in progress) – University of Chicago (advisor: Rick Stevens)
MS in Computer Science, June 2019 – University of Chicago
BA in Mathematics, June 2019 – University of Chicago

POSITIONS
Research Scientist RD I, Argonne National Laboratory, Data Science and Learning Division, 2019 to Present

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

AWARDS AND RECOGNITION
- Recognition in the Secretary's Honor Awards for Department of Energy National Virtual Biotechnology Laboratory for COVID-19 effort (May 2021)
- ACM Gordon Bell Prize Special Prize for High Performance Computing-Based COVID-19 Research (November 2020)
- Impact Argonne Award (2) (June 2020, August 2020

PUBLICATIONS
In-review, Journals
Austin Clyde, Thomas Brettin, Alexander Partin, Hyunseung Yoo, Yadu Babuji, Ben Blaiszik, Andre Merzky, Matteo Turilli, Shantenu Jha, Arvind Ramanathan, Rick Stevens, "Protein-Ligand Docking Surrogate Models: A SARS-CoV-2 Benchmark for Deep Learning Accelerated Virtual Screening." (In Review, June 2021).

Austin Clyde, Ashka Shah, Max Zvyagin, Arvind Ramanathan, Rick Stevens, "Scaffold-Induced Molecular Graph (SIMG): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery." (In review 2021).

Peer-reviewed Journals
Anda Trifan, Defne Gorgun, Zongyi Li, Alexander Brace, Maxim Zvyagin, Heng Ma, **Austin Clyde**, David A Clark, Michael Salim, David Hardy, Tom Burnley, Lei Huang, John McCalpin, Murali Emani, Hyunseung Yoo, Junqi Yin, Aristeidis Tsaris, Vishal Subbiah, Jessica Liu, Noah Trebesch, Geoffrey Wells, Venkatesh Mysore, Tom Gibbs, James Phillips, S Chakra Chennubhotla, Ian Foster, Rick Stevens, Anima Anandkumar, Venkatram Vishwanath, John E Stone, Emad Tajkhorshid, Sarah A Harris, Arvind Ramanathan. Intelligent Resolution: Integrating Cryo-EM with AI-driven Multi-resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action. Finalist for Gordon Bell Special Prize for HPC-Based COVID-19 Research 2021 (to appear, *The International Journal of High Performance).*

Daniel Kneller, Hui Li, Stephanie Galanie, Gwyndalyn Phillips, Audrey Labbe, Kevin Weiss, Qiu Zhang, Mark Arnould, **Austin Clyde**, Heng Ma, Arvind Ramanathan, Marti Head, Coates, John M. Louis, Peter Bonnesen, Andrey Kovalevsky, "Structural, electronic and electrostatic determinants for inhibitor binding to subsites S1 and S2 in SARS-CoV-2 main protease." Journal of Medicinal Chemistry (October 2021)

Austin Clyde, Stephanie Galanie, Daniel W Kneller, Heng Ma, Yadu Babuji, Ben Blaiszik, Alexander Brace, Thomas Brettin, Kyle Chard, Ryan Chard, Leighton Coates, Ian Foster, Darin Hauner, Vilmos Kertesz, Neeraj Kumar, Hyungro Lee, Zhuozhao Li, Andre Merzky, Jurgen G Schmidt, Li Tan, Mikhail Titov, Anda Trifan, Matteo Turilli, Hubertus Van Dam, Srinivas C Chennubhotla, Shantenu Jha, Andrey Kovalevsky, Arvind Ramanathan, Marti Head, Rick Stevens, "High Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Non-Covalent Inhibitor" in Journal of Chemical Informatics (October 2021).

Agastya P Bhati, Shunzhou Wan, Dario Alfè, **Austin R Clyde**, Mathis Bode, Li Tan, Mikhail Titov, Andre Merzky, Matteo Turilli, Shantenu Jha, Roger R Highfield, Walter Rocchia, Nicola Scafuri, Sauro Succi, Dieter Kranzlmüller, Gerald Mathias, David Wifling, Yann Donon, Alberto Di Meglio, Sofia Vallecorsa, Heng Ma, Anda Trifan, Arvind Ramanathan, Tom Brettin, Alexander Partin, Fangfang Xia, Xiaotan Duan, Rick Stevens, Peter V Coveney. "Pandemic Drugs at Pandemic Speed:

Accelerating COVID-19 Drug Discovery with Hybrid Machine Learning-and Physics-based Simulations on High Performance Computers." *Interface Focus.* (October 2021).

Lorenzo Casalino, Abigail C Dommer, Zied Gaieb, Emilia P Barros, Terra Sztain, Surl-Hee Ahn, Anda Trifan, Alexander Brace, Anthony T Bogetti, **Austin Clyde**, Heng Ma, Hyungro Lee, Matteo Turilli, Syma Khalid, Lillian T Chong, Carlos Simmerling, David J Hardy, Julio DC Maia, James C Phillips, Thorsten Kurth, Abraham C Stern, Lei Huang, John D McCalpin, Mahidhar Tatineni, Tom Gibbs, John E Stone, Shantenu Jha, Arvind Ramanathan, Rommie E Amaro. AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. *The International Journal of High Performance Computing Applications* (May 2021). 2021. Winner of Gordon Bell Special Prize for HPC-Based COVID-19 Research 2020.

Alexander Partin, Thomas Brettin, Yvonne A Evrard, Yitan Zhu, Hyunseung Yoo, Fangfang Xia, Songhao Jiang, **Austin Clyde**, Maulik Shukla, Michael Fonstein, James H Doroshow, Rick Stevens, "Learning Curves for Drug Response Prediction in Cancer Cell Lines," in *BMC Bioinformatics* (May 2021).

Conference Proceedings

Hubertus van Dam, Martin Purschke, Dean Hidas, Oleg Tchoubar, Maksim Rakitin, Xiaohui Qu, **Austin Clyde**, Arvind Ramanathan, Rick Stevens. "Autodock on Enamine Hit Locator Library and Drugbank." Provided data for conference attendees to utilize during hackathon. 2021 IEEE Healthcare Summit Data Hackathon. (October 2021)

Aymen Al Saadi, **Austin Clyde**, Dario Alfe, Yadu Babuji, Agastya Bhati, Ben Blaiszik, Thomas Brettin, Kyle Chard, Ryan Chard, Peter Coveney, Anda Trifan, Alex Brace, Ian Foster, Tom Gibbs, Shantenu Jha, Kristopher Keipert, Thorsten Kurth, Dieter Kranzlmüller, Hyungro Lee, Zhuozhao Li, Heng Ma, Andre Merzky, Gerald Mathias, Alexander Partin, Junqi Yin, Arvind Ramanathan, Ashka Shah, Abraham Stern, Rick Stevens, Li Tan, Mikhail Titov, Aristeidis Tsaris, Matteo Turilli, Huub Van Dam, Shunzhou Wan, David Wifling, "IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads" at 50th International Conference on Parallel Processing (ICPP). (August 2021).

Alexander Brace, Michael Salim, Vishal Subbiah, Heng Ma, Murali Emani, Anda Trifan, **Austin Clyde**, Corey Adams, Thomas Uram, Hyunseung Yoo, Andrew Hock, Jessica Liu, Venkatram Vishwanath, Arvind Ramanathan, "Stream-AI-MD: Streaming AI-driven Adaptive Molecular Simulations for Heterogeneous Computing Platforms" in the Platform for Advanced Scientific Computing (PASC '21). (July 2021).

Hyungro Lee, Andre Merzky, Li Tan, Mikhail Titov, Matteo Turilli, Dario Alfe, Agastya Bhati, Alex Brace, **Austin Clyde**, Peter Coveney, Heng Ma, Arvind Ramanathan, Rick Stevens, Anda Trifan, Hubertus Van Dam, Shunzhou Wan, Sean Wilkinson, Shantenu Jha, "Scalable HPC and AI Infrastructure for COVID-19 Therapeutics" in the Platform for Advanced Scientific Computing (PASC '21). (July 2021).

Yadu Babuji, Ben Blaiszik, Tom Brettin, Kyle Chard, Ryan Chard, **Austin Clyde**, Ian Foster, Zhi Hong, Shantenu Jha, Zhuozhao Li, Xuefeng Liu, Arvind Ramanathan, Yi Ren, Nicholaus Saint, Marcus Schwarting, Rick Stevens, Hubertus van Dam, Rick Wagner, "Targeting SARS-CoV-2 with AI-and HPC-enabled lead generation: a first data release." in the Platform for Advanced Scientific Computing (PASC '21). (July 2021).

Heng Ma, **Austin Clyde**, Anda Trifan, Venkatram Vishwanath, Arvind Ramanathan, Debsindhu Bhowmik, Shantenu Jha, "Benchmarking Machine Learning Workloads in Structural Bioinformatics Applications" at First International Workshop on Benchmarking Machine Learning Workloads on Emerging Hardware. (May 2020).

Austin Clyde, Arvind Ramanathan, Rick Stevens, "Virtual screening with deep learning using cancer cell line dose-response data" at American Association for Cancer Research. (Janurary 2020).

Workshops

Austin Clyde, Arvind Ramanathan, Rick Stevens, "Scaffold embeddings: Learning the structure spanned by chemical fragments, scaffolds and compounds." NeurIPS 2021 Machine Learning and Representation, Decemeber 2021.

Austin Clyde, "Created in our Likeness: Is Open-Source AI at Odds with Animal Rights?" MANCEPT Workshop "Politics, Animals, and Technology" organized by the Manchester Centre for Political Theory, September 2021.

Austin Clyde, Ashka Shah, Max Zvyagin, Arvind Ramanathan, Rick Stevens, "Scaffold-Induced Molecular Graph (SIMG): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery" in Sixth Computational Approaches to Cancer Workshop at Supercomputing 2020.

Austin Clyde, David Wright, Shantenu Jha, "Integrating High-Performance Simulations and Learning toward Improved Cancer Therapy" in Fifth Computational Approaches to Cancer Workshop at Supercomputing 2019.

DW Wright, A Devitt-Lee, **A Clyde**, K Palani, F Xia, M Turilli, J Karanicolas, S Jha, R Stevens, JD Chodera, PV Coveney, "Combining molecular simulation and machine learning to INSPIRE improved cancer therapy" at CompBioMed Conference 2019.

Book Chapters

Clyde, Austin. "Ultrahigh Throughput Protein–Ligand Docking with Deep Learning." In *Artificial Intelligence in Drug Design*, Methods in Molecular Biology, pp. 301-319. Springer, New York, NY, 2022.

Pre-prints

COVID Moonshot Consortium, (many authors, including **Austin Clyde**). Open Science Discovery of Oral Non-Covalent SARS-CoV-2 Main Protease Inhibitor Therapeutics. Preprint (2021).

Yulun Wu, Nicholas Choma, Andrew Chen, Mikaela Cashman, Érica T Prates, Manesh Shah, Verónica G Melesse Vergara, **Austin Clyde**, Thomas S Brettin, Wibe A de Jong, Neeraj Kumar, Martha S Head, Rick L Stevens, Peter Nugent, Daniel A Jacobson, James B Brown. Spatial Graph Attention and Curiosity-driven Policy for Antiviral Drug Discovery (2021).

Xia, Fangfang, Jonathan Allen, Prasanna Balaprakash, Thomas Brettin, Cristina Garcia-Cardona, **Austin Clyde**, Judith Cohn et al. "A cross-study analysis of drug response prediction in cancer cell lines." (2021).

COVID Moonshot Consortium, (many authors, including **Austin Clyde**), "COVID Moonshot: Open Science Discovery of SARS-CoV-2 Main Protease Inhibitors by Combining Crowdsourcing, High-Throughput Experiments, Computational Simulations, and Machine Learning." (Bioarxiv, October 2020).

Austin Clyde, Xiaotian Duan, Rick Stevens, "Regression enrichment surfaces: a simple analysis technique for virtual drug screening models." (Arxiv, June 2020)

Austin Clyde, Tom Brettin, Alexander Partin, Maulik Shaulik, Hyunseung Yoo, Yvonne Evrard, Yitan Zhu, Fangfang Xia, Rick Stevens, "A Systematic Approach to Featurization for Cancer Drug Sensitivity Predictions with Deep Learning." (Arxiv, April 2020)

PRESENTATIONS AND TALKS

- "AI and Democracy" at University of Chicago Department of Computer Science Seminar (November 2021)
- "The Human-in-the-Loop Learning Fallacy" at Harvard STS Fellows (September 2021)
- "Virtual Screening with Deep Learning: Understanding Speed and Accuracy in Context" at Emerging AI/ML Technologies for Drug Discovery, a Frontline Genomics Webinar June 2021
- "AI for Drug Discovery" at ATOM technical meeting, June 2021
- Panelist, "Intellectual Property Management: A Seminar Series." Argonne National Laboratory, April 2021 (Virtual)
- "Ensemble Models and Consensus Scoring for Computational Docking" at National Virtual Biotechnology Laboratory Celebration Seminar, February 2021 (Virtual)
- "Integrating Simulations and Learning Towards Improved Cancer Therapy" at CompBioMed Webinars, March 2021 (Virtual)
- "Tiered BFE Estimation Workflow" At CompBioMed2 Conference, March 2020 (Virtual)
- "Accelerating Virtual Docking Screens with Deep Learning" at Janssen Pharmaceuticals (Seminar)
- "Virtual Drug Screening with Deep Learning" at NIH.AI Workshop on Applications of Machine Learning for Next Generation Sequencing and Drug Data, November 2019
- "Computational Drug Discovery at Scale" at ComBioMed Kick-off meeting, October 2019
- "Molecule Generation, Search, and Optimization" at ATOM technical Meeting, April 2019

TEACHING EXPERIENCE

Instructor, *University of Chicago Department of Computer Science*
- (Summer 2021) CMSC 15200 Introduction to Computer Science II

Instructor, *University of Chicago Academic Achievement Program*
- (Summer 2021, Summer 2020) Introduction to Computer Science

Graduate Teaching Assistant, *University of Chicago Department of Computer Science*
- (Fall 2019, CMSC 25410) Machine Learning and Medicine

SERVICE AND OUTREACH

- Volunteer, Hour of Code, December 2018
- Reviewed for: Cell Patterns 2021 (2), NeurIPS 2021 workshop on Machine Learning and the Physical Sciences (3)
- Association for Computing Machinery (ACM) Member

SELECT COURSEWORK

- Technology, Anthropology, Ethics (PHIL 6300 Saint Louis University)*
- Science, Power, and Politics (IGA 513, Harvard Kennedy School)*
- Autonomous Laboratories (CMSC 35360, University of Chicago)
- The Value of Data (CMSC 33580, University of Chicago)
- Modern European Intellectual History (HIST 29416, University of Chicago)
- Art and Knowledge (ARTV 27214, University of Chicago)
- Buddhist Thought: India and Tibet (RLST 23900, University of Chicago)