Austin Clyde

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RESEARCH INTERESTS

Intersection of AI and "Science," drug discovery, representation learning

EDUCATION

PhD in Computer Science (currently) – 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, January 2019 to Present.

PUBLICATIONS

Peer-reviewed Journals

Casalino, L., Dommer, A. C., Gaieb, Z., Barros, E. P., Sztain, T., Ahn, S.-H., Trifan, A., Brace, A., Bogetti, A. T., **Clyde, A**., Ma, H., Lee, H., Turilli, M., Khalid, S., Chong, L. T., Simmerling, C., Hardy, D. J., Maia, J. D., Phillips, J. C., … Amaro, R. E. (2021). AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. The International Journal of High Performance Computing Applications (May 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 Review, May 2021)

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 Informatics (May 2021)

Conference Proceedings

Alexander Brace, Michael Salim, Vishal Subbiah, Heng Ma, Murali Emani, Anda Trifan^{1,5}, **Austin R. 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).

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).

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).

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 2020.

Workshops

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

Austin Clyde, "Ultra High-Throughput Protein-Ligand Docking with Deep Learning" in *Artificial Intelligence in Drug Design*, Methods in Molecular Biology (Springer). (To appear, August 2021).

Pre-prints

Austin Clyde, Arvind Ramanathan, Rick Stevens, "Scaffold embeddings: Learning the structure spanned by chemical fragments, scaffolds and compounds." (Arxiv, March 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." (Arxiv, March 2021).

Aymen Al Saadi, Dario Alfe, Yadu Babuji, Agastya Bhati, Ben Blaiszik, Thomas Brettin, Kyle Chard, Ryan Chard, Peter Coveney, Anda Trifan, Alex Brace, **Austin Clyde**, 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" (Arxiv, November 2020).

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).

Aymen Al Saadi, Dario Alfe, Yadu Babuji, Agastya Bhati, Ben Blaiszik, Thomas Brettin, Kyle Chard, Ryan Chard, Peter Coveney, Anda Trifan, Alex Brace, **Austin Clyde**, 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" (Arxiv,

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)

AWARDS AND RECOGNITION

- Recognition in the Secretary's Honor Awards for DOE 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)

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

- (Fall 2019, CMSC 25410) Machine Learning and Medicine

PRESENTATIONS AND TALKS

- "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

SERVICE AND OUTREACH

- Volunteer, Hour of Code, December 2018