AI-driven Multi-scale Simulations for COVID-19 Drug Discovery

Dr. Arvind Ramanathan, Computational Biologist
Data Science and Learning Division
Argonne National Laboratory, Lemont, IL

Our work addresses both the fundamental biological mechanisms of the SARS-CoV-2 virus and the disease, while simultaneously targeting the entire viral proteome to identify potential therapeutics. We will describe machine learning (ML), deep learning (DL) and artificial intelligence (AI) techniques to: (i) identify and build accurate three-dimensional structural models of the SARS-CoV-2 proteome by integrating experimental structural and systems biology datasets, (ii) accelerate adaptive conformational sampling of the viral proteins to potentially identify novel binding sites/ pockets that can be targeted by compound libraries, and (iii) rapidly filter, rank, and search for small molecules across widely available chemical libraries and to integrate virtual screening with experimental high throughput screening. The immediate impact of our current research is an ecosystem of open source AI/ML tools and conventional physics-based simulations that can accelerate timely response for treating such pandemics. We have made significant progress across the aforementioned goals, including the release of over 60 terabytes of machine readable data for various open-source chemical compound libraries (https://2019-ncovgroup.github.io/data/), development of scalable AI/ML methods for rapidly filtering the chemical space that can bind specifically to viral protein targets. The outputs from physics-based models are used iteratively to improve the prediction capabilities of our AI/ML approaches, thus successively improving the overall yield of drug candidates that can be refined further using biochemical and biological assays. Together, our integrated approach provides insights into how the overall drug-design and discovery process can be improved for emerging pandemics.

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Remote via https://www.utep.edu/science/bioinformatics/colloquium/zoom

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