CompBioMed

A Centre of Excellence in Computational Biomedicine

Webinar Series

Webinar #13:
"Are we there yet?" — Addressing emerging drug discovery challenges for SARS-CoV-2 with artificial intelligence driven molecular dynamics

16 September 2020

10am CST / 4pm BST (1h duration)

Register for free here: https://register.gotowebinar.com/register/3855043206817780493

This talk will primarily cover our ongoing efforts in using AI/ML techniques in addressing the COVID-19 pandemic. We outline how we have been using AI/ML strategies in (1) elucidating the molecular mechanisms by which drugs/ small molecules interact with the SARS-CoV-2 proteome, and (2) driving multi-scale molecular simulations to accelerate the sampling of 'rare' events in the conformational landscape of these proteins.

This is the 13th of a series of webinars organised by CompBioMed.
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Dr. Arvind Ramanathan received his MSc and PhD degrees in Computer Science and Computational Biology from Stony Brook University, NY and Carnegie Mellon University, PA in 2005 and 2010. From 2010, he undertook postdoctoral training and then became the team lead for the integrative systems biology team within the Computer Science division at Oak Ridge National Laboratory, TN. He has authored over 30 publications, and his work has been featured in several popular media outlets in the US. Since 2019, he works as a computational biologist at Argonne National Laboratory, IL. His research interests are at the intersection of data science, high performance computing and biological/biomedical sciences, with a specific focus on scalable statistical inference techniques.

Moderated by Katya Ahmad, University College London

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