



## DSICCR Tuesday Seminar Series

Tuesday at Noon, Click [Here](#) to Join

### AlphaFold: algorithm and deployment in an HPC environment

**David Shih, Ph.D., Yuntao Yang, Zhao Li**

Data Science and Informatics Core for Cancer Research  
School of Biomedical Informatics  
University of Texas Health Science Center at Houston

AlphaFold2, developed by Google DeepMind, is a breakthrough in the grand challenge of protein structure prediction. We will present an overview of this deep learning algorithm and discuss how to interpret its predictions. In addition, we will discuss about how we deployed the AlphaFold 2 pipeline in an HPC environment. Specifically, we will show how to split the AlphaFold 2 pipeline into CPU and GPU parts and run them on computer clusters and GPU servers separately to accelerate the workflow. We used the Frontera computer cluster in Texas Advanced Computing Center (TACC) to complete the CPU part of over 200 protein sequences within 10 hours. For the GPU part, over 50 structure predictions could be completed within 24 hours on a GPU server. The deployed workflow can efficiently use different computing environments to process many protein structure predictions to advance biomedical research.

Tuesday, March 8<sup>th</sup>, 2022. 12p – 1p. [Webcast](#)

Contact: Xiaohong.Bi@uth.tmc.edu

 #SBMIseminar

