



DSICCR Tuesday Seminar Series

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AlphaFold: algorithm and deployment in an HPC environment

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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 8th, 2022. 12p – 1p. [Webcast](#)

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