Continuum Computational Modeling of Biophysical Systems



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Abstract

This seminar will explore how continuum modeling and high-performance computing can be combined to study biophysical systems from the nano to the millimeter scale. Starting at the atomic scale, we will see how Poisson-Boltzmann calculations can help us understand the fundamental biophysical mechanisms of deforming proteins, focusing specifically on the opening of the covid-19 spike protein and its role in the infection pathway. Zooming out, we will then focus on cellular material transfer during cell division, a crucial process that could shed light on the propagation of prion diseases, such as mad cow and Creutzfeldt-Jakob. This seminar is intended for a broad computational audience and does not require any prior biophysical background.

Bio

Maxime Theillard is an Associate Professor of Applied Mathematics in the School of Natural Sciences at UC Merced. He completed his undergraduate training in engineering sciences and applied Mathematics at Ecole Polytechnique in France before moving to the Mechanical Engineering department at UC Santa Barbara in the Fall of 2009. There he received an MS with an emphasis in Computational Science in 2010 and defended his Ph.D. in 2014. The same year, he started a postdoc position in the Department of Mechanical and Aerospace Engineering at UC San Diego, which he held until joining UC Merced in July 2017. Maxime has leveraged his interdisciplinary training to create an innovative research program in Computational Sciences with a high potential for multidisciplinary studies. His scholarship impacted not only applied mathematics, and specifically the fields of scientific computing and numerical analysis, but also other related disciplines, biophysics, or fluid mechanics, through his collaborative work.