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Molecular dynamics simulation: at a crossroad between molecular biophysics and petascale computing[1] XIAOLIN CHENG, Oak Ridge National Laboratory — High-performance computing (HPC) has become crucial for most advances made in chemistry and biology today. In particular, biophysical simulation is capable of helping generate critical new insights and drive the direction of experimentation. In this talk, I will discuss our work towards addressing some fundamental membrane biophysical questions using HPC capabilities at Oak Ridge National Laboratory. I will first provide a synopsis of our current progress in developing molecular dynamics (MD) techniques that make efficient use of massively parallel supercomputers. I will then discuss a few examples of large-scale MD simulations of biomembrane vesicles, an effort aimed at shedding light on the lateral organization and cross-layer coupling in biologically-relevant membranes. In conclusion, I will discuss a few scientific and technical challenges faced by MD simulation at the exascale.

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