Affordable multiscale methods for simulating virus like particles

Sergio Pantano Gutierrez
Institut Pasteur de Montevideo
Biomolecular Simulations Group
Calle Mataojo 2020
11400 Montevideo
Uruguay

Abstract:

Multiscale simulations schemes combine different resolutions according to the relevance of particular regions in a molecular system. They can get the best of two worlds by achieving high resolution in regions of interest, and benefit from a significant decrease in computational cost by considering less relevant parts at a simplified level of representation. I will introduce a cost-effective, triple-scale solvation approach particularly well suited for the simulation of large macromolecular assemblies. This simulation approach is well suited for viral like particles, which require a massive amount of explicit bulk solvent for a proper description. Using this approach in combination with the coarse grained SIRAH force field it is possible to obtain dynamics insights on virus like particles at a moderate computational cost. The viability of this scheme is discussed in terms of the size of the currently reported viral structures on the Protein Data Bank and the affordability of simulations performed with GPU-accelerated desktop computers.