Numerical modelling of Enveloped Virus Hydrodynamics

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Abstract: Since 2019, the virus SARS-CoV-2 has been a critical issue worldwide because of its massive health impact. Here, we investigate the diffusion of SARS-CoV-2 virions using computational simulations. Due to the morphological features, virions can be modelled as decorated nanoparticles and characterized according to their translational and rotational diffusivity. Since they lack an active motion mechanism we used the Rigid Multi-Blob (RMB) [1] methodology and Smoothed Dissipative Particle Dynamics (SDPD) [2] to simulate the effect of the spike proteins on the virions transport. Using RMB, we construct virion models by discretizing the structures as rigidly connected spherical beads; later, we compute their mobility tensor to determine the diffusion. The results revealed the effect of spike arrangement, number, density, and morphology on virion transport and paves the way to look at possible effects on viral infectivity [3]. Moreover, using a similar blob discretization of RMB, we conduct SDPD simulations, treating the envelope and spikes as separate rigid bodies to introduce flexibility in the spikes. This approach allowed us to characterize the effects of flexible spikes and their effect on the rotational diffusivity of the virion. We identify that passive microrheology provide relevant information about viruses.

References:

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