A molecular simulation study for the packaging and the ejection processes of viral DNA

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DNAs are packaged into and ejected from a small viral capsid during the virus replication process. Single molecule experiments were performed to understand how the DNA could overcome a large entropy loss and a strong pressure during packaging. Theoretical studies also reported how the DNA was jammed in non-equilibrium states inside the capsid. It is also an issue how such non-equilibrium jammed conformation would affect the DNA ejection from a viral capsid. Unfortunately, however, packaging and ejection processes have been treated as independent processes under the assumption that the DNA would reach an equilibrium conformation. In this presentation, I would like to report that the ejection process of DNA from the viral capsid should depend significantly on how the DNA was packaged into the viral capsid. We perform Langevin dynamics simulation to package the DNA into a viral capsid and let the DNA eject from the capsid spontaneously. There should be three different regimes depending on the packaging rate: (1) knot dominant, (2) non-equilibrium dominant, and (3) intermediate regimes. When the DNA is packaged slowly, the DNA forms a complex knot easily during the packaging such that the ejection slows down (knot dominant regime). When the DNA is packaged quickly, the DNA is more likely to be jammed in non-equilibrium states, slowing down the ejection process (non-equilibrium dominant regime). When the packaging rate is intermediate, the probability of knot conformation is relatively low, and the DNA conformation may also relax easily, which facilitate the ejection most (intermediate regime).