Theory and modeling of virus assembly

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We plan to discuss the following three related issues:

(1) The genome packing in RNA/DNA viruses is investigated by considering conformational entropy of the constituent macromolecules and electrostatic interactions among them. The predicted general results, such as the genome size and genome density distribution inside the capsid, seem to be largely borne out by the available experimental data on diversely different viruses. Additionally, the stability of assembled virus structures will be addressed theoretically.

(2) The kinetics of virus assembly in the presence and absence of ssRNA is modeled by simulations. We find that the assembly of the capsid proceeds by the nucleation and growth mechanism and that the nucleation barrier is reduced by the presence of the genome. We further find that the growth stage involves another nucleation and growth process.

(3) The above results for ssRNA/DNA viruses will be contrasted with our modeling results for dsDNA phages where we have monitored the packing kinetics and ejection kinetics under idealized conditions.