Effects of pulling forces, osmotic pressure, condensing agents, and viscosity on the thermodynamics and kinetics of DNA ejection from bacteriophages to bacterial cells: a computational study

(Supplemental Material)

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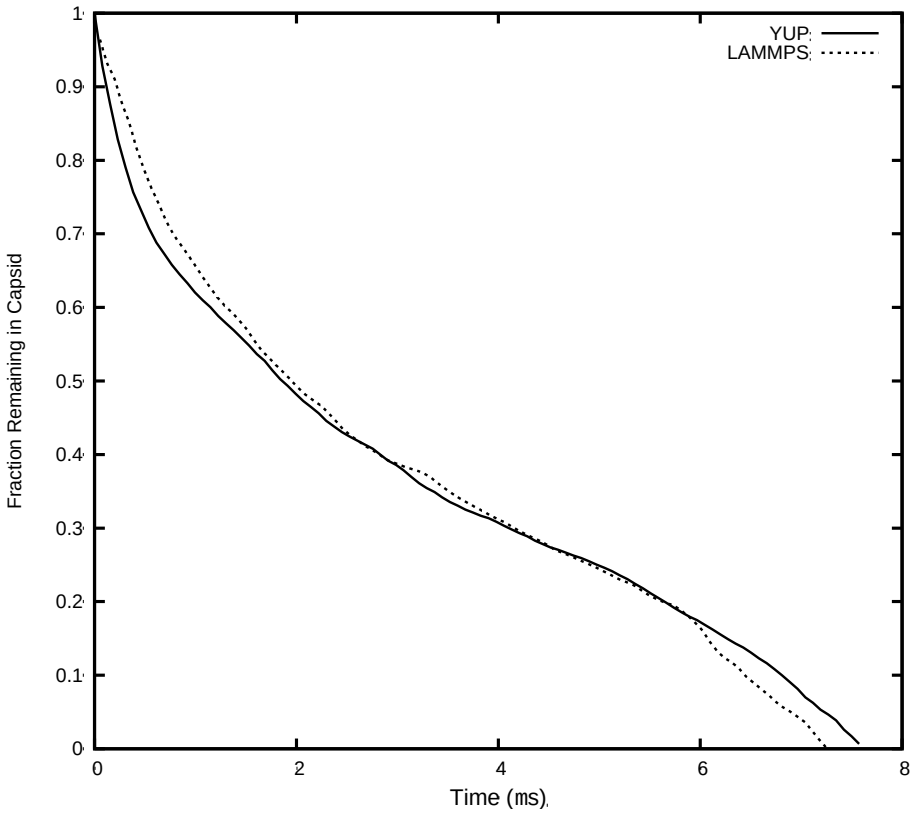


Figure 1S: Comparison of a fixed-viscosity (γ=10^{-3}) ejection run in our YUP implementation and in our LAMMPS implementation. For our purposes, the two implementations yield equivalent results.

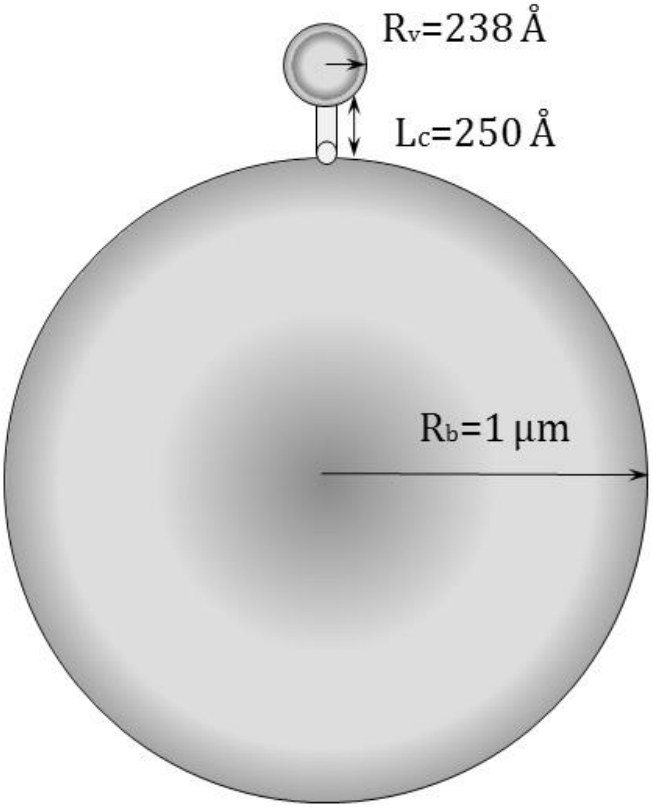


Figure 2S. A schematic description of the model used in the ejection simulations. A spherical capsid of radius, R_c = 238 Å is connected to the cell by a cylindical channel of length L_c = 250 Å (50 Å of which penetrates inside the capsid), and a bacterial cell modeled as a sphere with a radius R_b = 1 μm.

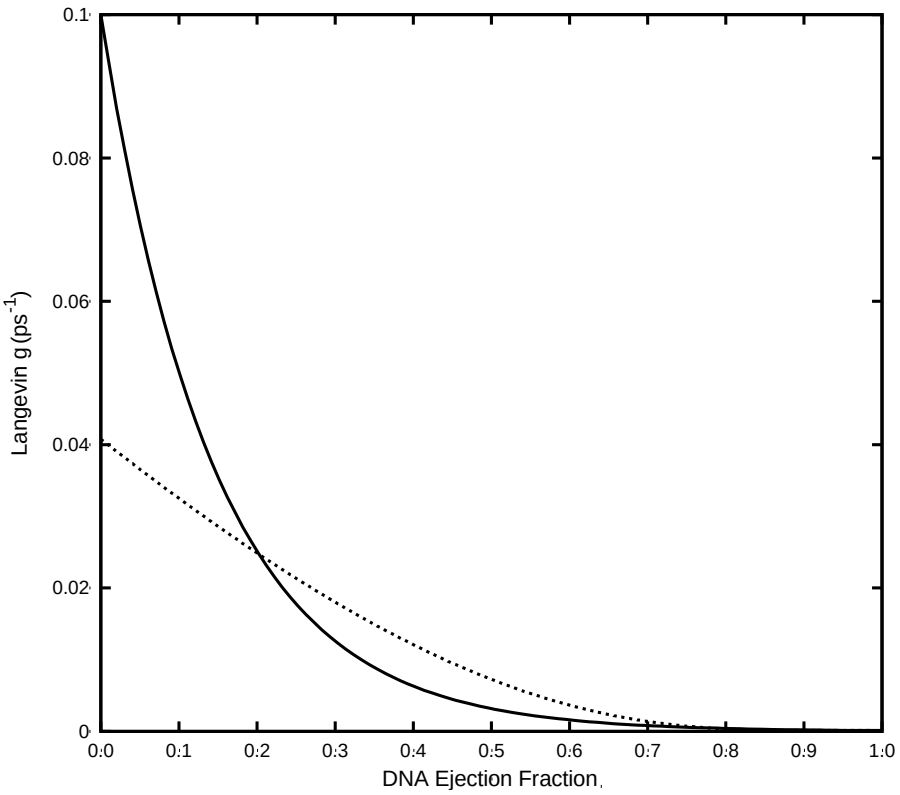


Figure 3S: Comparison of radical (dotted line) and semilogarithmic (solid line) functionals for a Langevin collision frequency with $\gamma_{high}=10^{-2}$ $ps^{-1}$and $\gamma_{low}=10^{-4}$ ps^{-1} calculated according Eqn. 4 and Eqn. 5. The scaling factor in the exponent of the radical functional was selected such that the starting γ inside the capsid was within a factor of ~2 of γ_{high}.

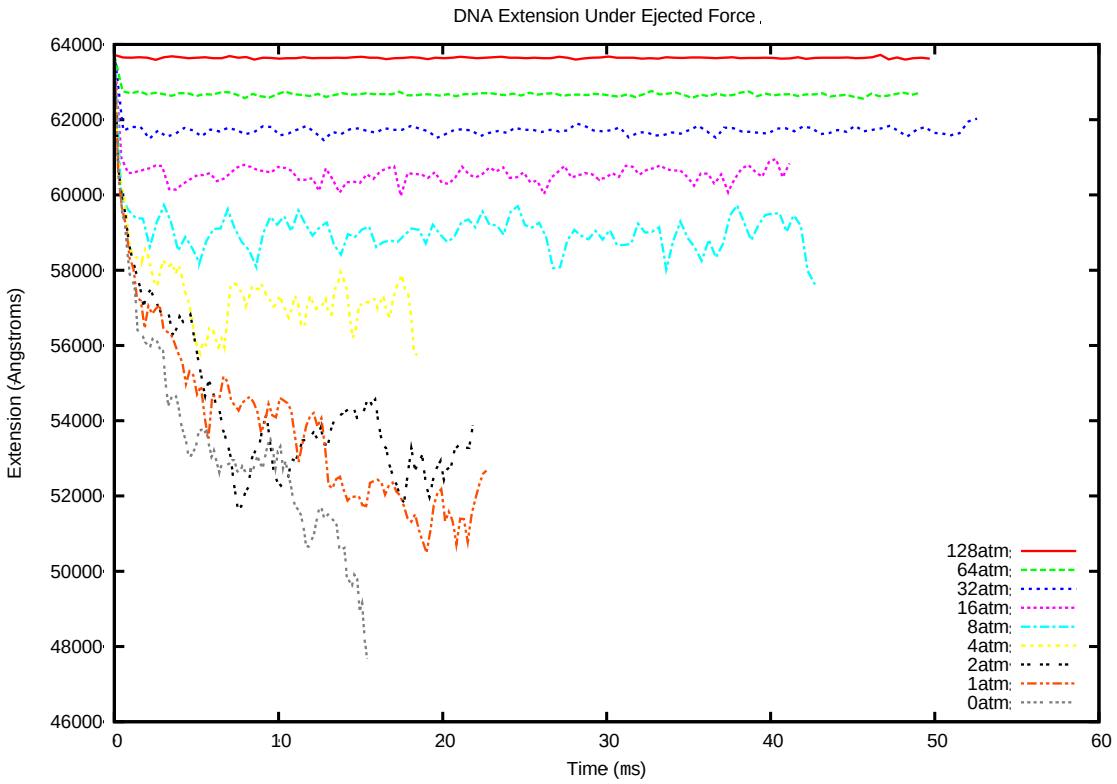
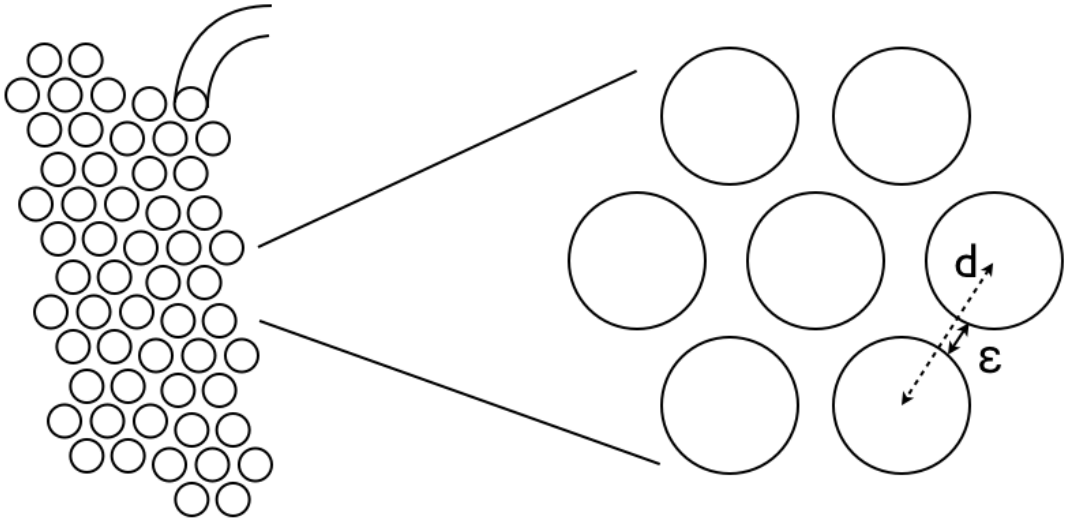


Figure 4S: Simulated DNA extension under "ejected" force (total force equally distributed among all pseudoatoms in the DNA chain; 1atm is equivalent to 1pN force). On the timescale of these simulations (larger than the timescale of ejection), the DNA straightens out at ~4atm.

Derivation of Equation 4

The DNA within the viral capsid can be idealized as hexagonally packed structures.The cross-sectional area of s DNA strands organized in such fashion is a 2D array of circles with a hexagonal symmetry. The fraction of packed DNA, F, equals the ratio of the instantaneous 2D density of these circles ρ to the fully-packed 2D density of circles ρ_0 as illustrated in the diagram below.



The average 2D density of the coils varies inversely with the square of the coils' center-center distance, so we have

$$F = \frac{\rho}{\rho_0} = \frac{{d_0}^2}{d^2},$$

By convention, we measure the fraction P of ejected DNA, $P = 1 - F$. Assuming uniform coil density, the average surface-surface distance between the coils ε is given by

$$\varepsilon = d - 2r = d_0(1 - P)^{-\frac{1}{2}} - 2r.$$

Assuming that the viscosity of the water depends exponentially on the distance between DNA surfaces in the packed capsid (as suggested by studies of Riedo

and co-workers[1]), the dependence of the collision frequency parameter on the distance between the DNA strands becomes:

$$\gamma_{in} = \gamma_{high} * exp\left(-0.15 * \left[\left(1 - f_{ejec}\right)^{-0.5} * d_{DNA,0} - d_{DNA}\right]\right) + \gamma_{low},$$

where γ_{in} is the Langevin collision frequency inside the viral capsid, $\gamma_{out} = \gamma_{low}$ is the Langevin collision frequency in the cell medium, $d_{DNA,0}$ is the center-center distance (28 Å) of DNA in a fully-packed capsid, and d_{DNA} (22 Å) is twice the radius of our DNA chain. The factor -0.15 was chosen empirically such that γ_{in} was within a factor of 2 of γ_{high} when ejection began. γ_{high} and γ_{low} were varied for each run.

Note that the segments of DNA do not actually spread monotonically throughout the capsid during ejection; rather, they tend to press against the walls, leaving a hollow region in the center of the capsid. The derivation above is meant only to provide a useful (though not necessarily rigorous) physical model for a new viscosity functional.

1 Li, T. D.; Gao, J. P.; Szoszkiewicz, R.; Landman, U.; Riedo, E. *Phys Rev B* **2007**, *75*