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Tethered DNA molecules stretched by an electric field: A Molecular Dynamics Study. GARY SLATER, MARTIN BERTRAND, University of Ottawa — It has been predicted by Long, Ajdari and Viovy (Phys. Rev. Lett., 1996, 76:3858) that the mechanical force necessary to stall a DNA molecule during electrophoresis is substantially smaller than the sum of the electrical forces applied on all of its monomers. In fact, it should be proportional to its hydrodynamic friction coefficient, which may vary with the molecular conformation. We have tested this prediction using coarse-grained Molecular Dynamics simulations in which we explicitly included the polymer, the solvent, the counterions and the salt. Our results show that the above prediction is indeed valid. In fact, our data demonstrate that there is a universal linear relationship between the stall force and the product of the electrical field and the radius of gyration of the polyelectrolyte. This remarkable relationship holds even when the electric forces stretch the DNA molecule near full extension. We thus conclude that an electrophoretic field is equivalent to a fluid flow, as suggested by Long, Ajdari and Viovy. This has profound implications for the development of a theoretical framework that can explain the electrophoresis of hybrid DNA-protein molecules.

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