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Langevin Equation for DNA Dynamics DAVID GRYCH, JEREMY COPPERMAN, Univ of Oregon Dept. of Physics, MARINA GUENZA, Univ of Oregon Dept. of Chemistry — Under physiological conditions, DNA oligomers can contain well-ordered helical regions and also flexible single-stranded regions. We describe the site-specific motion of DNA with a modified Rouse-Zimm Langevin equation formalism that describes DNA as a coarse-grained polymeric chain with global structure and local flexibility. The approach has successfully described the protein dynamics in solution and has been extended to nucleic acids. Our approach provides diffusive mode analytical solutions for the dynamics of global rotational diffusion and internal motion. The internal DNA dynamics present a rich energy landscape that accounts for an interior where hydrogen bonds and base-stacking determine structure and experience limited solvent exposure. We have implemented several models incorporating different coarse-grained sites with anisotropic rotation, energy barrier crossing, and local friction coefficients that include a unique internal viscosity and our models reproduce dynamics predicted by atomistic simulations. The models reproduce bond autocorrelation along the sequence as compared to that directly calculated from atomistic molecular dynamics simulations. The Langevin equation approach captures the essence of DNA dynamics without a cumbersome atomistic representation.

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