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DNA translocation through small channels and pores from molecular models. Hydrodynamic, electrostatic, and hybridization considerations.

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The flow and translocation of long DNA molecules are of considerable applied and fundamental interest. Design of effective genomic devices requires control of molecular shape and positioning at the level of microns and nanometers, and understanding the manner in which DNA is packaged into small channels and cavities is of interest to biology and medicine. This presentation will present an overview of hierarchical models and computational approaches developed by our research group to investigate the effects of confinement, hydrodynamic interactions, and salt concentration, on the structure and properties of DNA, both at equilibrium and beyond equilibrium. The talk will include a discussion of coarse grain descriptions of the flow of DNA in microfluidic and nanofluidic channels over multiple length and time scales, and a discussion of emerging, detailed models that are capable of describing melting and rehybridization at the single nucleotide level, as well as the packaging of DNA into viral capsids and small pores.