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Machine Learning as a Tool to Study Soft Matter in Confinement

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With the advent of robust nanoscale fabrication, the study of soft matter has become intertwined with nano- and microfluidic device design. Applications range from building nanoscale devices with which to isolate single biomolecules, to studying colloidal particles in nano- to microchannels. Modeling and simulation of soft matter have followed this shift and have become powerful tools both for characterizing the biological material and for aiding in the design of the devices. In such work, common tasks include solving electric fields in complicated geometries and extracting quantities of interest such as the mean first passage time of polymers or particles moving through the devices. Traditional approaches to solving these problem include mesh-based techniques such as the finite element method for electric fields, and particle simulations such as Langevin dynamics for the mean first passage time. In this talk, I will present work from my lab in which we use deep neural networks to replace both of these traditional methods. The "slit-well" device will be used as an exemplar system. I will discuss the benefits of this machine learning approach, such as being mesh-free and parameterizable, as well as some of the remaining challenges.

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