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Large-scale particle-based simulations of active nematic fluids in bulk and under confinement[1] ABHIJEET JOSHI, MATTHEW PETERSON, APARNA BASKARAN, MIKE HAGAN, Brandeis University — Active nematics are liquid crystals which are driven out of equilibrium by energy-dissipating active stresses. Experiments and theory have demonstrated that in such systems the ordered nematic state is unstable to the proliferation of topological defects, which undergo birth, streaming dynamics, and annihilation to yield a seemingly chaotic dynamical steady state. In this talk we describe large-scale simulations of a particle-based computational model for active nematic, motivated by an experimental active nematic system containing extensile bundled microtubules and molecular motor proteins. Extending upon previous theoretical and computational work, our model explicitly describes degrees of freedom internal to bundles. We explore how the properties of these internal modes affect large-scale emergent behaviors, such as defect shapes and inter-defect correlations, in bulk and under confinement. We quantitatively compare these defect behaviors observed in bulk and confined experimental systems.

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