Continuum Simulations of Liquid Crystal Droplets and Colloids

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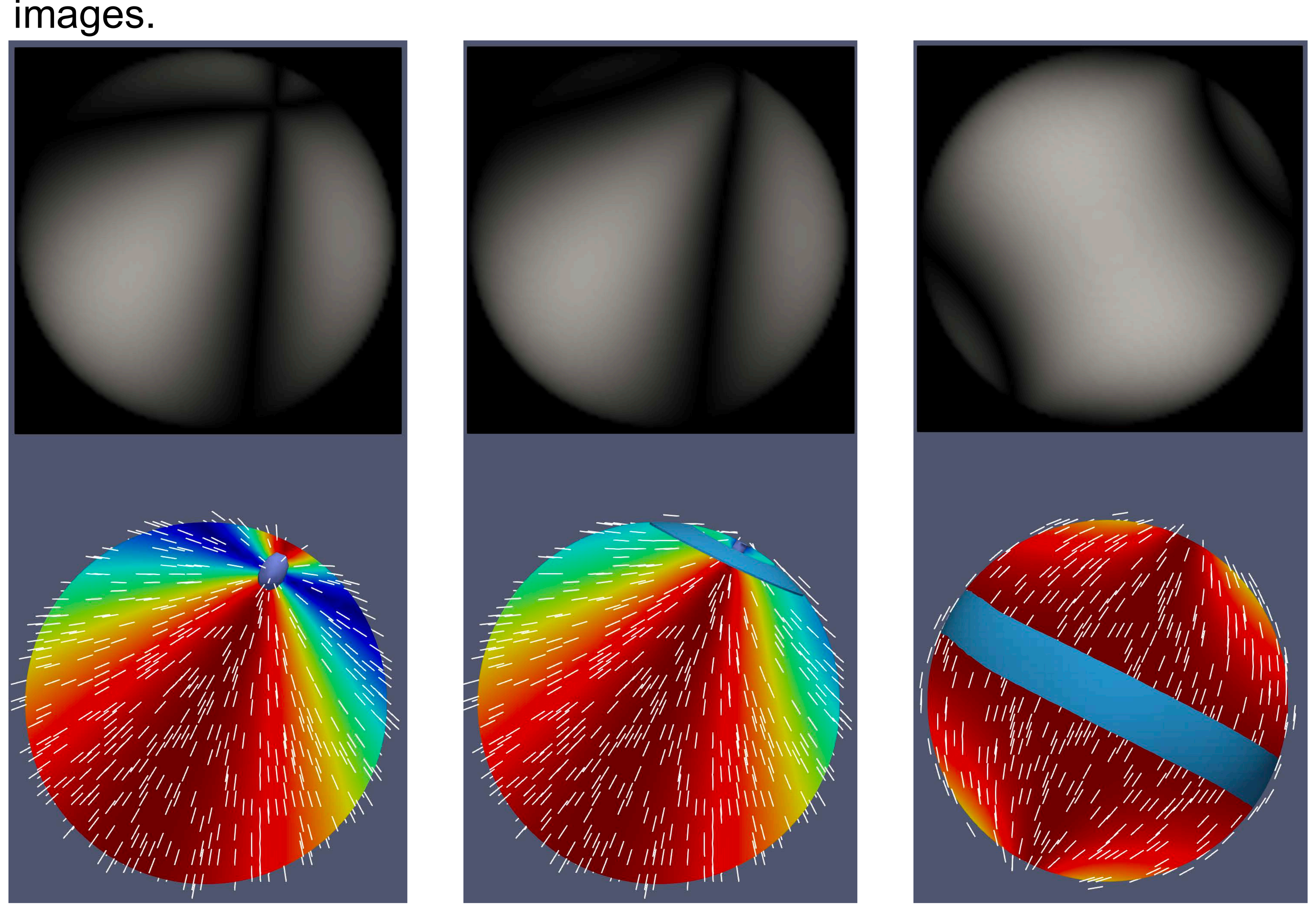
Introduction

Recent study of biocompatible liquid crystals (LCs) and the discovery of LC phases in biological systems have triggered a wave of fundamental research in LCs towards their biological applications. Although LC theory has mainly been developed in the last century, with the help of modern computational power, the new century has seen highly reliable, large-scale, continuum simulations of LCs that are comparable to and capable of guiding experiments for applications including design of novel biological sensors and autonomous materials. In the following, we show three ongoing projects in the de Pablo group to demonstrate the power and beauty of LC simulations.

Results

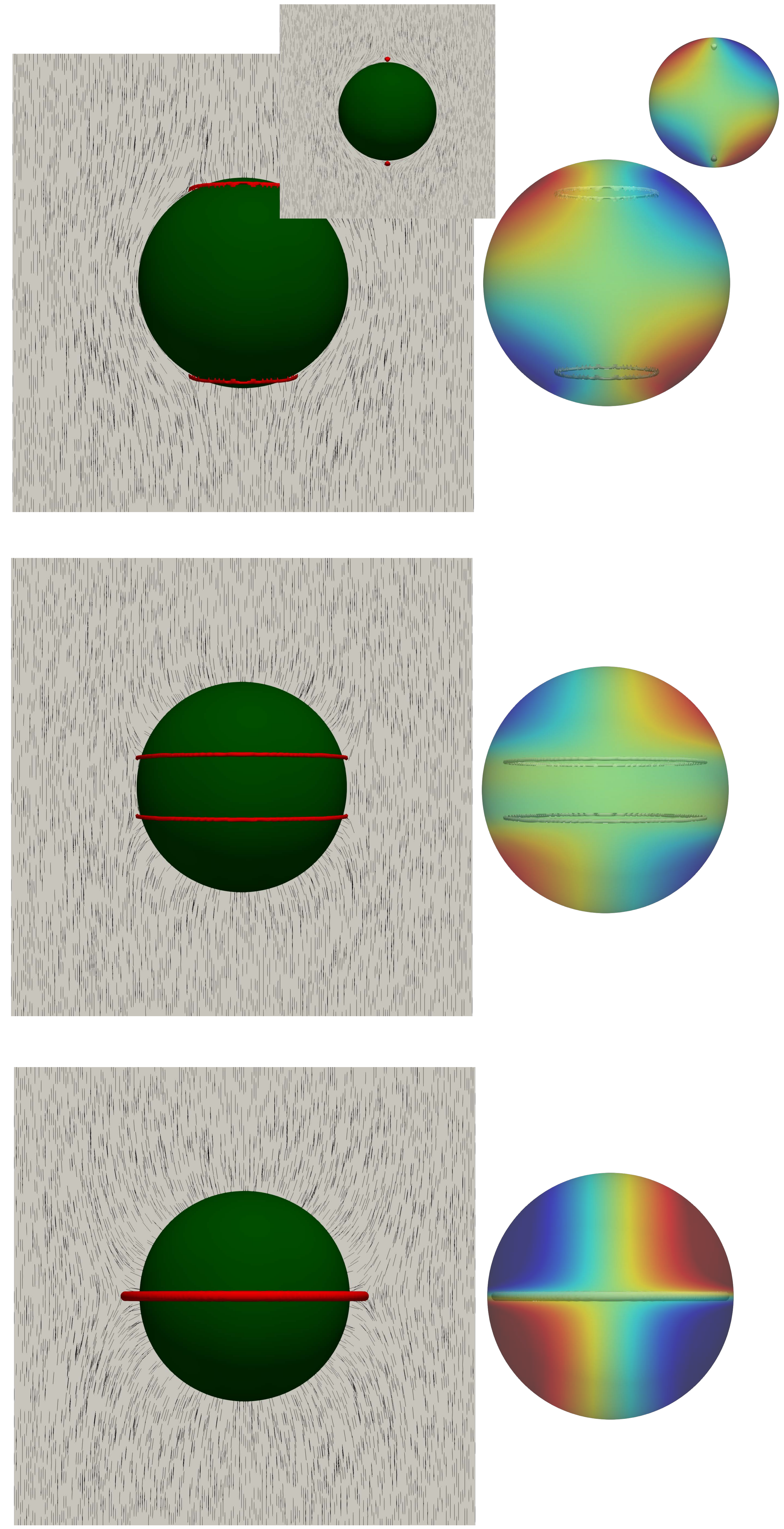
I. Structural Transition in a nematic LC droplet

We use continuum simulation to calculate the structural evolution of a micro-meter nematic LC droplet during a change of anchoring condition from normal to planar, experimentally due to the addition of certain surfactants. Coresponding optical appearance under crossed polarizers (top) and LC microstructures (bottom) are shown in the following images.



II. Structural Transition in a nematic LC Colloid

In this project, we explore the transformation of elastic multipoles around a nematic LC colloid filled with a diffusing surfactant species which alters the anchoring condition from planar to normal. We aim to unpack the mechanism of anchoring transformation and the emergence of new elastic multipoles at the droplet surface suspended in a nematic LC with the far-field uniform alignment of the nematic director. These series of figures display the transformation of topological defects from Boojums to Saturn.



III. Dynamics of 3D Active Nematic droplets

Here we use parallalized hydrodynamic simulation to study 3D active nematics confined in a droplet with normal anchoring. Snapshots show velocity (arrows), director fields (lines) and defects (red) for two activities. (a) Quasi steady-state for low activity with two small defects in the poles (b-d) Time evolution of active nematic for higher activity. b) is the onset, c-d) show the evolution of defect loops.