Chapter 6

Conclusions

A new scheme for a localized radial basis function method in three-dimensions is proposed. Shape parameter-dependent radial functions are required for the local scheme to work. The method optimizes shape parameter based on the highest gradients present in problem of interest. Two options are shown and validated through numerical simulations. For scattered data or problems that do not involve boundary conditions, the optimization is done through a known analytical function. On the other hand, transient partial differential problems require a global RBF that is applied directly to the operator. We found that shape parameter optimizations, following both approaches, depend on geometry, node distribution and density. Contrary to previous approaches, we did not observe shape parameter differences within the domain and a constant value was sufficient to provide good approximations.

For global and local schemes, the differential operator optimization resulted in better approximations to the function, gradient and laplacian. Shape optimizations, following previous works in two-dimensional domains, based on the matrix condition number, failed to provide acceptable approximations. Differential operators are calculated through direct (Kansa) and quadrature approaches. During global RBF interpolations, both methods were successful. On the other hand, the direct approach was the only method that provided good approximations in the LRBF. In general, approximation errors decrease as the node density and the stencil size increase.

To our knowledge, this method is the first consistent method to optimize local RBF schemes in three dimensional domains. It provides a platform to use meshless methods in complex and moving geometries following linear or non-linear dynamics.

We presented a comprehensive study of confined chiral nematics in spheroids from a continuum description of the free energy functional. Simulations were carried out minimizing the free energy following a theoretically informed Monte Carlo relaxation and a Finite Element discretizations. We built phase diagrams in terms of temperature and chirality for three families of spheroids under strong, moderate and low anchoring conditions. The droplet phase diagram was consistent with morphologies previously reported with similar ranges of stability. As the anchoring is weakened we observed the degeneracy of some phases and we discovered precursors to the BPs in the intermediate chirality regime.

In addition, we demonstrate how geometric frustration helps to stabilize and generate new BP morphologies that may have novel technological applications. The main consequences on changing the geometry is the widening or narrowing of some regions in the phase diagrams. High curvature regions attract surface defects inducing the formation of structures like the RSS. On the other hand, the constriction of one dimension interrupts the formation of defect networks and emulate structures found in nanochannels. Finally, the extension of one dimension enables the formation of a new hybrid BPs with a higher density of defects. The detailed phase description expands the family of configurations with blue phase characteristics and provides general understanding to increase its range of stability.

Additionally, we studied sets of nanoparticles adsorbed on bipolar droplets. This study comprises sets of planar and homeotropic particles. In past work, small sets of homeotropic particles were studied where it was found that they segregated towards regions were nematic distortions were present [43], and when particles group the nematic field distorts near the junctures between them. Here we report on larger sets where we found the same segregation phenomena and defect structure, but we also notice a degeneration on the stable configurations as the set size increases. Degenerate states account for the combinatorics of a set of size N organized in two groups. Sets composed of planar particles exhibit the same tendency to aggregate at the poles, coinciding with results reported in [44], however degenerate states exhibit particles roaming near the equator. The defect structure in these cases consist on half spherical shells or bridges between two nanoparticles near the boojum.

By studying large sets of particles, we were able to found an ample spectrum of configurations with different values of free energy thus indicating the emergence of novel assemblies based on probabilistic principles. However, the possible combinations and assembly geometries leads us to believe there are more configurations that remain unexplored due to the extensive coverage such study would require.

Chapter 7
Future projects

The theoretically informed Monte Carlo method presented in [60, 61], and employed for the study shown in chapters 4 and 5, has proven to be a versatile and elaborate tool when representing any type of LC system. The FEM implementation with linear and quadratic tetrahedral elements capture the nuance of any geometry and so intricate regions, or surfaces with curvatures are represented to perfection. An efficient sampling proves to reach configurations with lower free energy than those found with a Ginzburg–Landau relaxation. The next projects are directed towards three different effects: new geometries, colloidal interaction, and heterogeneous surfaces.

The role of curvature the formation of blue phases was evidenced in tactoids. The results showed how the cubic symmetry of BPI or BPII can be destroyed, and with a tight confinement disclination lines can be manipulated to form knots or links as reported by Orlova *et al.* in [183]. The next step in our research is directed towards cylindrical and toroidal cavities for LCs with different chiralities.

Regarding nanoparticles, the assembly of homeotropic colloids on the surface of a droplet has been studied in [43, 44]. From experiments [37] we know that a group of nanoparticles bigger than a pair, assemble in dfifferent combinations at the defects. However, the probability of finding specific configurations, and a physical explanation for the combinatoric character of such assembly remains an open field with minor exploration to date. We presented a study on the assembly of large sets of homeotropic and planar particles. The compendious study of mixed sets is to follow in the upcoming weeks.

Tetrahedral colloids immersed in a LC droplet were studied by Armas–Pérez *et al.* in [60]. It could be possible to control the distance between two tetrahedral opposite to each other, depending on its orientation and size. The results of this study serve as an introduction to photonic droplets and lasing technology.

For heterogeneous surfaces, janus colloids immerse in nematics have been reported [204, 205]. When this particular boundary conditions are imprinted on the surface of a chiral droplet, specific types of defects could be segregated to regions of the droplet or knotting and distortion of the blue phase is to be observed.

Blue phases confined in nanochannels form regular networks, but the orientation of the crystal-like defect structure is yet to be controlled. Specific wavelengths are reflected depending on the crystallographic plane of incidence. We aim to find the optimal design of patterned surfaces, with homeotropic and planar anchoring, in a channel that allow the stabilization of a specific crystallographic plane of BPI and BPII. This could prove the viability of some experimental strategies.

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