Theoretical modelling of liquid crystals

Liquid crystal are rod-like molecules that align to form structures visible to the naked eye. They are the best of both worlds: They flow like liquids, but have optical properties like solid crystals. Hence, their optical properties are easily modified, e.g. by electric fields. This explains their ubiquity in applications, such as Liquid Crystal Displays, and more recently optical computing, nonlinear optics, and visual arts.

While it is relatively easy to manipulate such crystals for technical applications, it is more difficult to understand the detailed physics, especially when one looks at the interplay between the flow and the crystal structure. Developing this understanding is the aim of the project. The project aim will be achieved by mathematical modelling of the Landau-de Gennes equations, which describe the liquid crystal structure. The PhD student will extend the model include the effects of flow effectively, by “coupling” the Landau-de Gennes equation to the Navier Stokes equations. The student will solve this set of equations to develop understanding of the liquid-crystal structure and flow properties.

The first question the student will focus on concerns the patterns formed by a liquid-crystal sample when the crystal is forced to flow in a thin film. The student will use simplified equations to predict and explain these patterns. The second concerns the crystal-defect morphology, specifically, how sharp jumps in the orientation field come about, and how the defects are affected by flow.

A mixture of different methodologies will be used. Firstly, the student will use analytical techniques (“pen and paper solutions”) to describe the thin-film liquid crystals. Thereafter, because the equations are so complicated, the student will resort to resort to computer models. In the final stages the student will look at three-dimensional liquid crystals, where the computer simulations will be performed using high-performance computers at the Irish Centre for High-End Computing (ICHEC).