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Topological and activity-induced constraints in nematic liquid crystals

Louise Catherine Head

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Abstract

Active matter encompasses a broad class of out-of-equilibrium materials with internally-driven components. A trademark feature of these materials is that energy injections at microscopic scales develop into complex pattern formation and collective flows on scales many times larger. Further, examples from cytoskeletal biopolymers, bacteria suspensions and biological tissues have additional constraints on their self-organisation, emerging from their elongated components forming orientational order.

To study the interplay between orientational order and emergent flow patterns, active nematic liquid crystal theory is often utilised. This hydrodynamic model accounts for instabilities that emerge from nematic deformation, and has elucidated the crucial role of topological defects in establishing the characteristic lengthscales of the steady-state structures. Numerical and analytical work on this model, has led to a popular viewpoint on active flow states as arising from point-like two-dimensional topological defects. However, this framework is insufficient for the recent experimental and numerical advancements in three-dimensional active nematics, where defects are points, lines and loops, with different conservation laws and interactions. In addition, colloidal inclusions can induce stable point defects in the orientation field. To understand the relationship between topological defects and self-organised dynamics in three-dimensional materials requires novel numerical methods and theoretical frameworks.

This thesis contributes three advancements towards topological active nematics. The first study adapts a versatile mesoscopic algorithm to include colloids that are responsive to the bulk nematohydrodynamic fields. The elastic interactions between colloids and their passive nematic environment are demonstrated, in addition to the topological properties of three-dimensional defect loops accompanying colloidal particles. This work contributes a useful simulation package that can study inclusions in complex geometries and active settings.
The second study explores how topology can be engineered to control active flow patterns. By tuning the number of inclusions inside an active nematic emulsion, the bulk fluid alternates between topologically-charged disclination loops, and defect-free states. Simulations reveal that, in addition to direct topological constraints, the inner emulsions fix particular geometric constraints on the loop, supporting dynamical states resembling a rotor through to a chaotic oscillator. This work contributes to the understanding of three-dimensional active defect dynamics in the presence of colloidal particles. The third study revisits defect dynamics in two-dimensional active films, to discover a mesoscopic bridge between topological structures in the coupled orientation and flow field. Analysing simulation and experimental data shows that +1/2 defects are constrained to specific isosurfaces of the $Q$ criterion, a parameter that indicates the topology of the local streamlines. The relationship between defects and the $Q$ criterion offers a new framework for understanding two- and three-dimensional defect dynamics. These results reveal a previously invisible, yet dominant, class of defects that locally break mirror-symmetry, with regards to the local streamline structure.

Overall, we demonstrate that defect dynamics can be understood through the framework of nematic topological, geometric, and activity-induced self-constraints. This work may guide future studies on exploring how biological fluids constrain their own dynamics.
Lay summary

Liquid crystals are a phase of matter that are between solids and liquids, which flow and possess orientational order. The simplest type of liquid crystal is the nematic phase, where molecules preferentially align along a common axis. However, there can be places where the alignment becomes discontinuous, called topological defects. In two-dimensions, topological defects exist as point singularities, whereas in three-dimensions they form lines and loops. Generally, passive liquid crystals rearrange their molecular orientations to remove defects and restore global alignment.

A variety of spontaneously-flowing biological or bio-inspired fluids display orientational order and are termed active nematic liquid crystals. Unlike traditional nematics, these may continuously regenerate defects. Further, studies have found complex dynamical behaviours associated to defects—including self-propulsion of point-like defects, and disclination loop growth, shrinking, merging and splitting. Understanding how these dynamical defect behaviours relate to the emergent flows is an ongoing topic of research.

In this thesis, we study the structure and dynamics of topological defects in bio-inspired liquid crystals. We utilise methods to artificially create defects and explore how these singularities control and respond to emergent flows. These results could help to understand biological dynamics and provide insight on how to control their collective flows.
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Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

Parts of this work have been published in


* Denotes co-first author.

Several authors have contributed to parts of this work

- Chapter §4: Y.A.G. Fosado and D. Marenduzzo calculated the defect loop writhe.
- Chapter §5: G. Negro performed all simulations and analysed the single inner emulsion.
- Chapter §6: C. Doré and T. López-León provided experimental data. Simulation data was provided by R.R. Keogh, K. Thijssen, L. Bonn and G. Negro. L. Bonn averaged the flows in Fig. 6.7d-f. K. Thijssen performed the numerical solutions in Fig. 6.13

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4.13 Relaxation pathways for dimer-associated disclination loops following a thermal quench, as measured via the disclination contour lengths $L$ scaled by colloid radius $R = 6$.

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b. Figure-of-omega transitioning to Saturn rings.  
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4.1 Classification of each of the eight identified nematic disclination states (Fig. 4.9) in terms of topological and geometric information. Disclination properties include the writhe (Wr) and twist (Tw), which combine to give the topologically-protected self-linking number $S_l = Wr + Tw$. Topological point charge $p$ associated with colloidal dimers combine to give a trivial nematic texture (even), allowing even contributions from each $n = 1$ or two odd contributions for states with $n = 2$ loops. The properties are calculated directly for the frames shown in (Fig. 4.9).
Chapter 1

Introduction
Topological defects are ubiquitous across many physical systems with broken symmetries, including vortices in superfluids [6], dislocations in crystals [7] and ferromagnets [8]. In each, topological defects are crucial to the material properties and dynamical response. This arises from the fact that topological defects cannot be smoothly removed from a system and they impart geometric signatures on the local order parameters.

A fruitful playground for testing topological phenomena is in nematic liquid crystals, which are fluids composed of rod-like molecules that align along a special axis, called the director. In general, nematics favour configurations where the director is continuous everywhere in space. However, situations can arise in which discontinuities in the orientational order can emerge [9]. In two-dimensions these topological singularities are isolated points, which behave a bit like electric charges. Nematic point defects are characterised by a topological charge, and the sum of all charges in a system must adhere to global conservation laws. In three-dimensions, topological defects are more complicated and can be nonlocal singularities: disclination lines that terminate at boundaries or close their ends together to form loops [10]. These topological structures are still associated with charge-like properties and conservation laws, but this information is contained over the entire structure. One method of probing these topological structures is to introduce colloidal particles in a nematic host [11]. These particles frustrate the smooth nematic order and can lead to the formation of topological defects in their vicinity [12]. Accordingly, many fascinating configurations have been found such as defect rings that surround the colloid’s equator, through to loops that entangle multiple colloids [3].

The behaviour of topological defects are further compounded in a class of spontaneously flowing biological fluids with orientational order. These materials have elongated components that are continuously moving or exerting forces on their environment, categorising these fluids as *active* [13, 14]. Examples include cytoskeletal biopolymers with motor proteins [15] and bacterial suspensions [16]. Such systems are considered to be *active liquid crystals*. Active liquid crystals exhibit striking features, including characteristic turbulent-like disorderly flows [17, 18] and a steady-state population of point-like topological defects [19]. These defects have been identified as crucial to the self-organised flow structures. They are found to tune the geometric features of the local flow field [20] and exhibit dynamical behaviours such as self-propulsion [17]. As such topological point defects are identified as control centres of active turbulent flow states [21, 22].
and theoretical models have been developed where hydrodynamic flows follow directly from the defect configuration [23].

In recent years, the first experimental synthesis of three-dimensional bulk active nematics has been performed [24]. This, and numerical work [25, 26], has uncovered a sea of defect loops that are a variety of sizes, shapes and perform elaborate dynamical behaviours. This finding includes defects that can grow, shrink, but also split up and recombine with other loops [27]. These non-equilibrium topological behaviours are unlike those seen in near-equilibrium passive liquid crystals and have been identified as a major mystery to understanding the self-organisation of three-dimensional active fluids with broken symmetries [28]. However, studying the dynamics of topological structures is a difficult task. Aside from experimental difficulties, visualising and characterising three-dimensional fields requires simplification into scalar isosurfaces or projections onto two-dimensional slices. Recently, tensor-based numerical methods have been proposed that can characterise the local geometric properties of disclinations lines/loops [29, 30], but characterising non-local topological structures remain elusive. Building an understanding of the structure and dynamics of topological defects in non-equilibrium environment would provide insight into biological processes and inform how topology can be utilised for the design of bio-inspired technologies.

This thesis is motivated by the complexities of three-dimensional defects and how they couple to activity-generated flows. To explore this topic, we draw inspiration from passive nematics—utilising colloidal particles to induce and stabilise defect loops. We refer to this approach as topologically-induced constraints. These control mechanisms have not been thoroughly explored in active fluids. Here, we apply these constraints in two settings: first, in a passive liquid crystal to study near-equilibrium topological structures and second, in an active setting where induced defect loops govern the emergent flows. Another perspective that we examine is the dependency of defects on the surrounding flow structures, a relationship that is not understood in two- or three-dimensions. Our work uncovers that an activity-induced constraint exists between topological defects and the borders of coherent flow structures. Studying topological defects within the framework of these constraints allows for the identification of fundamental relationships within the intricate interplay of coupled orientation and flow fields.

We utilise a novel tensor-based formalism to characterise local properties [29], while also developing our own numerical methods to assemble non-local
information. This includes the twisting and coiling of defect loops, their total length, and variation of local director patterns over the entire defect. Our analysis also reveals the crucial influence of extended nematic and flow structures on the dynamics of topological defects. We provide details on the scalar fields that are used to obtain these conclusions. Further, we detail a numerical hydrodynamic algorithm that is employed to investigate the dynamics of topological defects and colloidal inclusions. This algorithm incorporates thermal stochasticity and has been applied to study variety of fluids and solutes, but the accuracy of resolving topological structure had not been fully recognised. These methods are provided in Chapter §3.

In Chapter §4 we apply our fluctuating hydrodynamics algorithm to study topological constraints in a passive nematic liquid crystal. We embed colloidal particles in a passive nematic and study the associated dynamics and defect structures. Within this study, we explore the topological properties of defect loops which entangle pairs of colloids, and study the relaxation dynamics of defects initialised out of equilibrium. This chapter demonstrates the algorithm’s ability to simulate the dynamics of topological structures.

In Chapter §5 we numerically study topological constraints in an active nematic liquid crystal. We utilise a multiple emulsion; a nematic emulsion which encapsulates a tunable number of inner emulsions (cores), which controls the bulk topology. We reveal a variety of dynamical regimes for a defect-free single core emulsion, which include spontaneous translation and rotation. On introduction of a second core, we explore the rich dynamical behaviours associated with an induced defect loop. The loop exhibits rotational dynamics at low activity, whereas it stretches, splits and recombines at high activity, while adhering to topological constraints. This chapter identifies the important role of geometric constraints on active defect dynamics.

In Chapter §6 we discover that two-dimensional point defects are constrained to reside on specific contours of the flow structure. Through experiments and simulations we explore the nature of this constraint and demonstrate the role of flow structures on defect trajectories and pair creation/annihilation events. This work elucidates the influence of larger scale deformation structures in the activity-induced cross-talk between nematic and flow fields. We demonstrate the generality of this constraint, which extends to three-dimensional topological defect lines and loops.
Overall, this thesis demonstrates how constraints can be utilised to control defects and active flow states. We show that topological constraints establish rules on defect configurations, and geometric or cross-field constraints fine-tune the characteristics of defects and emergent flows.
Chapter 2

Background
2.1 Liquid crystals

2.1.1 Introduction

A little over 100 years ago, the first liquid crystal phases were classified as a mysterious class of materials with intermediate properties between simple solids and isotropic fluids [31]. Liquid crystals are generally composed of molecules with an elongated shape. These molecules align to form long-range orientational order and typically little positional order. This means that they can flow, have an inherent elasticity to restore alignment, and are strongly anisotropic [32]. The classic mesophases are the simple nematic, cholesteric and smectic phases [9]. Nematics (Fig. 2.1a), which are the focus of this thesis, tend to align their molecules along an average apolar direction. Cholesterics (Fig. 2.1b) feature molecules with inherent chirality, and spontaneously form a bulk twisted state with a preferred handedness. In contrast to the nematic phases, smectics (Fig. 2.1c) have a degree of positional ordering into layers, as well as orientational order.

Liquid crystals are most famous for their pivotal role in optical technologies [33]. Their strong responsiveness to external fields [34] and birefringent properties [9] have been utilised in design of pixels [35]. However, among the most recent trends in liquid crystals is the ubiquity of orientational order in biologically active and living systems, including bacterial colonies [36], DNA [37], cytoskeletal fluids [17] and cellular membranes [38]. Accordingly, understanding the self-organisation of active materials is benefiting from an expanding interdisciplinary bridge between biology and the condensed matter physics of ordered media.

This section reviews the fundamentals of nematic liquid crystals, characterising molecular order and orientational elasticity. We then discuss the classification and properties of singularities in the nematic order, which are central to the theme of topological and activity-induced constraints. We close this section by discussing colloidal particles embedded in nematics. This background forms a basis for interpreting structures in confined and active liquid crystals in later chapters.
2.1.2 Nematic order parameters

Order parameters are a vital tool in characterising phases of matter [39]. As measurable properties of materials, they represent the symmetries of the system and illustrate the nature of phase transitions [9]. The average direction \( \mathbf{n} \), that the constituents point in is one of the nematic order parameters. The director has unit magnitude \((\mathbf{n} \cdot \mathbf{n} = 1)\) and is head-tail symmetric \((\mathbf{n} \rightarrow -\mathbf{n})\), meaning that \( \mathbf{n} \) is a line field rather than a vector field. However, the alignment direction alone is not sufficient to describe all features of the molecular ordering. For molecules \( i \) with an orientation \( \mathbf{u}_i \), there can be variation in the degree of alignment along \( \mathbf{n} \). This introduces another parameter, called the scalar order parameter [32],

\[
S = \frac{1}{d - 1} \left( d \left( \mathbf{u}_i \cdot \mathbf{n} \right)^2 - 1 \right),
\]

where \( d \) is the dimension. The scalar order parameter quantifies the magnitude of alignment over an ensemble average in a chosen measuring volume. The values of \( S \) lie in the interval \([-1/2,1]\], where \( S = 1 \) corresponds to perfect nematic order, \( S = 0 \) is isotropic (or uncorrelated orientations) and \( S = -1/2 \) has molecular orientations everywhere in the plane perpendicular to \( \mathbf{n} \).

Instead of working with \( \mathbf{n} \) and \( S \) individually, the entire information of the nematic state can be conveniently obtained from a tensorial averaging of the molecular order [40]

\[
\mathbf{Q} = \frac{1}{N} \sum_i \left( \mathbf{u}_i \otimes \mathbf{u}_i - \frac{1}{d-1} \mathbf{I} \right).
\]
Here, \( Q \) is the tensor order parameter, which is symmetric and traceless. The tensor \( Q \) is valuable as an order parameter because it captures quadrupolar symmetry. This automatically accounts for the head-tail orientational nature, which would otherwise cancel in a dipolar (or vectorial) ensemble average. Furthermore, \( S \) and \( n \) are extracted directly from \( Q \) as the largest eigenvalue and corresponding eigenvector. This thesis utilises the uniaxial form of \( Q \)

\[
Q(r) = S \left( n \otimes n - \frac{1}{d^2} \mathbf{1} \right),
\]

which assumes no special molecular ordering in the perpendicular plane to \( n \). There is a mixture of convention of whether to multiply \( Q \) by the factor \( \frac{d}{d-1} \). We only multiply by this factor for the particle-based simulations in Chapter §4.

2.1.3 Nematic free energy

The emergence of equilibrium global nematic order is determined by the minima of the free energy. This section introduces the free energies that are used to underpin the theoretical descriptions of passive and active liquid crystals. These free energies are used in the continuum modelling of Chapters §5 and §6.

2.1.3.1 Bulk free energy

Many descriptions of the free energies of ordered materials utilise Landau expansions of their order parameters [7]. Within these expansions, only the lowest order terms are kept that capture the essential symmetries and nature of the phase-transitions. For liquid crystals, the bulk contribution to the Landau-de Gennes free energy is [9]

\[
\mathcal{F}_{\text{bulk}} = \int dV \left[ \frac{A}{2} Q^2 + \frac{B}{3} Q^3 + \frac{C}{4} (Q^2)^2 \right],
\]

where each \( Q^p \) to the \( p \)th power is \( \text{Tr}(Q)^p \) and \( A, B, C \) are phenomenological constants. In the nematic phase, \( A \) and \( B \) are negative, and \( C \) is positive to ensure thermodynamic stability. As a simplification, the constants can be written
Figure 2.2  Schematic of liquid crystal deformation modes.  

- a, Splay.  
- b, Twist.  
- c, Bend. The director is represented by orange rods.

in terms of two independent variables [42]

\[ \mathcal{F}_{\text{bulk}} = \int dV \left[ A_0 \left( \frac{1 - \gamma/3}{2} \right) Q^2 - \frac{A_0}{3} Q^3 + \frac{A_0}{4} \gamma (Q^2)^2 \right], \]  

(2.5)

where \( \gamma \) controls the transition and \( A_0 \) sets the magnitude of the free energy. This form is used as the bulk free energy in Chapters §5 and §6.

One detail to note is that the \( Q^3 \) term is only required for three-dimensional liquid crystals to ensure that the phase transition is first order. For two-dimensional systems, the isotropic to nematic transition is continuous, so this term can be omitted.

2.1.3.2 Elastic free energy

While the power expansion in \( Q \) (Eq. (2.5)) describes the bulk free energy for a uniform nematic order, gradients in \( Q \) account for spatial inhomogeneities in the direction of alignment. For interpreting these gradients, we turn to the director description of free energy cost due to deviations from a uniaxial ground state. The Oseen-Frank free energy is [43]

\[ \mathcal{F}_{\text{elastic}} = \int dV \left[ \frac{1}{2} K_1 s^2 + \frac{1}{2} K_2 t^2 + \frac{1}{2} K_3 b^2 \right], \]

(2.6)

written in terms of the basic deformation modes: splay \( s \), twist \( t \), and bend \( b \). The elastic constants associated with each mode are given by the Frank elastic constants \( K_1, K_2, K_3 \). Each mode has a particular geometric meaning:

- **Splay** is a scalar \( s = (\nabla \cdot \mathbf{n}) \), which measures the inwards or outwards tilting
of $\mathbf{n}$. Because $s$ is odd in $\mathbf{n}$, splay is constructed as a vector $\mathbf{s} = \mathbf{n}(\nabla \cdot \mathbf{n})$ (Fig. 2.2a).

- **Twist** is a pseudoscalar $t = \mathbf{n} \cdot (\nabla \times \mathbf{n})$, which measures the left or right-handed rotation of $\mathbf{n}$ in the orthogonal plane to $\mathbf{n}$ (Fig. 2.2b).

- **Bend** is a vector $\mathbf{b} = \mathbf{n} \times (\nabla \times \mathbf{n})$, which measures the curvature of $\mathbf{n}$ in the plane perpendicular to $\mathbf{n}$ (Fig. 2.2c).

For many analytical and numerical purposes, the elastic free energy is simplified by assuming that the splay, twist and bend elastic constants are equal. This assumption is the one-constant approximation $K_1 = K_2 = K_3 = K$ [9], and Eq. (2.6) becomes

$$ F_{\text{elastic}} = \int dV \frac{1}{2} K |\nabla \mathbf{n}|^2. \quad (2.7) $$

The elastic free energy can be written in terms of $\mathbf{Q}$, which further accounts for elastic influences when $S$ is not uniform in space [44]. This is particularly relevant when the scalar order parameter is locally isotropic ($S \approx 0$), which can occur when orientations are frustrated at the cores of topological defects (§2.1.4). In this thesis, modelling the free energy uses the one-constant approximation of the $\mathbf{Q}$ elastic energy

$$ F_{\text{elastic}} = \int dV \frac{1}{2} K |\nabla \mathbf{Q}|^2. \quad (2.8) $$

Combining Eq. (2.8) and Eq. (2.5) gives the free energy

$$ F = F_{\text{bulk}} + F_{\text{elastic}}. \quad (2.9) $$

This free energy creates a lengthscale from the competition between the bulk thermodynamic and elastic energy contributions. This is the nematic coherence length $\ell_K = \sqrt{K/A_0}$, which roughly determines the spatial scale for the variation of nematic ordering, such as the defect core size [9]. Minimisation of $F$ gives the equilibrium director configuration of the nematic order.
2.1.3.3 Phase fields

In Chapter §5 a nematic multiple emulsion is studied. A nematic liquid crystal is encapsulated inside of a droplet and one or two smaller isotropic droplets (cores) are placed inside. To model this system, we require an additional order parameter that represents the distinct nematic and isotropic phases. This order parameter is the phase field $\phi_i$, which can be qualitatively thought of as a concentration field. Here $i \in [1, \cdots, N]$ is the index for each of the $N$ phases.

To ensure a phase separated mixture at equilibrium, the following free energy is used [45]

$$F_{\phi}^{\text{phase}} = \int dV \sum_{i=1}^{N} \left[ \frac{a}{4} \phi_i^2 (\phi_i - \phi_0)^2 + \frac{k_\phi}{2} (\nabla \phi_i)^2 \right]. \quad (2.10)$$

The first term represents a double-well potential that ensures there are two coexisting minima at $\phi_i = 0$ and $\phi_i = \phi_0$. The second term controls the interfacial energy. This has an elastic constant $k_\phi$, which penalises spatial variations of the phase fields near an interface. The combination of these terms establish a surface tension $\sigma = \sqrt{8ak_\phi/9}$ and interfacial thickness $\xi_{\phi} = \sqrt{2k_\phi/\alpha}$ [46].

The bulk properties of the liquid crystal phase are controlled by the Landau de Gennes free energy Eq. (2.5) but with the isotropic-nematic transition parameter a function of the phase fields $\gamma(\bar{\phi})$. Following other works [45, 46], the phase transition parameter is constructed as $\gamma = \gamma_0 + \gamma_s \bar{\phi}$, where $\bar{\phi} = \sum_i^N \phi_i$ and $\gamma_0$ and $\gamma_s$ are constants that determine the boundary of the coexistence region.

To prevent the inner cores from merging, a further free energy term is added

$$F_{\phi}^{\text{rep}} = \int dV \sum_{i,j, i<j} \epsilon \phi_i^2 \phi_j^2, \quad (2.11)$$

which is a soft core repulsion with magnitude controlled by the positive constant $\epsilon$. A physical interpretation of this term could be a surfactant adsorbed onto the droplet interface.

Overall, the free energy for simulating a double emulsion is

$$F_{\phi} = F_{\text{bulk}} + F_{\text{elastic}} + F_{\phi}^{\text{phase}} + F_{\phi}^{\text{rep}}. \quad (2.12)$$
2.1.3.4 Anchoring

Thus far, the free energy descriptions control the material response of the bulk liquid crystal (Eq. (2.9)) and nematic emulsion (Eq. (2.12)). In many practical situations, it is desirable to externally impose specific features on the equilibrium nematic order. This can be done through surface anchoring, where an easy axis is imposed on a boundary for the nematic molecules to align with. Experimentally, this is achieved through chemical or mechanical surface treatment [47, 48]. Anchoring has been invaluable in optical technologies for fixing a desired background alignment, and controllably switching the orientation using external fields to modulate polarised light [49]. In this thesis, anchoring is used in all results chapters as a mechanism to impose geometric and topological features onto the bulk director. The mechanisms for controlling topology are discussed in §2.1.7. Here, we detail the types of anchoring alignment and free energies used for the numerical implementations.

Two types of anchoring alignment are typically imposed [9]:

- **homeotropic**: normal alignment at the surface (Fig. 2.3a).
- **planar**: tangential alignment at the surface (Fig. 2.3b). In three-dimensions, planar anchoring is further distinguished between planar-aligned and planar-degenerate anchoring. Planar-aligned means that molecular orientations have an imposed easy axis within the tangent plane of
the surface, whereas planar-degenerate can align parallel to any tangential direction.

Surface anchoring is built into the free energy framework by including a surface free energy term for each boundary. A commonly used anchoring energy for imposing an alignment easy axis is

$$F_{\text{anch}} = \frac{1}{2} W \int dS (\mathbf{Q} - \mathbf{Q}^0)^2,$$

which penalises deviations of \( \mathbf{Q} \) from a surface-preferred order parameter \( \mathbf{Q}^0 \) with an energy cost \( W \). This anchoring energy (Eq. (2.13)) is well suited to modelling homeotropic anchoring conditions. We provided this anchoring energy as the simple case for achieving homeotropic anchoring in free-energy modelling. However, the two applications of homeotropic anchoring in Chapter §4 and §5 use alternative methods. The anchoring methods for §4 are detailed in §3.2.3. For multiple emulsions (Chapter §5), imposing director alignment at the nematic interfaces uses

$$F_{\phi}^{\text{anch}} = W_\phi \int dV \sum_{i} N \left[ (\nabla \phi_i \cdot \mathbf{Q} \cdot (\nabla \phi_i)) \right],$$

where \( W_\phi < 0 \) enforces homeotropic anchoring [50].

For anchoring that is planar-degenerate, the free energy seeks to obtain a minima where \( \mathbf{Q} = S_0 (\mathbf{v} \otimes \mathbf{v} - \frac{1}{d} \mathbf{1}) \). Here, \( S_0 \) is the surface-preferred degree of order and \( \mathbf{v} \) is an arbitrary orientation parallel to the surface. To achieve this, two terms are required [51]

$$F_{\text{anch}} = \int dS \left[ W_1 \left( \mathbf{Q} - \mathbf{Q}^\perp \right) : \left( \mathbf{Q} - \mathbf{Q}^\perp \right) + W_2 \left( \mathbf{Q} : (\mathbf{Q} - S_0^2) \right) \right].$$

The first term imposes alignment on the tangent plane with an energy cost \( W_1 \). Here, \( \mathbf{Q} = \mathbf{Q} + \frac{1}{d} S_0 \mathbf{1} \) and \( \mathbf{Q}^\perp = \mathbf{P} \cdot \mathbf{Q} \cdot \mathbf{P} \) in terms of the projection operator \( \mathbf{P} \) on the plane perpendicular to the surface normal. The second term sets the degree of order \( (S_0) \) on the plane, with energy cost \( W_2 \). Planar-degenerate anchoring is used in Chapter §6.

For the imposed-constraints theme of this thesis, greatest control of topological and geometric features desire strong anchoring. Strong refers to nematic orientations aligning tightly with the anchoring axis, as opposed to weak
anchoring for which there can be variation of the molecular ordering at the surface. To quantify the strength of anchoring, the Kleman-de Gennes extrapolation length is constructed [9]

\[ \xi_K = \frac{K}{W}, \]  

which measures the competing influence of nematic elasticity against anchoring strength. In Chapter §4, we utilise \( \xi_K \) to compare methods of anchoring strength in a particle-based hydrodynamics solver.

### 2.1.4 Introduction to topological defects

The emergent properties and dynamics of ordered media are strongly influenced by topological defects [52]. These are singularities that form in materials with broken symmetries, such as superfluid helium [6], ferromagnets [8], and crystals [7]. For nematic liquid crystals, the breaking of rotational symmetry permits defects in orientational order, known as disclinations—which can exist as isolated points or lines, either terminating at boundaries or forming closed loops [10] [52]. Topological defects are fundamental to this thesis. This section will detail the topological and geometric properties of topological defects in two- and three-dimensions.

One of the most influential features of topological defects is their role in imposing constraints on material response to internal or external stimuli [7]. This is because, as discontinuous structures, they cannot be smoothly removed by any continuous transformation. Characteristic deformation patterns in the disclination proximity render defects as excitations, and facilitate defect-interactions through minimising nematic gradients. Their large distortion means that defects are a signature of a liquid-crystal that is out-of-equilibrium, and strongly control the relaxation pathways towards equilibria [53].

To characterise the essential properties of defects, homotopy theory has provided the natural framework since the 1970s [52] [54] [55]. Scalar values are sought out that describe how discontinuities are similar up to continuous deformations of their surroundings. The process of classifying defects involves enclosing the defect with appropriate measuring surface, and studying the nematic textures on this surface [52]. Possible textures form an order parameter space, which can vary depending on the symmetry of the order and dimension. Constructing
maps between the measuring domain and the order parameter space results in
the formation of homotopy classes, grouping features that remain unchanged
under continuous deformation. The homotopy group structure forms the basis
for conservation laws of topological charges, which dictate how defects are created
and annihilated [10].

2.1.5 Topological defects in two-dimensions

In two dimensions, the nematic director field $\mathbf{n}(\mathbf{r})$ can be written in terms of an
orientation angle field $\theta(\mathbf{r})$

\[\mathbf{n}(\mathbf{r}) = (\cos \theta(\mathbf{r}), \sin \theta(\mathbf{r})).\]  

(2.17)

Since nematics are invariant under the transformation $\mathbf{n} \rightarrow -\mathbf{n}$, the angle $\theta$ forms
an order parameter space that takes values in the interval $[0, \pi]$ with endpoints
identified [52]. This space is the real projective line $\mathbb{R}P^1$. Defects in $\mathbf{n}(\mathbf{r})$, are
point singularities that can be classified by constructing a measuring loop that
surrounds the defect core and counting how many times $\theta(\mathbf{r})$ turns on a closed
anticlockwise circuit. This assigns defects a topological charge from the winding
number [7]

\[k = \frac{1}{2\pi} \oint d\theta.\]  

(2.18)

If the director enclosed by the measuring loop is devoid of defects, Eq. (2.18)
returns $k = 0$. Otherwise, $k$ returns an integer or half-integer value $\frac{1}{2}\mathbb{Z}$. Half-
integer values are possible since $\pi$ turns of $\theta$ are permitted by $\mathbf{n} = -\mathbf{n}$. More
formally, the winding number is an element of the homotopy group $\pi_1(\mathbb{R}P^1) = \frac{1}{2}\mathbb{Z}$, where $\pi_1$ is the fundamental group, the group structure corresponding to measuring loops. Director profiles for $k \in [-1, -1/2, +1/2, 1]$ are shown in Fig. 2.4.

Minimum energy solutions of the Frank free energy Eq. (2.6), that satisfy Eq. (2.18), give the orientation angle field

$$\theta = k\phi + \theta_0,$$

(2.19)

where $\phi = \tan^{-1}(y/x)$ is the polar angle and $\theta_0$ is an arbitrary orientation. The winding number $k$ dictates the local symmetry of the director field (Fig. 2.4), but also controls the energy cost associated with a defect. The elastic energy of a defect scales with $k^2$ [9], meaning that $k = \pm 1/2$ vastly dominate systems with nematic defects, while $|k| \geq 1$ are rare.

The conservation of topological charge governs how defects are created and annihilated [52]

$$\sum_i k_i = 0,$$

(2.20)

where the sum is taken over individual defects with index $i$. For example, Eq. (2.20) allows $+1/2$ and $-1/2$ defects to be created and annihilated in pairs, and single $+1$ defects can split into two $+1/2$ defects. Under this constraint, the free energy controls the details of defect interactions and evolution (Eq. (2.9)).

2.1.6 Topological defects in three-dimensions

Nematic textures in three-dimensions are topologically distinct from two-dimensions, since the director can rotate out of plane, and orient in any direction on a unit sphere (with antipodal equivalence) [10]. This order parameter space corresponds to the real projective plane $\mathbb{R}P^2$. For classifying defects, the choice of measuring surface varies depending on whether the disclination is a point, line or loop.
2.1.6.1 Point defects

To classify three-dimensional point defects, the measuring surface is a sphere $S^2$. By writing the director as a vector $\mathbf{n}(\theta, \phi)$, the point charge $p$ (also known as hedgehog charge), is measured from the number of times the director wraps around the measuring sphere \[^{56, 57}\]

$$p = \frac{1}{8\pi} \int dS \epsilon_{ijk} \mathbf{n} \cdot (\partial_j \mathbf{n} \times \partial_k \mathbf{n}). \quad (2.21)$$

Here, the integral is taken over the spherical surface enclosing the core. In Eq. (2.21), $\epsilon_{ijk}$ is the Levi-Civita, $x_i$ are Cartesian coordinates and summation convention is applied. Throughout, $p$ corresponds to the 3D topological point/hedgehog charge, while $k$ corresponds to the winding number, which is equivalently the topological charge of a defect in 2D. The point charge returns values from the second homotopy group, $\pi_2(\mathbb{R}P^2) = \mathbb{Z}$, which are integer values.

By convention, director patterns associated with $p = 1$ are called radial hedgehogs (Fig. 2.5a) and $p = -1$, hyperbolic hedgehogs (Fig. 2.5b) \[^{10}\]. In principle, combinations of hedgehog charges are additive. However, there arises some ambiguity on whether point defects add or subtract, since $p$ is odd under $\mathbf{n} \to -\mathbf{n}$ (Eq. (2.21)). This means that combinations of two point charges could either combine to $p = 0$ or 2. Therefore, in interpreting the conservation of topological
point charge

\[ \sum_i p_i = 0 \pmod{2}, \quad (2.22) \]

which accounts for the sign ambiguity. Charged point defects are rarely observed in bulk systems as they cost large elastic energy \[9\]. However, they can be stabilised by surfaces, which is discussed in §\[2.1.7\] and utilised in Chapters §\[4\] and §\[5\].

### 2.1.6.2 Disclination lines

In systems with confining or embedded surfaces, disclination lines form, with endpoints connected to surfaces \[58\]. In a similar manner to two-dimensional point defects, these structures are characterised by placing measuring loops around the line and computing the local winding number \[10\]. However, because the director can rotate out of plane, \(k\) may smoothly transform between \(+1/2\) and \(-1/2\) profiles on the same line—giving topological equivalence to both profiles in 3D (Fig. \[2.6a\]). Disclination lines with integer winding numbers \(k = \pm 1\) are homotopic (equivalent under continuous transformation) to a defect-free state, as the director can rotate out of plane and form an escaped configuration, removing the singularity \[10\]. This means that topology only distinguishes between two types of disclination line \(\mathbb{Z}_2\): trivial (integer winding) and non-trivial (half-integer winding). These two elements belong to the group structure \(\pi_1(\mathbb{R}P^2) = \mathbb{Z}_2\), the fundamental group \(\pi_1\) of the order parameter space \(\mathbb{R}P^2\).

Despite the limited topological variety of disclination lines, the geometric details of the emergent director patterns can be rich. This can be uncovered by the relationship between two locally-defined, and continuously-varying, vectors defined at each point of the disclination \[59\]: the line tangent vector \(\mathbf{T}\), and the rotation vector \(\Omega\) specifying the normal of the plane that the director winds (Fig. \[2.6a\]). By constructing the twist angle \(\cos \beta = \Omega \cdot \mathbf{T}\), \(+1/2\) director profiles are identified as \(\cos \beta = 1\) \(\Omega\) parallel to \(\mathbf{T}\), \(-1/2\) director profiles as \(\cos \beta = -1\) \(\Omega\) anti-parallel to \(\mathbf{T}\) and twist-type intermediate profiles if \(\cos \beta = 0\) \(\Omega\) perpendicular to \(\mathbf{T}\). Identifying these profiles not only give a convenient interpretation of disclination structure, but provide insight for dynamical behaviours of disclinations, such as twisted defects in phase transitions \[60\], behaviours of patterned defects \[58\ \[61\], and motile behaviours in active
Figure 2.6  **Schematic of topological line and loop defects.**  

*a*, Disclination line (coloured tube) smoothly transitions from +1/2 to −1/2 profiles via an intermediate twist (green). The director is represented by orange rods. The line is coloured by \( \cos \beta = \Omega \cdot T \), where \( \Omega \) is the director winding plane (red arrows) and \( T \) is the line tangent (blue arrows). A plus half profile forms when these vectors are parallel (\( \cos \beta = +1 \); yellow), a twist profile when perpendicular (\( \cos \beta = 0 \); green), and a minus half profile when anti-parallel (\( \cos \beta = -1 \); purple).  

*b-d*, Defect loops illustrated the same as in *a*.  

*b*, Charge-neutral wedge-twist loop alternates once between a +1/2 profile and −1/2 profile, smoothly connected via twist. The rotation vector, \( \Omega \), is uniform within the plane of the loop.  

*c*, Neutral pure-twist loop with \( \Omega \) uniformly oriented perpendicular to the loop.  

*d*, Charged Saturn ring with pure −1/2. The rotation vector turns by \( 2\pi \) over the loop.

2.1.6.3 Disclination loops

Disclinations can also form loops—defect lines with endpoints joined to form a closed structure. Disclination loops are self-generated by active nematics [24], and stabilised by colloidal particles [11], consequently dominating the deformation patterns and elastic free energies. Here, we will first review the topological properties of disclination loops and then discuss the types of loops that are relevant to this thesis.
Topological classification

In comparison to the other disclination structures described in this section, which have local classifications, disclination loops are particularly intriguing from a topological perspective because they inherit the same local winding patterns as disclination lines, but additionally contain non-local information of how these textures vary as a loop reconnects with itself [62]. Further, disclinations can be enclosed by a spherical measuring surface, and may return a hedgehog charge (Eq. (2.21))—demonstrating that loops also have features of point defects [10]. To capture the local and non-local nature of their topology, disclination loops are classified using toroidal measuring surfaces [63]. Here, we explain how the toroidal classification identifies four possible defect classes.

The torus can be parameterised in terms of a local meridional circuit $u$ and a non-local longitudinal circuit $v$ (Fig. 2.7), as following the framework by Čopar and Žumer in [1]. Then the director on the toroidal surface can be defined as $n(u, v)$. Once a reference director profile is established $n(u, 0)$, the director elsewhere on $v$ can be matched by the rotation transformation $R(v)$

$$n(u, v) = R(v)n(u, 0).$$  \hspace{1cm} (2.23)
By writing $R(v) = R_0(v)R'(v)$, the transformations can be decomposed into two operations; $R_0(v)$ transforms the Cartesian basis $\{e_x, e_y, e_z\}$ into a local basis with $e_z$ axis aligned to the disclination loop tangent $T$. We denote the local basis as $\{m, m_\perp, T\}$, where $m$ and $m_\perp$ are unit vectors that form an orthonormal triad with $T$. The operator $R'(v)$ performs transformations about the local basis. On closing the loop ($v = 2\pi$), the initial conditions ($v = 0$) must be maintained. The tangent vector $T(v)$ has a continuous circulation direction and so $T(2\pi) = T(0)$. The director must also return back to the start orientation, up to head-tail symmetry, $n(u, 2\pi) = \pm n(u, 0)$. To ensure the closure constraints on $n$ and $T$, the transformation $R(2\pi)$ is constrained to take four particular forms, encoding the topology of the loop. The limited degrees of freedom arise since director can flip on return $n(u, 0) \rightarrow -n(u, 2\pi)$ or the local frame can change parity, $\{m, m_\perp, T\} \rightarrow \{m_\perp, m, T\}$.

To capture both properties, studies of $R(2\pi)$ adopt the quaternion representation [1]. For a general rotation transformation

$$q_Q = \cos \frac{\phi}{2} + (a_x i + a_y j + a_z k) \sin \frac{\phi}{2},$$

(2.24)

where $a = (a_x, a_y, a_z)$ is a specified rotation axis and $\phi$ is the rotation angle about that axis. The unit quaternions ($i$, $j$, $k$) represent the rotation basis, which for $R(v)$ is $\{e_x, e_y, e_z\}$, or $R'(v)$ is $\{m, m_\perp, T\}$. Note that here $k$ is a quaternion and not the winding number. The quaternions obey the relations $i^2 = j^2 = k^2 = -1, ij = -ji = k, jk = -kj = i$ and $ki = -ik = j$. From Eq. (2.24), rotation transformations by $2\pi$ about any axis yield $q_Q(2\pi) = -1$.

Representing $R_0(2\pi)$ and $R'(2\pi)$ using quaternions, one finds that $R_0(2\pi) = -1$ since the local coordinate frame simply rotates by $2\pi$ on the loop circuit [1]. Therefore, all four of the transformations are encoded $R'(2\pi)$. Since $R'(2\pi)$, refers to the local basis in which $k$ is aligned with $T$, $R'(2\pi)$ is independent of $i$ and $j$. This is because any net rotation about $i$ or $j$ will not satisfy $T(2\pi) = T(0)$. Therefore, the four possibilities can be encoded by one of $R'(v) \in \{-1, -k, 1, k\}$. Combining with $R_0(2\pi) = -1$,

$$R(2\pi) \in \{1, k, -1, -k\} = k''.$$

(2.25)

The notation here is that $\{\ldots\}$ denotes the cyclic group of allowed rotations, which can be accessed by the integer $\nu \in \{0, 1, 2, 3\}$. These elements of $\mathbb{Z}_4$ coincide with the global defect index $\nu$ first proposed by Janich in 1987, characterising each of
the four possible loop topologies \[63\].

For the purpose of this thesis, we are concerned only with \(\nu = 0, 2\) which correspond to unlinked loops that have no hedgehog charge (neutral) and a hedgehog charge (charged) respectively \[1\]. The other classes \(\nu = 1, 3\) are linked disclination loops, which simulations and experiments suggest do not naturally occur in nematic fluids with activity or colloidal particles \[24, 64\]. The details of obtaining \(\nu\) from \(\mathcal{R}\) provides an understanding of the topological classes from geometric arguments. This framework will be used for exploring constraints on purely -1/2 type disclinations that accompany nematic colloids, which is relevant for analysis performed in Chapter §4.

**Geometry**

As we saw previously with disclination lines, the geometric description of local disclination profiles can be identified through the rotation vector \(\Omega\) and the tangent vector \(T\). For disclination loops, this is helpful to the themes of this thesis for two purposes. The first is that deformation profiles are important for understanding active motility behaviours (§2.2.6.2). The second is that the twist angle (\(\cos \beta = \Omega \cdot T\)) is insightful for visually distinguishing between different types of loops.

For uncharged loops (\(\nu = 0\)), distinctions are made between wedge-twist loops (Fig. 2.6b) and pure twist loops (Fig. 2.6c). Wedge-twist loops have a +1/2 wedge profile that is concurrent on the same loop with a −1/2 wedge, with twist smoothly connecting between them \[24\]. In contrast, twist loops observe only twist and have no wedge profiles. Both loops are associated with uniform \(\Omega\) along the loop (red arrows). For charged loops (\(\nu = 2\), in passive liquid crystals only purely -1/2 disclination loops have been reported \[3\]. The geometric patterns of charged disclination loops in active scenarios have not previously been addressed and are one of the themes visited in Chapter §5.

2.1.7 **Connection between defects and surfaces**

Imposing geometric or topological constraints to the director field is most simply performed through tuning the geometry of surfaces \[56\]. With application of strong surface anchoring, surface-related curvatures can be imprinted onto the director field itself, and can form topological defects. However, a clear
distinguishing factor between the types of defects imposed, depends on whether
the anchoring is homeotropic or planar.

For the planar case, defects form directly on the imposed surface and are referred
to as *surface defects*. While the total number of surface defects may be dependent
on internal or external factors, the overall topological charge (sum of all winding
numbers) is fixed by the surface geometry. This constraint is, in fact, applicable
to any form of tangential vector (or line) field on a surface, and is known as the
the Poincare-Hopf theorem [65]

\[ \sum_i k_i = \chi. \]  

(2.26)

Here, \( \chi \) is the Euler characteristic which is a topological invariant of the geometry
of the surface, and \( k_i \) is the winding numbers of each surface defect (Eq. (2.18)).

The Euler characteristic is defined by converting the surface into a polygonal
mesh and counting the number of vertices \( V \), edges \( E \) and faces \( F \)

\[ \chi = V - E + F, \]  

(2.27)

which gives the same value of \( \chi \) independent of the choice or resolution of mesh.

An even simpler interpretation is in terms of the *genus* of the surface \( g \), which
simply counts the number of holes

\[ \chi = 2(1 - g). \]  

(2.28)

For example, a torus has one hole \( (g = 1) \) so \( \chi = 0 \) by Eq. (2.28) and the surface
may remain defect free by Eq. (2.26). Alternatively, a spherical surface has no
holes \( (g = 0) \), so \( \chi = 2 \) and the total charge of all defects must add up to
\( k = 2 \). The Poincare-Hopf theorem (Eq. (2.26)) enters when considering planar
anchoring on colloidal spheres (Chapter §[4]).

The homeotropic anchoring case is different from planar anchoring in that any
imposed topological defect is formed in the bulk, rather than on the surface. This
is because each surface imprints on the immediate director a hedgehog charge \( p \)
(Eq. (2.21)) that depends on the surface invariant \( \chi \) (or \( g \)) [56]

\[ p = \pm \chi/2 = \pm(1 - g). \]  

(2.29)

However, whether a topological defect is induced or not depends on if the *global*
charge is satisfied by each surface addition. In particular, the sum of all of
hedgehogs inside the fluid must equal the imposed hedgehog charge $p$ of the
confining geometry (mod 2). If this is not satisfied by the surfaces alone, then
charged topological defects must be formed by the bulk fluid.

In this thesis, equation Eq. (2.29) arises in two different situations. First in
Chapter §4, where we study nematic colloids, each spherical colloidal inclusion
with homeotropic anchoring forms a hedgehog $p = 1$. Second in Chapter §5
emulsions are studied in situations with inverted and tunable numbers of inner
emulsions. Inverted emulsions (i.e. the fluid inside of a droplet) mean that
Eq. (2.29) forms a global constraint, and the inner emulsions tune the number of
imposed hedgehogs.

2.1.8 Colloidal inclusions

The section expands on the emergent physics that colloidal inclusions ($\chi = 2$) with homeotropic and planar anchoring impart on their liquid crystalline
hosts. We focus on the homeotropic anchored case, as planar anchoring is only
considered briefly in Chapter §4.

2.1.8.1 Competition between anchoring and deformation

Embedding particles in liquid crystals induces an abundance of interesting
topological and elastic behaviours [11, 66], emerging from the competition
between anchoring constraints and free-energy minimisation of the director. To
appreciate these behaviours, it is helpful to define a dimensionless number that
quantifies this competition [12]. For a colloidal particle with radius $R$, the bulk
director penalises deformation with an elastic energy $\sim KR$ (Eq. (2.6)). On the
other hand, the anchoring energy scales as $\sim WR^2$ (Eq. (2.13)). The ratio of
these energies form a dimensionless number

$$Z = \frac{WR}{K}.$$  

For small $Z$, the inclusion only weakly deforms the local director. However, at
large $Z$, the director becomes frustrated, leading to the formation of a hedgehog
charge $p = 1$ (Eq. (2.29)). Consequently, the bulk director nucleates a topological
defect to satisfy charge conservation (Eq. (2.22)). For a single colloid, three
possible defect structures have been observed: i) a hyperbolic point hedgehog [67], ii) a purely -1/2 disclination ring that surrounds the colloidal equator (Saturn ring) [68, 69] and iii) a surface ring [70]. Of these, the hedgehog defect is associated with the largest values of $Z$ and the surface ring the lowest. The exact values of the $Z$ transitions between these states have been debated [66, 71]. In Chapter §4, nematic colloids are studied at large, but finite, $Z$ where defect loops dominate.

### 2.1.8.2 Electrostatic analogy

One perspective of nematic colloids that has captured interest is the potential for designing soft materials through colloidal self-assembly [72, 73]. This self-assembly occurs because colloids form far-field deformation, which is influenced by the type and positioning of accompanying topological defects [11]. Elastic forces form between colloids to minimise their deformation, which is measured in Chapter §4. To make predictions on the nature of the far-field interactions, colloid-associated deformation is often simplified using electrostatic analogies [57].

For an isolated colloid, with a far-field director aligned with $e_z$, the director can be approximated as $n \approx e_z + \delta n$ [74], assuming a small perturbation $\delta n =$
\( \delta n_x \mathbf{e}_x + \delta n_y \mathbf{e}_y \) in the perpendicular plane \( \mathbf{e}_x, \mathbf{e}_y \). Director solutions are found by minimising the Frank free energy (Eq. (2.7)), which result in the Euler-Lagrange equation for the perturbation field

\[
\nabla^2 \delta \mathbf{n} = 0.
\]

(2.31)

In analogy with electrostatics, solutions of the Laplace equation can be expanded as a multipoles \[57, 74]\n
\[
\begin{align*}
\delta n_x &= m \frac{x}{r^3} + p \frac{xz}{r^5} + 3c \frac{\mathbf{e}_x}{r^5}, \\
\delta n_y &= m \frac{y}{r^3} + p \frac{yz}{r^5} + 3c \frac{\mathbf{e}_y}{r^5}.
\end{align*}
\]

(2.32)

Here, \( m, p \) and \( c \) are the monopole, dipole and quadrupole elastic moments and \( r \) is the radial distance from the colloid \[75\]. Higher order terms rapidly decay with distance and can be neglected \[74\]. The dominant terms in the expansion can be identified from the symmetries of the colloid-defect complex and far-field alignment. For instance, the companion hyperbolic-hedgehog defect (Fig. 2.8a) and colloid combination has only axial symmetry. This symmetry is incompatible with the monopole terms, but compatible with the dipole and quadrupole terms. Further if the hedgehog switches to the opposite side of the colloid, then the dipolar part can accommodate a sign change. Therefore, the hedgehog-colloid complex form an elastic dipole \[57\]. Alternatively, the Saturn ring (Fig. 2.8b) and surface defects configurations are considered to be elastic quadrupoles, since both the monopole and dipole terms are incompatible with the axial and equatorial symmetry of the colloid-defect complex \[66, 76\].

The director solution in Eq. (2.32) considers isolated colloids. However, the electrostatic analogy is particularly useful for understanding the interactions between colloids or their confining surfaces \[75\]. This has been observed and verified in studying the power-law interactions \[67, 77, 78\] and angular attraction-repulsion behaviours between combinations of dipoles and quadrupoles \[75\]. The elastic forces between colloids and confining walls find that the power-law repulsion can be understood as dipole-dipole or quadrupole-quadrupole interactions—in line with theoretical treatment using the method of images \[79\] or Green functions \[75\].
2.1.8.3 Entangled disclinations

Disclination structures accompany more than one homeotropic-anchored inclusion as well. This is relevant for the study of induced topological constraints in passive (Chapter §4) and active (Chapter §5) nematics. With each inclusion contributing $p = 1$ (Eq. (2.29)), a rich and non-trivial topological interplay can occur where disclinations are required to balance the global charge (modulo 2).

The first hints of exotic defect structures were identified by Guzman et al. in 2003 [80] and Araki and Tanaka in 2006 [81], finding disclinations that can encircle two colloidal particles. Such defect structures have been termed entangled disclinations and many possible configurations have since been observed (Fig. 2.9a,b), which multiply up in complexity with additional inclusions [82–84]. Entangled configurations are metastable and can be formed by locally melting the director [3]. However, entanglement can naturally arise in the case of many colloids (Fig. 2.9c). Above a critical colloidal volume fraction, a single percolated disclination wraps around colloidal clusters [84], contrasting with individual Saturn rings, which are favoured at low volume fractions.

Entangled disclinations are found to have -1/2 profiles throughout their entire structure [3], similar to the Saturn ring (Fig. 2.6d). Because of this constraint, Čopar and Žumer revealed that a connection can be made between the $-1/2$ winding along the loop and the topological class $\nu$ [1]. Here, we outline this mapping, and use the resultant tools in Chapter §4.

The connection between $-1/2$ disclination loop geometry and topological class
Figure 2.10 *Angles used to identify the minus half defect profile windings.* Left: The $-\frac{1}{2}$ profile (red rods) is parameterised in terms of $u$, where $u = 0$ is a reference director orientation (tangentially oriented in this case). The vector $\mathbf{m}$ is defined at $u = 0$ and $\mathbf{m}_\perp$ is orthogonal. The director orientation relative to $\mathbf{m}$ is indicated by the angle $\alpha$. Right: A director rotation of $\phi = \pi$ about the $z-$axis corresponds to a $-\frac{1}{2}$ profile rotation of $\psi = \frac{2\pi}{3}$. Adapted from [1].

builds on the toroidal parameterisation (Eq. (2.23)), which maps a reference director $\mathbf{n}(u, 0)$ to another point on the loop $\mathbf{n}(u, v)$ via the transformation $\mathcal{R}(v)$. As discussed in §2.1.6.3, $\mathcal{R}(2\pi)$ encodes the topological properties of the disclination, returning one of four classes $\nu \in \mathbb{Z}_4$. In the special case of $-\frac{1}{2}$ disclinations, $\mathcal{R}(2\pi)$ is simplified since the director always resides in a plane with normal vector $\mathbf{\Omega}$ anti-parallel to $\mathbf{T}$. In the local frame $(\mathbf{m}, \mathbf{m}_\perp, \mathbf{T})$, this means that the director rotation axis is fixed along $\mathbf{T}$. An angle can be specified $\cos \alpha(u, v) = \mathbf{n}(u, v) \cdot \mathbf{m}$. This identifies the director rotation about $\mathbf{T}$ as $\phi(v) = \alpha(u, v) - \alpha(u, 0)$. This director rotation $\phi(v)$ can be mapped to the profile rotation by $\phi(v) = \frac{3}{2} \psi$ [1]. The mapping is visualised in Fig. 2.10, which demonstrates that a $\phi = \pi$ rotation of the director is equivalent to a $\psi = \frac{2\pi}{3}$ rotation of the $-\frac{1}{2}$ profile.

The mapping between the director and profile rotation is helpful because the $-\frac{1}{2}$ profile has a constrained number of total rotations along the loop. This can be labelled by the self-linking number $\text{Sl} = \frac{\psi(2\pi)}{2\pi}$ [85, 86]. The self-linking number is a topological invariant traditionally associated with ribbons [87]. Ribbons are
distinct from one-dimensional curves since they are associated with a tangent curve $T$ and a perpendicular framing vector $w$, which describes the ribbon orientation. Therefore, the analogy with $Sl$ treats $-\frac{1}{2}$ disclinations as ribbon, but with three-fold symmetry accounted for in the allowed framing rotations. Hence, $Sl$ is permitted to take third integer values $Sl \in \frac{n}{3}$.

The topological classification can be obtained through the deconstruction $R(v) = R_0(v)R'(v)$ (§2.1.6.3). As before $R_0(2\pi) = -1$, while Eq. (2.24) gives

$$R'(2\pi) = \cos \frac{(3/2)2\pi Sl}{2} + k \sin \frac{(3/2)2\pi Sl}{2}.$$ (2.33)

This transformation is in terms of the unit quaternion $k$, which is aligned with the local tangent axis $T$. Combining $R_0(2\pi)$ and $R'(2\pi)$, the possible rotations are restricted to take the form $R(2\pi) = k^{3Sl+2}$. Therefore, the mapping between the index $\nu$ and the ribbon invariant $Sl$ is

$$\nu = 3Sl + 2 \pmod{4}.$$ (2.34)

This mapping implies that uncharged loops with $\nu = 0$ can be identified as $Sl = \frac{2}{3}$ and charged loops with $\nu = 2$ as $Sl = 0$.

A benefit of using ribbon invariants to characterise $-\frac{1}{2}$ loop topological classification is that the self-linking number can be calculated from geometric properties of the disclination. The Călugăreanu-White-Fuller theorem relates the self-linking number to the writhe (Wr) and twist (Tw) of the loop [88]

$$Sl = Wr + Tw.$$ (2.35)

Writhe is a non-local geometric property that describes the change of direction of the tangent along the curve [86], or the coiling of the curve. This is calculated by the double integral

$$Wr = \frac{1}{4\pi} \oint_C ds \oint_C ds' T(s) \times T(s') \cdot \frac{r(s) - r(s')}{|r(s) - r(s')|^3},$$ (2.36)

where $r(s)$ are position vectors for points along the loop, $L$ is the length of the loop, $T(s) = \frac{dr(s)}{ds}$ is the local tangent vector [65], and $C$ is a closed curve composing the disclination loop. Twist measures the rotation of the framing $w$. 

30
The writhe and twist are calculated in Chapter § 4 for characterising -1/2 disclination configurations. However, the ribbon analysis is not extendable to the active nematic disclination loops in Chapter § 5, which have a variety of disclination profiles. The twist $T_w$ of the ribbon, and elastic deformation twist $t = n \cdot (\nabla \cdot n)$ have the same name but describe different geometric quantities. To avoid future confusion, we will refer to twist as the deformation mode $t$. If the ribbon property is required, then the label $T_w$ will accompany the description.
2.2 Active nematics

2.2.1 Introduction

Active materials are composed of individual components that consume energy from their environment to perform mechanical work, which is a feature they share with living matter [89]. This active work can drive collective motion, such as spontaneous flow [90–92], or generate intrinsically non-equilibrium steady-state self-organised structural order [93, 94]. The connection between activity and self-organisation motivates the role of symmetry breaking and order parameters in active matter [13]. Furthermore, the individual components may possess their own intrinsic symmetries. For instance, polar units have a well-defined head and tail and may be self-propelled in the direction of their orientation. Such polar units may align to form a polar vector field $\mathbf{P}$ [95–97]. Alternatively, they might antialign and cancel their polarity to form a head-tail symmetric nematic phase described by the tensor $\mathbf{Q}$ [98, 99]. Nematic phases can form also from apolar units [100], that have zero mean motion. Many examples of active units have a rod-like elongated nature, and can form states with nematic orientational order [16, 36]. Viewing active matter in terms of their symmetries simplifies continuum descriptions, in terms of evolution of order parameter fields and their structural properties, such as deformation and their singularities [101–103]. Such systems have been described as active liquid crystals [104].

This section provides background for active nematic liquid crystals. First we discuss the form for the active stress and how it drives flows through the continuum active nematohydrodynamic equations. We then discuss how long-wavelength orientational fluctuations drive a hydrodynamic instability into a turbulent-like flow state with dynamic structures in the orientation and velocity fields. The properties of active nematic defects in two and three dimensions will then be reviewed. The literature to-date has focussed on two-dimensional films and this section will follow that precedent, but will briefly discuss recent studies in three-dimensions.
Figure 2.11 Schematic of types of active nematic stress. a, Extensive stress with force (red) directed outwards along particle orientation (orange rod). b, Contractile stress with inwards force. Lilac arrows shows the local dipolar flows associated with each type of stress.

2.2.2 Active nematic stress

For active liquid crystals with apolar ordering, the stress tensor

\[ \sigma^\zeta = -\zeta Q, \]

is constructed with nematic symmetry [14]. The phenomenological parameter that describes the sign and magnitude of the active stress is the activity \( \zeta \), which can be thought of as a fuel, converting chemical energy into motion. When \( \zeta > 0 \), the stress extends outwards along \( n \), known as extensive stress (Fig. 2.11a), whereas when \( \zeta < 0 \), the stress contracts inwards, called contractile stress (Fig. 2.11b).

The most popular experimental system for testing active nematic emergent order is in vitro microtubules cross-linked by kinesin molecular motors, combined with a depletion agent to promote the formation of densely ordered bundles [17]. The dense ordering is required for a nematic phase, since microtubules are polar entities. Microtubules and other biopolymers are a staple in the cell’s cytoskeletal fluids [15], with molecular motors that walk along the filaments, exerting sliding forces along the filament axis—to push outwards two adjacent filaments (extensive), or to pull in (contractile). Microtubules are primarily associated with extensive active stress [17], but another biopolymer, actin, can form contractile stress through the action of myosin molecular motors [105]. In both biopolymer cases, the motion of the molecular motors is fuelled by Adenotriphosphate (ATP), which is hydrolysed into Adenodiphosphate (ADP).
The concentration of ATP modulates the activity \( \zeta \), and, hence, is responsible for maintaining the out-of-equilibrium behaviours \( \eta \).

The results in Chapter \( \S5 \) and \( \S6 \) are centred on the extensile active nematics formed by the *in vitro* microtubule-kinesin system. This is the basis for the experimental analysis in Chapter \( \S3 \) and motivates the continuum extensile active nematic models that are detailed in the next section.

### 2.2.3 Active nematic hydrodynamics

Building from active stress towards a full description of the evolution of the hydrodynamic fields depends on the nature of the hydrodynamic interactions. Distinctions are made between *dry* and *wet* active matter \( \eta \). Dry active matter is overdamped \( \eta \). Wet active matter is momentum conserving and hydrodynamic modes are able to propagate. Systems can be continuously tuned between the two limits of dry/wet by adding friction to the hydrodynamic description \( \eta \). Continuum equations hydrodynamics of wet active nematics are a standard description for microtubule-kinesin systems \( \eta \) and form the basis for the numerical simulations in Chapter \( \S5 \) and \( \S6 \) with additional extensions provided for non-zero friction.

The active nematohydrodynamic equations are formed as coupled evolution equations of three hydrodynamic (slow) variables, which are each fields defined for all positions \( r \) at time \( t \). The density field \( \rho(r, t) \) is a conserved quantity, whereas the velocity field \( v(r, t) \) and orientational field \( Q(r, t) \) are soft modes formed by the breaking of isotropy \( \eta \).

The dynamics of the tensor order parameter field are given by \( \eta \) \( \eta \),

\[
\frac{DQ}{Dt} - S = \Gamma Q H, \tag{2.39}
\]

where \( \frac{D}{Dt} = \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) \) is the material derivative, meaning a derivative taken with respect to a coordinate system moving with \( v \). The evolution of \( Q \) towards lowest free energy \( F \) configurations is controlled by the molecular field \( H = -\frac{dF}{dQ} + \frac{1}{3} \text{Tr} \left( \frac{dF}{dQ} \right) \) and the rotational diffusivity \( \Gamma Q \), which controls the relaxation timescales \( \eta \). Here, \( F = F_{\text{bulk}} + F_{\text{elastic}} \), but may also include \( F_{\text{anch}} \) if anchoring is applied or \( F_{\phi} \) for emulsions (\( \S2.1.3 \)). The co-rotation term \( S \) accounts for the coupling of the orientation to gradients in the velocity field, \( A = \nabla v \). Splitting
\[ A = E + W \] into the symmetric (rate of strain \( E \)) and antisymmetric components (rate of rotation \( W \)), the corotation is

\[
S = (\lambda E + W) \cdot \left( Q + \frac{1}{3}I \right) + \left( Q + \frac{1}{3}I \right) \cdot (\lambda E - W) - 2\lambda \left( Q + \frac{1}{3}I \right) (Q : A).
\] (2.40)

The tumbling parameter \( \lambda \) determines the dominant influence between \( E \) and \( W \) on the alignment of orientation under flow. In shear flow, nematogens preferentially align with the principle axis (stretching axis) of \( E \) when \( \lambda > 9S/(3S + 4) \). On the other hand, \( W \) favours tumbling motion when \( \lambda < 9S/(3S + 4) \) \[110, 111\]. These two regimes are referred to as flow-aligning and flow-tumbling, respectively.

The density field obeys the conservation law

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,
\] (2.41)

which is also referred to as the continuity equation. For many fluid flows, the density can be treated as spatially uniform and the continuity equation simplifies to the incompressibility condition

\[
\nabla \cdot \mathbf{v} = 0,
\] (2.42)

which describes that the velocity is everywhere divergence free.

The flow field is described in terms of the momentum balance equation,

\[
\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \mathbf{\sigma} + f_E.
\] (2.43)

The right hand term describes the forces generated by internal stress \( \mathbf{\sigma} \) and any external force density \( f_E \). In an isotropic fluid, stress is composed only of pressure \( P \) and viscous forces

\[
\mathbf{\sigma}^I = -P \mathbf{1} + 2\eta \mathbf{E},
\] (2.44)

where \( \eta \) is the dynamic viscosity. The pressure, \( P \), is non-local, and adjusts to all stress contributions to ensure the incompressibility condition (Eq. (2.42)) is satisfied. For active liquid crystalline fluids, the stress \( \mathbf{\sigma} = \mathbf{\sigma}^I + \mathbf{\sigma}^N + \mathbf{\sigma}^\zeta \) additionally requires elastic \( \mathbf{\sigma}^N \) and active contributions \( \mathbf{\sigma}^\zeta = -\zeta Q \) (Eq. (2.38))
The elastic contributions are 

\[
\sigma^N = 2\lambda \left( \mathbf{Q} + \frac{1}{3} \right) \left( \mathbf{Q} : \mathbf{H} \right) - \lambda \mathbf{H} \cdot \left( \mathbf{Q} + \frac{1}{3} \right)
\]

\[
-\lambda \left( \mathbf{Q} + \frac{1}{3} \right) \cdot \mathbf{H} - \nabla \mathbf{Q} \frac{\delta F}{\delta \mathbf{Q}} + \mathbf{Q} \cdot \mathbf{H} - \mathbf{H} \cdot \mathbf{Q}.
\]

(2.45)

These equations are sufficient for the usual modelling of wet active nematics, and composes the majority of numerical simulations in Chapter §6. However, for the study of friction in §6.6.3, an external force \( f_E = -\kappa \cdot \mathbf{v} \) with friction tensor \( \kappa \) is applied [111].

The study of active nematic emulsions (Chapter §5) requires an additional hydrodynamic variable, the passive scalar phase field \( \phi_i \). The index \( i \) denotes each phase, which takes values \( i = 1, 2 \) or \( i = 1, 2, 3 \). The phase fields evolve according to the Cahn Hilliard equation

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = M_\phi \nabla^2 \mu_i,
\]

(2.46)

where \( M_\phi \) is the mobility and \( \mu_i = \frac{\delta F}{\delta \phi_i} \) is the chemical potential with the total free energy given by (Eq. (2.12)) [50]. An additional term is added to the stress tensor \( \sigma \) to account for the interfacial stress [46]

\[
\sigma^\phi = \sum_{i=1}^{N} \left[ (f - \phi_i \frac{\delta F}{\delta \phi_i} ) \mathbf{1} - \frac{\partial f}{\partial (\nabla \phi_i) \nabla \phi_i} \right].
\]

(2.47)

Here, \( f \) is the free energy density \( \mathcal{F} = \int f dV \) and \( N \) is the total number of phase fields \( (N = 2 \) or 3).

### 2.2.3.1 Dimensionless numbers

Dimensionless numbers and characteristic lengthscales arise from comparing terms in the equations of motion. These are informative for characterising the emergent flow patterns (§2.2.4) and to inform simplifications of the hydrodynamic equations needed for analytical treatments.

One of these dimensionless numbers is the Reynolds number. The Reynolds
number gives the ratio of inertial to viscous forces \[ \text{Re} = \frac{\rho \bar{U} \bar{L}}{\eta}, \] (2.48)

where \( \bar{U} \) and \( \bar{L} \) are characteristic velocities and lengths. In passive fluids, the Reynolds number is commonly used to characterise the transition between laminar (\( \text{Re} < 1 \)) and turbulent motions in inertial fluids (\( \text{Re} \gg 1 \)). For active nematics composed of cytoskeletal fluids, the characteristic velocities and small scales are associated with low Reynolds number [114]. In this limit, inertial terms (\( \rho \frac{Dv}{Dt} \) in Eq. (2.43)) can be neglected. This gives the Stokes regime, where dynamics can be captured by the force balance

\[ \nabla \cdot \sigma = 0. \] (2.49)

A feature observed in many active fluids is spontaneous flow [93, 115], which can appear disorderly or turbulent-like. These flows are referred to as active turbulence [109], despite the fact that they occur in the low-Re limit. Unlike high-Reynolds number turbulence, which is scale invariant, active nematic flow patterns have a characteristic scale. The active lengthscale is set by the competition between the active stress \( \sim \zeta \) and elastic stress \( \sim K/\ell_\zeta^2 \) over lengths \( \ell_\zeta \). Comparing these two stresses gives [116]

\[ \ell_\zeta = \sqrt{\frac{K}{\zeta}}. \] (2.50)

Introducing another lengthscale (such as system size \( L \)) can compete with \( \ell_\zeta \). In strongly confined systems (\( L \ll \ell_\zeta \)) active turbulence is suppressed, while in large systems (\( L \gg \ell_\zeta \)) flow domains are disordered [109]. When the confinement and active length scales are comparable (\( L \sim \ell_\zeta \)) spatio-temporally ordered flows can emerge [117]. Therefore, the transition to turbulent-like flows can be posed in terms of the dimensionless activity number [118]

\[ A = \sqrt{\frac{\zeta L^2}{K}}, \] (2.51)

which can be tuned by increasing activity or system size, or by decreasing nematic elasticity \( K \). Alternatively, a controlling lengthscale can be imposed through
friction $\kappa$. This introduces a hydrodynamic screening lengthscale

$$\ell_{\kappa} \sim \sqrt{\frac{\eta}{\rho \kappa}},$$  \hspace{1cm} (2.52)

which is set by the balance of viscosity and friction ($\kappa = |\kappa|$).

A further simplification of the Stokes equation is to assume negligible elastic stress relative to active stress ($A \gg 1$). In this case, $\sigma^N$ is neglected and Eq. (2.49) becomes

$$\eta \nabla^2 \mathbf{v} - \nabla P - \zeta \nabla \cdot \mathbf{Q} = 0.$$ \hspace{1cm} (2.53)

This has been used in analytical models of flow structures around defects \cite{20,119} and will be applied in Chapter §\hspace{0.5cm}6.

### 2.2.4 Active turbulence

Active turbulence is observed in many biological systems with orientational order, such as bacteria suspensions \cite{93,115} and cytoskeletal fluids \cite{17}. Characterising active turbulence is relevant to the study of self-organised dynamics; however, this is a complex task because of the nonlinearities in Eq. (2.39) and Eq. (2.43).

Here, we introduce the characteristic features of active nematic turbulence with particular emphasis on its emergent structures and topological defects.

The most utilised experimental system for studying active nematic turbulence is the \textit{in vitro} microtubule-kinesin active nematic films \cite{17}, assembled at an oil-water interface (Fig. 2.12). Microtubules (grey) can be seen to form a complex pattern with swirly-like strokes (Fig. 2.12a). Accompanying these strokes are topological defects, where the microtubule orientation field is discontinuous. Since the film is quasi two-dimensional, defects are points (§\hspace{0.5cm}2.1.5) and emerge as subpopulations of $k = \pm 1/2$, where $k$ is the winding number (Eq. (2.18)). A difference to the topologically imposed constraints using boundaries (§\hspace{0.5cm}2.1.7) is that these defects are generated by active energy injection at the smallest scales \cite{17,120}. Defects emerge in pair-creation events, in which $+1/2$ and $-1/2$ are simultaneously formed to maintain global charge neutrality (Eq. (2.20)). Likewise, defects also annihilate in pairs. Together, these processes form a steady-state population of topological defects with equal numbers of $+1/2$ and $-1/2$ \cite{19}.
Through the maintenance of a roughly constant population of defects over time, a characteristic lengthscale can be identified from the average spacing between defects \[ \ell_\zeta \] (Eq. (2.50)). This lengthscale is found to be proportional to the active lengthscale \[ \ell_\zeta \] (Eq. (2.50)). A further illustration of the active lengthscale exists in the flow field. Fig. 2.12 shows the velocity field (arrows) and vorticity field (colour) for the same experimental snapshot. The vorticity field shows a distribution of rotational flow domains of varying sizes \[ \ell_\zeta \], but with a characteristic scale that is comparable to the defect spacing and proportional to the active lengthscale \[ \ell_\zeta \].

2.2.5 Hydrodynamic instability

The formation of flow patterns is closely tied to fluid instabilities \[ \zeta \]. The first linear stability analysis of the active nematohydrodynamic equations (§ 2.2.3) was conducted by Simha and Ramaswamy in 2002 \[ \zeta \]. This showed that active nematics are inherently unstable to long wavelength disturbances in the orientation field. For extensile stress \( (\zeta > 0) \), the dominant unstable mode is bend \[ \mathbf{b} = \mathbf{n} \times \nabla \times \mathbf{n} \]. For contractile stress \( (\zeta < 0) \), splay \[ \mathbf{s} = \mathbf{n} (\nabla \cdot \mathbf{n}) \] is unstable. These unstable modes are evident in the emergent patterns, with sharp line-like
bands of accentuated bend (extensile; Fig. 2.13a) or splay (contractile) \[125\]. These sharp kink structures are colloquially referred to as *elasticity bands* \[126\], or *bend/splay walls* \[111\]. During the instability-driven transient onset of active turbulence \[126\], the distance between kink walls is the same active lengths scale \( \ell_\zeta \) that characterises defect separation \[116\] and vortex size \[122\] in fully formed turbulence (Fig. 2.13b).

Defect pair creation has been associated with these walls. This process can be qualitatively understood by examining the active force density \( f^\zeta = \nabla \cdot \sigma^\zeta \). Using (Eq. (2.38)), the force density is

\[
f^\zeta = -\zeta \nabla \cdot (n \otimes n) = -\zeta (s - b),
\]

under the simplifying assumption that the scalar order \( S = 1 \). This shows that activity generates forcing that is directed parallel to splay \( s \) and bend \( b \). These forces act to accentuate the original deformation, forming a feedback loop. Gradients in nematic order cost elastic free energy (Eq. (2.6)), which are eventually released by opening up the walls through defect pair creation (Fig. 2.13b) \[17\], a process known as defect unbinding \[127\] (Fig. 2.14).
2.2.6 Defect dynamics in active nematics

In §2.1, we introduced how defect creation and annihilation is constrained by the conservation of topological charge, and that their associated elastic energy control their relaxation dynamics towards equilibrium. Topological defects in active liquid crystals, too, obey these fundamental topological rules, although their energetics and dynamics are strikingly different to their passive counterparts. One such difference is that the profile of strong deformation at the core of a defect can highly influence the active flow generation [20], supporting self-motility in the case of positive half integer defects [17, 20]. The flow structures associated with active topological defects, form the basis of an emerging perspective of defects as “organisation centres” of active flow structures [22], an important viewpoint for Chapters §5 and §6 when studying defect dynamics.

2.2.6.1 Two-dimensions

The theoretical understanding of the active flow structure around two-dimensional topological defects was formulated by Giomi et. al. [20], which followed from experimental [17] and numerical [19, 121, 128] insights of the importance of defects in controlling flow structures. The derivation builds upon the director angle solution $\theta(k)$ for a defect with winding number $k$ (Eq. (2.19)). An arbitrary orientation $\theta_0 = 0$ is set so that the splay-side of each defect is aligned with $e_x$. This gives the director field $\mathbf{n} = \cos(k\phi)e_x + \sin(k\phi)e_y$, in terms of the domain-
Figure 2.15  Activity generated force and flow fields associated with isolated $+1/2$ and $-1/2$ defects.  a-b, Active force (blue arrows) for $+1/2$ (a) and $-1/2$ defect (b) from Eq. (2.56). The director is shown by black lines and background colouring is the splay-bend parameter $S_{SB}$ (Eq. (3.32)), which indicates localised nematic deformation.  c-d, Active flow fields (arrows) for $+1/2$ (c; Eq. (2.59)) and $-1/2$ (d; Eq. (2.60)) defects. The background is coloured by vorticity.

space polar angle $\phi = \tan^{-1}(y/x)$. For the two lowest energy $k = \pm 1/2$ defect cases, the active force density (Eq. (2.54)) is

$$f^\zeta(r) = -\frac{\zeta}{2r} \begin{cases} e_x, & k = +1/2, \\ -\cos(2\phi)e_x + \sin(2\phi)e_y, & k = -1/2, \end{cases}$$

(2.56)

with radial distance from the origin $|r| = r$. For $+1/2$ defects, Eq. (2.56) reveals that extensile active forcing is directed parallel to the defect orientation axis. This forcing is outwards-pointing through the bend side and inwards-pointing through the splay side (Fig. 2.15a). The $-1/2$ disclinations present a three-fold
symmetric force profile (Fig. 2.15b). In both \( k = \pm 1/2 \) cases, the force magnitude is strongest at the defect core and decays with \( 1/r \).

The flow fields \( \mathbf{v}(\mathbf{r}) \) are obtained by solving the Stokes equation (Eq. (2.53)) under the simplifying assumption that active stress dominates over elastic restoring forces (\( A \gg 1 \)). These solutions are found by integrating \( f^\zeta \) at each point \( \mathbf{r}' \) within a domain \( S \)

\[
\mathbf{v}(\mathbf{r}) = \int dS' \mathbf{G}(\mathbf{r} - \mathbf{r}') \cdot f^\zeta(\mathbf{r}').
\]  

(2.57)

This uses the two-dimensional Oseen tensor \( \mathbf{G} \)

\[
\mathbf{G}(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi\eta} \left[ \left( \ln \frac{\tilde{L}}{|\mathbf{r} - \mathbf{r}'|} - 1 \right) + \frac{(\mathbf{r} - \mathbf{r}') \otimes (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} \right],
\]  

(2.58)

which is the Greens function for the Stokes equation between points \( \mathbf{r}' \) and \( \mathbf{r} \). The integration lengthscale \( \tilde{L} \) must be included because of the logarithmic nature of hydrodynamic interactions in two-dimensions. Flow solutions for \( k = +1/2 \) \( (\mathbf{v}_+) \) and \( k = -1/2 \) \( (\mathbf{v}_-) \) defects are found to be

\[
\mathbf{v}_+(\mathbf{r}, \phi) = -\frac{\zeta L}{12\eta} \left[ \left\{ \left( 1 - \frac{r}{L} \right) + \frac{r}{L} \cos 2\phi \right\} \mathbf{e}_x + \frac{r}{L} \sin 2\phi \mathbf{e}_y \right],
\]  

(2.59)

\[
\mathbf{v}_-(\mathbf{r}, \phi) = -\frac{\zeta r}{12\eta} \left[ \left\{ \left( \frac{3}{4} \frac{r}{L} - 1 \right) \cos 2\phi - \frac{1}{5} \cos 4\phi \right\} \mathbf{e}_x - \left\{ \left( \frac{3}{4} \frac{r}{L} - 1 \right) \sin 2\phi + \frac{1}{5} \sin 4\phi \right\} \mathbf{e}_y \right].
\]  

(2.60)

These equations present several interesting features, which are visualised in Fig. 2.15c,d. The first is that \( +1/2 \) disclinations have a ‘self-propulsion’ speed since \( |\mathbf{v}_+| = \zeta \tilde{L}/(4\eta) \) at the defect core \( (r = 0) \). Fig. 2.15c illustrates this as two counter-rotating vortices that superpose at the defect. For \( -1/2 \) disclinations, \( |\mathbf{v}_-| = 0 \) at their core. Fig. 2.15d shows that \( -1/2 \) defects are associated with 6 vortices of alternating handedness that cancel at their centre.

The identification of two distinct motility behaviours for \( k = \pm 1/2 \) topological defects laid the groundwork for theoretical models to understand the statistics of steady-state active turbulence. One popular approach is to formulate the hydrodynamic description in terms of defects as interacting quasi-particles [127, 129, 130]. The statistical description of a dilute active-nematic defect gas on a substrate (neglecting hydrodynamic interactions) has been performed by Shankar
et al. [23, 127]. A mixture of motile (+1/2) and passive (-1/2) defects interact through Coulomb-like interaction forces and active alignment torques [127]. In working towards the wet hydrodynamic limit, Angheluta et al. [119] built in screened hydrodynamic interactions (with frictional forces), in an incompressible Stokes flow. This model accounts for the non-local effects, by solving for the pressure arising from active stress contributions.

Other recent studies have explored the relationship between topological defects and the unsteady features of the turbulent flows. These have measured exponential stretching of fluid parcels through chaos theory methods such as topological entropy [21] and Lyapunov exponents [22]. As a result, +1/2 defects have been identified as ‘special points’ for generating chaotic mixing and maximising topological entropy [131, 132].

2.2.6.2 Three-dimensions

Studies of active nematics have mostly been limited to two-dimensional materials, due to experimental difficulties in synthesising and obtaining nematic field data in three-dimensions. However, the pivotal work of Duclos et al. introduced an experimentally viable approach to study the mysteries of three-dimensional active turbulence [24]. This was achieved through state-of-the-art high-speed and resolution light-sheet microscopy. In this, the standard microtubule-kinesin was supplemented with filamentous viruses to ensure a fluidic state.

One of the major findings of these experiments, which complemented numerical expectations [25, 27], is the complex role of topology in active liquid crystals. Unlike the free point defects in two-dimensions (§2.2.6.1), three-dimensional active turbulence has a topologically rich structure with an assortment of charge-neutral disclination loops (Fig. 2.16), some of which are system spanning in numerical studies [26]. Disclination loops are generated by the hydrodynamic instability (§2.2.5), but instead of nucleating pairs of \( k = \pm 1/2 \) point defects, rings emerge that can connect half-integer winding profiles together as one structure (§2.1.6.3). The simplest loops smoothly connect local \( \pm 1/2 \) profiles as a wedge-twist loop (Fig. 2.6b), or arise as pure twist loops (Fig. 2.6c). Of yet, no linked (\( \nu = 1, 3 \)) or charged disclinations (\( \nu = 2 \)) have been found in experiments or simulations of bulk active turbulence [24, 64]. All observed loops are topologically trivial \( \nu = 0 \). This means that each loop can be created by smoothly expanding from a defect-free nematic texture. Likewise, any existing
Figure 2.16  **Network of disclination loops form in three-dimensional bulk active turbulence.** Disclinations coloured by twist angle $\cos \beta$ (as in Fig. 2.6). Yellow indicates local $+1/2$ wedge profile, green twist-type profile and blue $-1/2$ wedge profile. Data from Chapter §6.

A loop can be smoothly contracted to remove the singularity. The majority of disclination loops and lines in extensile active turbulence are observed to be twist-type [24, 133, 134]. However, the probability can be tuned in favour of wedge-twist loops in confinement [135] or in contractile active nematics [134].

The complex dynamics of active defect loops has been revealed in experiments [24] and simulations [27, 64, 136]. Loops can grow, shrink, coalesce with other loops, and split via self-interactions [27, 136]. These dynamical behaviours can also exist in passive liquid crystals [3, 137], but generally merge and shrink to reach equilibrium. In active nematics, dynamical behaviours of disclinations are driven out of equilibrium by activity [24, 136].

In several of these studies it was noticed that, akin to two-dimensions [20], motility features of loops relate to the local director geometry [4, 135]. In Binysh et al. the active backflow solutions are derived for three-dimensional director profiles [4]. The local profiles are constructed in terms of a local orthonormal basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{T})$. Here, $\mathbf{e}_1$ is a radially-outward pointing vector on the plane perpendicular to the tangent vector $\mathbf{T}$ (Fig. 2.17a). The binormal vector is $\mathbf{e}_2$. From this frame, the
Figure 2.17 *Three-dimensional defect profiles and active flows.* a, Defect profile is parameterised by a twist angle $\beta$ and a phase offset angle $\alpha$. b, Active flows (blue arrows) generated by a $+1/2$ wedge ($\alpha = \beta = 0$). The director is represented as green rods. Figure adapted from [4].

director profile geometry is indicated by two angles ($\alpha, \beta$). The twist angle $\beta$ is defined as $\cos \beta = \Omega \cdot T$, where $\Omega$ is the rotation vector and $T$ is the local disclination line tangent (§2.1.6.2). This indicates whether the profile is locally +1/2, −1/2, twist, or intermediate. The other angle $\alpha$ is the phase offset of the director from a radially-outward configuration (Fig. 2.17a). For all wedge profiles, $\alpha = 0$ since the director has an outwards/inwards pointing component (Fig. 2.4b,c). For twist type profiles, $\alpha$ can be non-zero. With the local defect geometry established, the flow-field solutions to the Stokes equation (Eq. (2.53)) are

$$v(\alpha, \beta) = -\frac{\zeta R_\perp}{16\eta}(1 + \cos \beta)^2(\cos 2\alpha e_1 + \sin 2\alpha e_2) - \frac{\zeta R_\parallel}{4\eta} \sin \beta (1 + \cos \beta) \sin \alpha T.$$  

(2.61)

Here, $R_\perp$ and $R_\parallel$ are lengthscales that roughly correspond to the typical defect spacing [4]. For +1/2 profiles, $v(0, 0) = -\zeta R_\perp e_1$, indicating self-propulsion in their bend direction (extensile) and splay (contractile). This is illustrated by the local dipolar flows in Fig. 2.17b. The magnitude of the +1/2 self-propulsion is proportional to activity. For -1/2 disclinations, $v(0, \pi) = 0$. Therefore, the theoretical self-propulsion velocity of wedge-type defect profiles are equivalent to the two-dimensional case (§2.2.6.1). However, a difference arises because three-dimensional disclination lines/loops are non-local—they are singular structures that smoothly connect multiple defect profiles. Thus, the locally generated active flows influence loop morphology rather than body self-propulsion. The connection between the local defect geometry and motility (Eq. (2.61)) has motivated studies to visualise defects in terms of $\cos \beta$ [24, 133, 135], which is used to understand the dynamical features of disclination lines and loops (Chapters §5 and §6).
Chapter 3

Methods
3.1 Introduction

In this chapter, we introduce the simulation and analysis methods used to study the interplay between topology and self-organised dynamics. The first section (§3.2), details the simulation methods and algorithm developments of a mesoscale particle based hydrodynamics solver, Multi-Particle Collision Dynamics (MPCD). The algorithm implementations are used to study nematic colloids and their topological defects in Chapter §4. The majority of the results are in three-dimensions, where visualisations are important to obtain physical insight of complex behaviours. The second section (§3.3) discusses the visualisation software used. Finally, we provide the analysis methods used for analysing topological defects (§3.4) and emergent flow structures (§3.6).

Active nematic simulations (Chapters §5 and §6) and experimental methods (Chapter §6) are not introduced in this section. These methods and the data they produced are contributed by collaborators. As such, an outline of the experiments and simulations are provided in the relevant results chapters.
3.2 Multi-Particle Collision Dynamics

3.2.1 Motivation for coarse-grained algorithms

One particularly fruitful approach for imposing topological constraints is via colloidal inclusions with strong anchoring conditions. Inclusions not only disturb the nematodynamic fields, imposing far-field deformation and topological constraints, but also dynamically respond to features in the nematic and flow fields [11]. Choosing the appropriate numerical method to investigate the dynamical behaviours associated with topologically imposed disclinations requires an assessment of the physical system and the strengths/weakness of each approach.

No numerical method can simulate all situations and choosing a computational approach must be tailored to the known or hypothesised most significant physics. For example, most simulation methods that are used to study colloidal dispersions in passive nematic fluids are unsuitable for active environments. Likewise, Landau de-Gennes free energy minimisation techniques [44], have provided valuable insight into equilibrium colloidal self-assembled structures and defect configurations [83, 138], but neglect fluid flow. Molecular models of nematic fluids, can simulate defects [139, 140] and microrheology [141], but are too computationally exhausting to run for the system sizes and timescales required for active dynamics or self-assembly. One approach is to use neither a macro- nor microscopic approach, but rather turn to mesoscale hydrodynamic algorithms that coarse-grain the molecular details to greater efficiency [142]. Hybrid lattice Boltzmann algorithms are certainly one candidate approach, and have been applied to the study of inclusions in passive [143] and active nematics [144, 145]. A particularly versatile approach, which we utilise for Chapter §4 is a particle-based hydrodynamics solver known as Multi-Particle Collision Dynamics (MPCD). This algorithm has been employed to simulate nematic fluids [146, 149], passive nematic colloidal inclusions [150, 152] and active nematics [64, 153, 154]. However, the existing work simulating nematic colloids using MPCD have been hybridised with Molecular Dynamics (MD) to simulate inclusions. This hybrid approach is non-ideal for coupling nematic stresses to colloidal dynamics, and for further extensions to complex environments or active nematics.

In this section, we introduce MPCD and the methodology required to simulate
nematic fluids and colloidal inclusions. A portion of this section is dedicated to establishing a new simulation method to model nematic colloids, which we do as a fully inbuilt boundary method. The methodology developed here can be simply extended for future studies of more complicated inclusions or the dynamics of colloids in active environments.

3.2.2 Multi-Particle Collision Dynamics algorithm

Multi-Particle Collision Dynamics (MPCD) is a coarse-grained algorithm that simulates fluids using point-like particles \([155]\). Hydrodynamic evolution increments in discrete time intervals, where two characteristic steps take place i) *streaming* and ii) *collision*. These steps describe how particles move and interact with their local environment. Within this simple framework, many possible classes of fluids can be simulated \([156]\). The hydrodynamic and relevant order parameter fields are discretised into particle properties, accompanied by an appropriately defined mechanism for inter-particle interactions.

The bottom-up approach of modelling fluid flows through particles, offers a simple means of accounting for the environment. Influences from external fields, confinement, and embedded solutes can be accounted for through direct transformation rules on the particle properties. Accordingly, MPCD has been utilised in studying an assortment of solutes, such as polymers \([157]\), colloids \([150, 158]\), blood cells \([159]\), bacteria \([160, 161]\) and even fish schools \([162]\). Further, the intrinsic thermal noise, built into the collision operator’s design, creates an ideal environment for studying these micro to nano-scale suspensions where fluctuations are non-negligible.

We utilise a nematic MPCD algorithm (N-MPCD) \([146]\). For this, the continuous nematohydrodynamic fields for mass (Eq. (2.41)), momentum (Eq. (2.43)), and nematic order (Eq. (2.39)) are carried by particles indexed by \(i\), each having a mass \(m_i\), position \(r_i\), velocity \(v_i\), and orientation \(u_i\). Orientations have unit magnitude (\(u \cdot u = 1\)) and are apolar (\(u_i = -u_i\)). Further, the particle masses are set to equal \(m_i = m\). The spatial evolution of these fields takes place as particles stream ballistically over the time interval \(\delta t\) (Fig. 3.1a)

\[
\mathbf{r}_i(t + \delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\delta t.
\] (3.1)

With just this step, the fluid would act as an ideal non-interacting gas. Therefore,
Figure 3.1 *Schematic of MPCD hydrodynamic evolution.* a, *Streaming step* in which point-like particles (blue circles) move ballistically with their velocity (black arrows) for time $\delta t$. b, *Collision step* in which particles are binned into cells (enclosed by grey dashed lines). Cell-based collision operators stochastically exchange particle momentum and orientations within each cell, while conserving each cell’s total momentum and director.

Interactions are required between particles to allow hydrodynamic modes to propagate. MPCD works with interactions in a coarse-grained manner: particles are binned into cells where they interact only with the cell-localised collision operator $[155]$ (Fig. 3.1b). However, by discretising space into MPCD cells, Galilean invariance is broken. A solution for this is to apply a random grid shift each time step $[163]$.

Operators, $\Xi_{i,c}$, are built from each of the $N_c$ composite particles in a cell $c$, encompassing the average field properties. Further, the operators are designed to reproduce continuum hydrodynamic fields over sufficiently long length and timescales. This avoids the demanding computational cost of explicitly accounting for pair-wise interactions between particles, which is the approach used by many micro-scale simulation methods $[164]$. The evolution equations for velocity $v_i$ and orientation $u_i$ are defined in terms of collision operators for the velocity $\Xi^\text{vel}_{i,c}$ and orientation $\Xi^\text{ori}_{i,c}$

$$v_i(t+\delta t) = v^\text{cm}_c(t) + \Xi^\text{vel}_{i,c}, \quad (3.2)$$
$$u_i(t+\delta t) = n_c(t) + \Xi^\text{ori}_{i,c}, \quad (3.3)$$

which contribute stochastic perturbations about the cell’s centre of mass velocity.
\( v_{c}^{\text{cm}} \) and local director \( \mathbf{n}_{c} \). There is a broad range of choices in designing a collision operator, but the essential feature is that the hydrodynamic conservation laws are maintained.

### 3.2.2.1 Velocity collision operator

The collision operator on the velocity has two additive contributions

\[
\Xi_{i,c}^{\text{vel}} = \Xi_{i,c}^{I} + \Xi_{i,c}^{N},
\]

(3.4)

an isotropic \( \Xi_{i,c}^{I} \) and a nematic operator \( \Xi_{i,c}^{N} \). The isotropic component uses the Andersen locally-thermostatted collision operator \[165, 166]\n
\[
\Xi_{i,c}^{I} = \xi_{i} - \langle \xi_{i} \rangle_{c} + (I_{c}^{-1} \cdot \delta L_{\text{vel}}) \times r'_{i},
\]

(3.5)

where \( \xi_{i} \) is noise generated from a Gaussian distribution with variance \( k_{B}T/m \) and \( \langle \xi_{i} \rangle_{c} \) is a residual term designed to conserve the net linear momentum. The final term is a correction to conserve the net angular momentum introduced by the collision operator \( \delta L_{\text{vel}} = \sum_{i}^{N_{c}} m_{i} \{ r'_{i} \times (v_{i} - \xi_{i}) \} \). Here, \( r'_{i} = r_{i} - r_{c}^{\text{cm}} \) is the position of a particle \( i \) about the cell’s centre of mass and \( I_{c} \) is the cell’s moment of inertia tensor. One consequence of a thermostatted collision operator is that the MPCD does not strictly adhere to energy conservation, but has a set temperature.

In line with the continuum nemato-hydrodynamic equations (§ 2.2.3), \( \mathbf{n}(\mathbf{r}) \) and \( \mathbf{v}(\mathbf{r}) \) have an interdependent coupling—nematogens are rotated by velocity gradients, and director reconfiguration drives flow. The former effect is accounted for in \( \Xi_{i,c}^{\text{ori}} \), while the latter effect is captured in \( \Xi_{i,c}^{N} \). The flow generated by director reconfiguration, otherwise known as backflow, is implemented as a correction to conserve the net angular momentum associated with director reorientation \( \delta L_{\text{ori}} \)[146]

\[
\Xi_{i,c}^{N}(t) = (I^{-1} \cdot \delta L_{\text{ori}}) \times r'_{i},
\]

(3.6)

which is discussed next.
3.2.2.2 Orientation collision operator

The aligning interactions between particle orientations is accounted for in $\Xi_{ori,i,c}(t)$, where we utilise the collision operator designed by Shendruk and Yeomans [146].

The cell-based nematic tensor order parameter $Q_c = \frac{1}{d-1} \langle u_i \otimes u_i - \mathbf{1} \rangle_c$ (Eq. (2.2)) enables the scalar order parameter $S_c$ and the director $n_c$ to be constructed from the largest eigenvalue and corresponding eigenvector — determining the degree and direction of alignment within the cell ($\S$ 2.1.2). These order parameters are passed into a Maier-Saupe mean field theory [167], replacing pairwise orientational interactions with an effective field that all particles locally produce and respond to. The collision operator $\Xi_{ori,i,c}(t)$ is then a stochastic noise drawn from the equilibrium probability distribution $f_{ori} = f_0 \exp \left( \frac{US_c}{k_BT} (u_i \cdot n_c)^2 \right)$, centred about $n_c$ with normalisation constant $f_0$ and mean field interaction constant $U$.

The constant $U$ provides an input parameter that controls how tightly aligned the drawn orientations are with $n_c$. For large $US_c/(k_BT)$, the nematic is strongly aligned, while small $US_c/(k_BT)$ has equally-probable orientations, corresponding to an isotropic state. The expected first-order (3D) and second-order (2D) isotropic to nematic phase transition emerges with intermediate values of $U$. The constant is linearly proportional to the Frank elasticity (Eq. (2.7)) under the one-constant approximation $U \propto K$ [146].

While the stochastic orientation operator $\Xi_{ori,i,c}(t)$ describes the fluid’s thermodynamic nature and material elasticity, including additional terms for the coupling of orientations to flows are more conveniently recast in terms of a torque balance equation. The total torque on each particle $i$ over time $\delta t$ is

$$\Gamma^\text{col}_i + \Gamma^\text{Jeff}_i + \Gamma^\text{diss}_i = 0. \quad (3.7)$$

The first two terms $\Gamma^\text{col}_i + \Gamma^\text{Jeff}_i = \gamma_R u_i \times \left( \frac{\delta u^\text{col}_i}{\delta t} + \frac{\delta u^\text{Jeff}_i}{\delta t} \right)$ describe the over-damped torque for the stochastic collision (col) and hydrodynamic flows (HI) with a rotational friction coefficient $\gamma_R$. From Eq. (3.3), the collision contribution is $\frac{\delta u^\text{col}_i}{\delta t} = (n_c(t) + \Xi^\text{ori}_{i,c}(t))/\delta t$, while the hydrodynamic contribution uses the Jeffery equation [168] [169],

$$\frac{\delta u^\text{Jeff}_i}{\delta t} = \chi \left[ v_i \cdot W + \lambda (u_i \cdot E - u_i u_i u_i : E) \right], \quad (3.8)$$

with flow tumbling parameter $\lambda$ ($\S$ 2.2.3) and shear coupling coefficient $\chi$. The final term $\Gamma^\text{diss}_i = - (\Gamma^\text{col}_i + \Gamma^\text{Jeff}_i)$ is the dissipative torque. This identifies the net

53
angular momentum in the cell from each particle’s net torque Eq. (3.7), \( \delta L_{\text{ori}} = \sum_{i}^{N_{c}} \Gamma_{i}^{\text{diss}} \delta t \). The net angular momentum is passed as the backflow contribution in Eq. (3.6).

3.2.3 Boundaries

All simulations require boundary conditions—these conditions define the space that the fluid can occupy and determine specific features of the fluidic environment. In our implementation of N-MPCD, boundary conditions are simply carried out by particles via two steps i) defining surface equations and ii) establishing transformation rules on particles that make contact with the surface [158]. These two steps can realise many possible environments, from complex confining geometries [170], internal obstacles [171], porous media [172], and microfluidic channels [158].

3.2.3.1 Surfaces

Each boundary \( b \) has a surface equation with an implicit form \( S_{b}(r) = 0 \), where \( r = (x, y, z) \) satisfy points on the surface. There are an endless number of possible surfaces; however, a useful form is

\[
S_{b}(r) = A_{x}(x - q_{x})^{p_{x}} + A_{y}(y - q_{y})^{p_{y}} + A_{z}(z - q_{z})^{p_{z}} - R^{p_{R}} = 0, \tag{3.9}
\]

where the surface parameters represent the surface’s position \( q_{b} = (q_{x}, q_{y}, q_{z}) \), with scaling coefficients \( A = (A_{x}, A_{y}, A_{z}) \), surface powers \( (p_{x}, p_{y}, p_{z}, p_{R}) \) and radius \( R \). The two types of surfaces used are

- **Planes:** \( S_{b}(r) = A \cdot r - R \), for planes with normal vector \( A \) at a distance \( R \) from the origin. Planes are used for all confining surfaces (periodic and solid walls).
- **Spheres:** \( S_{b}(r) = (r - q_{b})^{2} - R^{2} \), for spherical colloids with centre coordinate \( q_{b} \) and a radius \( R \).

The utility of defining surfaces as implicit functions through \( S_{b}(r) = 0 \) is that there is a clearly defined space inside or outside of the surface. This establishes
a condition for whether particles have violated (found inside) a surface, if

\[ S_b(r) \leq 0. \]  \hfill (3.10)

If true, then the fluid domain is regulated by i) ray-tracing particles back to the surface (to position \( r^*_i \), at time \( t^* \leq \delta t \)), ii) applying particle transformation rules, and iii) continuing the stream for the remaining time \( (\delta t - t^*) \).

### 3.2.3.2 Transformation rules

With the particle residing on the boundary (at \( r^*_i \)), boundary rules are applied that operate on the particle’s position, velocity and orientation

\[
\begin{align*}
\mathbf{r}_i &\rightarrow \mathbf{r}_i + D_{\nu} \nu_b, \\
\mathbf{v}_i &\rightarrow M_{\nu_b} \text{proj}_{\nu_i}(\nu_b) + M_{t_b} \text{proj}_{\nu_i}(t_b), \\
\mathbf{u}_i &\rightarrow M_{\nu_b} \text{proj}_{\nu_i}(\nu_b) + M_{t_b} \text{proj}_{\nu_i}(t_b).
\end{align*}
\]  \hfill (3.11)

The position operator is defined as an additive shift, with magnitude \( D_{\nu} \) in the direction defined by the surface normal \( \nu_b \). If periodic boundary conditions are applied (Fig. 3.2a), then \( D_{\nu} \) is set equal to the system size \( L \), otherwise this is simply set to zero. The velocity operator is defined as a multiplier on the normal and tangential components of the velocity, with multiplier magnitudes \( M_{\nu_b} \) and \( M_{t_b} \) respectively. These are required for solid impermeable walls. For example, no-slip boundary conditions are achieved by setting \( M_{\nu_b} = M_{t_b} = -1 \), which reverse the particle velocity to create zero velocity at the surface (Fig. 3.2b). Additionally, ghost particles are required to enforce no-slip, ensuring that \( v_c \) extrapolates to zero in cells that are intersected by walls [173]. Finally, the orientation boundary conditions (anchoring conditions) are defined as multiplier operators on the normal and tangential components of the orientation, but with the constraint that \( \mathbf{u}_i \) needs to remain with unit magnitude (\( \mathbf{u}_i \cdot \mathbf{u}_i = 1 \)).

Homeotropic (normal) anchoring is achieved with \( \mathcal{M}_{\nu_b} = 1 \) and \( \mathcal{M}_{t_b} = 0 \) (Fig. 3.2c), and planar (tangential) anchoring with \( \mathcal{M}_{\nu_b} = 0 \) and \( \mathcal{M}_{t_b} = 1 \) (Fig. 3.2d). The surface normal projection is defined as \( \text{proj}_f(\nu_b) = (\nu_b \cdot f)\nu_b \) and surface tangent as \( \text{proj}_f(t_b) = f - (\nu_b \cdot f)\nu_b \), where \( f \) is the vector being projected. This method is a hard anchoring condition on the particles, but does not ensure the cell-based anchoring is infinitely strong, as will be investigated in § 4.3.
Figure 3.2  Particle transformations at boundaries. a, Periodic boundary conditions: MPCD particle (blue circle) passes through a wall (orange) and has its position shifted to the opposite end of the simulation domain. b, No-slip: particle’s velocity is reversed at the boundary. c, Homeotropic anchoring: particle’s orientation (black rod) aligns with surface normal $\nu_b$. d, Planar anchoring: particle’s orientation aligns with the surface tangent.

3.2.4 Colloids

One existing method for colloidal inclusions is to include them as embedded molecular dynamics particles with radial interaction potentials [150]. This method was applied to the study of topological defects around spherical [150] and anisotropic [151, 174] particles. However, these studies did not account for the response of the colloid to features of the nematic orientational field.

An alternative approach, which has been used to resolve hydrodynamic stresses on a colloid interface [158], is to construct the colloid as an in-built surface and resolve the surface stresses directly from particle transformations at the surface (Eq. (3.11)). To account for nematohydrodynamic stresses, we extend this method to resolve elastic stresses via particle orientation transformations.

3.2.4.1 Simulating mobile boundaries

Colloids are modelled as mobile boundaries. This means that their surface equations (Eq. (3.9)) have temporally dependent parameters. We only consider
spherical colloids with

$$S_b(r) = [r - q_b(t)]^2 - R^2 = 0,$$

(3.12)

which have centre coordinates \(q_b(t)\) that vary with time, and a constant radius \(R\). Each colloid \(b\) is further associated with a velocity \(v_b(t)\) and an angular velocity \(\omega_b(t)\). In a similar fashion to the particle streaming step, (Eq. (3.1)), \(v_b(t)\) is used to evolve \(q_b(r)\)

$$q_b(t + \delta t) = q_b(t) + v_b(t) \delta t,$$

(3.13)

which is up to first order in \(\delta t\) since the solvent is thermally fluctuating and higher order integrators would not gain significant accuracy benefits. However, this assumption is less valid for high Péclet numbers (when the rate of advection is much greater than the rate of diffusion). The surface equation Eq. (3.12) does not vary with \(\omega_b(t)\) since spheres have full rotational symmetry.

The evolution equations for \(v_b(t + \delta t)\) and \(\omega_b(t + \delta t)\) are determined directly from conserving the linear and angular impulse generated by each of the particle transformations

$$v_b(t + \delta t) = v_b(t) + \sum_i^{N^*_b} \delta v_{b,i}^{vel} + \sum_i^{N^*_b} \delta \omega_{b,i}^{ori}$$

(3.14)

$$\omega_b(t + \delta t) = \omega_b(t) + \sum_i^{N^*_b} \delta \omega_{b,i}^{vel} + \sum_i^{N^*_b} \delta \omega_{b,i}^{ori}.$$  

(3.15)

These update \(v_b(t)\) and \(\omega_b(t)\), with the incremental changes \(\delta v_{b,i}^{vel}\) and \(\delta \omega_{b,i}^{ori}\) from the velocity (superscript vel) and orientation (superscript ori) transformations (Eq. (3.11)). The sum is performed over the \(N^*_b\) particles that violate the surface equation Eq. (3.10) in a given timestep. In § 4.3, we will find that this does not simulate sufficiently strong anchoring and so we modify the sum to be over all the MPCD particles in cells that intersect a colloidal surface \(N^*_c\) in order to enhance the anchoring strength.

### 3.2.4.2 Velocity transformation

To obtain \(\delta v_{b,i}^{vel}\) and \(\delta \omega_{b,i}^{vel}\), the linear impulse due to the change in momentum of the particle’s velocity, \(J_i = m_i v_i(t + \delta t) - m_i v_i(t)\), is balanced with an impulse
on the colloid $J_b = -J_i$. The impulse can be split into normal and tangential components at the collision point on the surface ($r_i^*$). This gives the velocity and angular velocity increments as \[ m_b \delta v_{vel}^{b,i} = \text{proj}_{J_b}(\nu_b) \] \[ \delta \omega_{vel}^{b,i} = \mathbf{I}_b^{-1} \cdot (r_{b,i} \times \text{proj}_{J_b}(t_b)) \ , \] where $m_b$ is the mass of the colloid, $\mathbf{I}_b^{-1}$ is the inverse of the colloid’s moment of inertia and $r_{b,i} = r_i^* - q_b$ is the radial vector from the centre of the colloid to the point on the surface where the transformation is applied.

### 3.2.4.3 Orientation transformation

To obtain $\delta v_{ori}^{b,i}$ and $\delta \omega_{ori}^{b,i}$, the angular impulse due to a particle reorientation, $\Gamma_{i}^{\text{anch}} \delta t$, is conserved. Here, $\Gamma_{i}^{\text{anch}}$ is the anchoring torque that rotates an initial orientation $u_i(t)$ to a final orientation $u_i(t + \delta t)$. Therefore, angular impulse can be balanced by

\[ \Gamma_{i}^{\text{anch}} + \Gamma_{b,i}^{\text{anch}} = 0 , \] \[ (3.18) \]

where $\Gamma_{b,i}^{\text{anch}}$ is the torque experienced by the colloid. The torques each have a pivot axis that coincides with the $i$th particle centre. The contributions to the colloid’s linear and angular velocity apply following steps: i) find $\Gamma_{b,i}^{\text{anch}}$ using Eq. (3.18), ii) convert $\Gamma_{b,i}^{\text{anch}}$ into a point force acting at the boundary, iii) use the force to calculate $\delta v_{ori}^{b,i}$ and $\delta \omega_{ori}^{b,i}$.

To find $\Gamma_{b,i}^{\text{anch}}$, we first identify the torque experienced by the particle

\[ \Gamma_{i}^{\text{anch}} = \gamma R u_i(t) \times \frac{u_i(t + \delta t)}{\delta t} . \] \[ (3.19) \]

To compute the cross-product, the orientation is written as $u(t) = \text{proj}_{u_i}(\nu_b) + \text{proj}_{t_b}(t_b)$ in terms of an easy axis $\nu_b$ and perpendicular component $t_b$. Here, we only consider homeotropic and tangential anchoring, so $\nu_b$ is the surface normal and $t_b$ is the tangent. From Eq. (3.11), the final orientation is $u_i(t + \delta t) = M_{\nu_b} \text{proj}_{u_i}(\nu_b) + M_{t_b} \text{proj}_{t_i}(t_b)$. Computing the cross-product finds

\[ \Gamma_{i}^{\text{anch}} = \frac{\gamma R}{\delta t} M_{\Delta}(u_i \cdot \nu_b)(u_i \times \nu_b) , \] \[ (3.20) \]
where $\mathcal{M}_\Delta = (\mathcal{M}_\nu - \mathcal{M}_{tb})/\left(\sqrt{\mathcal{M}_{\nu}^2 + \mathcal{M}_{tb}^2}\right)$ and the denominator has been introduced to ensure that $\mathbf{u}_i(t + \delta t)$ has unit magnitude. By defining the angle $\cos \alpha_i = \mathbf{u}_i \cdot \mathbf{\nu}_b$, the torque magnitude can be written in terms of a single variable

$$
\Gamma_{i}^{\text{anch}} = \frac{\gamma R}{2\delta t} \mathcal{M}_\Delta \sin(2\alpha_i).
$$

(3.21)

Since $\Gamma_{i}^{\text{anch}}$ is odd with respect to $\alpha_i$, Eq. (3.18) is satisfied by

$$
\Gamma_{b,i}^{\text{anch}} = \frac{\gamma R}{2\delta t} \mathcal{M}_\Delta \sin(-2\alpha_i).
$$

(3.22)

Therefore, we consider Eq. (3.22) to be satisfied by a virtual particle, oriented initially at $-\alpha_i$ to $\mathbf{\nu}_b$ (with orientation unit vector $\mathbf{u}_{b,i}$). Over the time $\delta t$, the virtual particle reorients to align with $\mathbf{\nu}_b$, through application of the torque Eq. (3.22). The initial orientation of the virtual particle $\mathbf{u}_{b,i}$ is related to the N-MPCD particle $\mathbf{u}_i$ by a mirror reflection about $\mathbf{\nu}_b$ (Fig. 3.3).

As the next step towards determining $\delta \mathbf{v}_{\text{ori}}_{b,i}$ and $\delta \omega_{\text{ori}}_{b,i}$, the torque $\Gamma_{b,i}^{\text{anch}}$ must be converted into a force $\mathbf{F}_{b,i}^{\text{anch}}$ at the boundary. Since $\Gamma_{b,i}^{\text{anch}}$ is accounted for by the virtual particle, the force at the boundary is related to the torque by

$$
\mathbf{F}_{b,i}^{\text{anch}} = \mathbf{r}_{b,i} \times \Gamma_{b,i}^{\text{anch}},
$$

(3.23)

where $\mathbf{r}_{b,i} = \frac{\ell_u}{2} \mathbf{u}_{b,i}$ and $\ell_u$ is introduced to represent the length of the N-MPCD/virtual particle. However, because the torque is a pseudovector, converting a torque into a force is not generally possible. This is because there can be a colinear contribution between $\mathbf{F}_{b,i}^{\text{anch}}$ and $\mathbf{r}_{b,i}$ that returns the same torque value. The non-unique nature of the force is demonstrated by the identity

$$
\mathbf{F}_{b,i}^{\text{anch}} = \frac{\mathbf{r}_{b,i} \cdot \mathbf{F}_{b,i}^{\text{anch}}}{\mathbf{r}_{b,i} \cdot \mathbf{r}_{b,i}} - \frac{\mathbf{r}_{b,i} \times \Gamma_{b,i}^{\text{anch}}}{\mathbf{r}_{b,i} \cdot \mathbf{r}_{b,i}}.
$$

(3.24)

Since virtual particles and N-MPCD only rotate under the torque action (no translation), the colinear contribution is assumed to be zero ($\mathbf{r}_{b,i} \cdot \mathbf{F}_{b,i}^{\text{anch}} = 0$). Therefore,

$$
\mathbf{F}_{b,i}^{\text{anch}} = \frac{\Gamma_{b,i}^{\text{anch}} \times \mathbf{u}_{b,i}}{\ell_u/2}.
$$

(3.25)

The final detail remaining on inferring the force, is that Eq. (3.25) is odd under $\mathbf{u}_{b,i} \rightarrow -\mathbf{u}_{b,i}$. Since $\mathbf{u}_{b,i}$ is a head-tail vector, this results in an ambiguity on the
Figure 3.3  Schematic of the torque balance due to particle orientation transformation at a boundary. A particle (green rod) with orientation \( \mathbf{u}_i \) experiences a torque \( \Gamma_{\text{anch}}^{i} \) to align with the anchoring easy axis (shown as surface normal \( \mathbf{\nu}_b \)). A virtual particle (pink rod) oriented at \( \mathbf{u}_{b,i} \) is constructed that experiences and equal and opposite torque \( \Gamma_{\text{anch}}^{b,i} \). A colour wheel of the torque magnitude is shown (green/purple circle) with angular deviation of the orientation from \( \mathbf{\nu}_b \).

sign of the force. To establish a unique force, the sign of \( F_{\text{anch}}^{b,i} \) is chosen to be oriented towards the boundary \( F_{\text{anch}}^{b,i} \cdot \mathbf{\nu}_b < 0 \). This choice ensures that the colloid moves away from large elastic stress.

These steps find an inwards-pointing force \( F_{\text{anch}}^{b,i} \) at the boundary, that conserves the angular impulse associated with a N-MPCD orientation transformation. This force is converted into linear and angular velocity contributions by projecting in the surface normal and tangent directions,

\[
m_b \delta \mathbf{v}_{b,i}^{\text{ori}} = \text{proj}_{F_{b,i}}(\mathbf{\nu}_b) \delta t
\]

\[
\delta \mathbf{\omega}_{b,i}^{\text{ori}} = \mathbf{I}_{b}^{-1} \cdot (\mathbf{r}_{b,i} \times \text{proj}_{F_{b,i}}(\mathbf{t}_b) \delta t)
\]
Figure 3.4  Mayavi scene and interactive pipeline. Left: Mayavi scene is shown with two colloids (spheres), an entangled defect loop (purple) and director field (grey rods). Right: the interactive pipeline with red circles indicating the scene, data sources, filters and modules applied to make the image. The director is loaded as a VectorField (data source) and visualised using a VectorCutPlane (module). The defect loop is loaded as a ScalarField, and several filters are applied to form the isosurface and to load the twist angle as an attribute for colouring the isosurface. The loop is visualised using a surface module. Colloids are individually loaded as a ScalarScatter and visualised using a Glyph module, which forms a sphere.

3.3 Visualisations

All three-dimensional visualisations use Mayavi, an open-source scientific visualisation package written in Python [175]. In this section, we provide a brief overview of how Mayavi constructs images. These details are included to assist future studies which need to manipulate raw data for visualisation purposes.

Visualisations use the in-built pipeline architecture, defining how data is operated on to form an image. This works through the steps:

Scene → Data source → Filters → Modules

All objects and information belong to a scene. Inside the scene, scalar, vector and tensor fields, established as NumPy arrays, can be stored as VTK (Visualisation Toolkit) [176] objects to form data sources. The VTK objects are combined with traits (Traited VTK or TVTK), enabling attributes to be assigned. Filters are applied that operate on the data. Finally, modules define how the filtered data is visualised, which then produce the image. One of the strengths of the Mayavi pipeline, is that each part can be directly interacted with, and tested, through
the generated TVTK scene. Alternatively, Python methods can directly write
the pipeline and perform visualisations without needing to directly interact with
it. An example of the interactive pipeline is shown in Fig. 3.4.
3.4 Defect analysis

This section outlines the numerical methods used to identity, characterise and analyse nematic disclinations in two- and three- dimensions.

3.4.1 Two-dimensions

3.4.1.1 Topological charge density

Topological defects in both experiments and two-dimensional simulations are identified by calculating the topological charge density \[ q = \frac{1}{4\pi} \left( \partial_x Q_{x\alpha} \partial_y Q_{y\alpha} - \partial_x Q_{y\alpha} \partial_y Q_{x\alpha} \right) , \] (3.28)
in terms of \( Q \) (given here in index notation) and summation convention applied on Greek indices. The form of \( q \), arises from converting the winding number loop integral (Eq. (2.18)) into a surface integral and taking the integrand as a diffuse charge density to give Eq. (3.28). This relationship between \( q \) and \( k \) results in \( \text{sgn}(q) = \text{sgn}(k) \), and the sign and magnitude can be used to identify and characterise defects simultaneously. For example, regions without defects return \( q \approx 0 \) and therefore comprise most of the field. Defects can be identified with \( q > 0 \) (\( k = +1/2 \)) or \( q < 0 \) (\( k = -1/2 \)). To distinguish topological defects from numerical artifacts close to \( q = 0 \), a cut off is introduced \( q_{\text{cut}} \) chosen to be multiples of standard deviations of \( q \) about the mean (\( q = 0 \)). The \( q_{\text{cut}} \) values are provided in Chapter §6.

3.4.1.2 Defect orientation

Topological defects in active nematics have active backflows that are dependent on geometry of the local director (§2.2.6.1). In the case of +1/2 defects, this aids self-propulsion. In extensile active nematics (\( \zeta > 0 \)), self-propulsion is in the direction of bend, while it is in the direction of splay for contractile nematics (\( \zeta < 0 \)) [20] [178]. The defect orientation is therefore important for interpreting motility behaviours.

To obtain the defect orientations, we employ the method proposed by Vromans
and Giomi \[179\]. Motivated by the fact that \(+1/2\) active-nematic defects self-propel in the direction of average active force (Eq. (2.56)), the disclination polarity can be calculated from the divergence of the nematic \(Q\) tensor (\(\cos \psi, \sin \psi\) = \(\nabla \cdot Q / |\nabla \cdot Q|\)). The defect orientation angle \(\psi\) captures the direction where the director \(n\) points radially outwards/inwards towards the defect core and is defined modulo \(2\pi\) for a \(+1/2\) disclination due to 1-fold symmetry \[180\]. Calculating the orientational properties of defects with different values of \(k\) is more complicated with \(2|1-k|\)-fold director symmetry. It was found that the orientation angle of a defect with charge \(k\) can be calculated by

\[
\psi = \frac{k}{1-k} \tan^{-1} \left[ \frac{\langle \text{sgn}(k) \partial_x Q_{xy} - \partial_y Q_{xx} \rangle}{\langle \partial_x Q_{xx} + \text{sgn}(k) \partial_y Q_{xy} \rangle} \right],
\]

(3.29)

where \(\langle \cdots \rangle\) denotes an average over a closed loop around the disclination \[179\]. This form adjusts the divergence to include sign functions (\(\text{sgn}\)) on the off-diagonal elements of \(Q\), which accounts for negative \(k\) having mirror-reflected director angles compared to their positive \(k\) counterparts. The traceless condition on \(Q\) is applied so that \(Q_{yy} = -Q_{xx}\). The prefactor \(k/(1-k)\) ensures that \(\psi\) is defined modulo \(\pi/|1-k|\), respecting the symmetry of the local director. In Chapter §6, we use Eq. (3.29) to calculate the orientations of \(k = \pm1/2\) defects in experiments and simulations.

### 3.4.2 Three-dimensions

#### 3.4.2.1 Disclination density tensor

Characterising the topological properties of disclinations is insightful for understanding the relaxation processes of passive defects towards a lower free energy (Chapter §4), or for interpreting activity-induced motility (Chapter §5). Traditional methods of identifying three-dimensional disclinations use isosurfaces of the scalar order parameter, since small values indicate the locally-melted defect core \[181, 182\]. The biaxiality parameter has also been used to locate defects \[46\]. However, a methodology is required that can identify disclinations and extract \(\Omega\) and \(T\) \[24, 30, 64\].

A novel tensor-based formalism was proposed in 2022 by Schimmings and Viñals, which encodes geometric and topological properties simultaneously \[29\]. The disclination density tensor \(D\) is conveniently constructed from derivatives of \(Q\).
In index notation, the disclination density tensor is

\[ D_{ij} = \epsilon_{i\mu\nu} \epsilon_{j\eta\delta} \partial_\mu \theta_{\nu\alpha} \partial_\delta \theta_{\eta\alpha}, \]  

(3.30)

with summation convention applied on the repeated tensor indices \(i, j, k, \alpha, \mu, \nu\). The tensor \(D\) can be directly interpreted as the dyad

\[ D = s(r) \Omega \otimes \mathbf{T}, \]  

(3.31)

composed of the tangent vector \(\mathbf{T}\) of the disclination line and the rotation vector \(\Omega\), which defines the plane that the local director field lies and winds in (§2.1.6.2). The scalar field \(s(r)\) is non-negative and approaches a maximum at the core of the disclination. Therefore, \(s\) provides a useful quantity for identifying disclinations when using an appropriately defined lower bound \(s_{\text{cut}}\). The process of extracting \(s, \Omega\) and \(\mathbf{T}\) from Eq. (3.31) is outlined in [29].

For each results chapter, three-dimensional disclinations are identified by isosurfaces of \(s = s_{\text{cut}}\). The chosen values of \(s_{\text{cut}}\) will be provided in each chapter. In all three-dimensional visualisations, the defect isosurfaces are coloured by \(\cos \beta = \Omega \cdot \mathbf{T}\), which allows the local defect profile (+1/2, −1/2 or twist) to be inferred (§2.1.6.2). Presenting \(\cos \beta\) uses two methods:

1. Isosurfaces of \(s\) coloured by \(\cos \beta = \text{Tr}(D)/s\). This takes advantage of Eq. (3.31) without needing to further calculate \(\Omega\) and \(\mathbf{T}\).

2. A tube that connects identified ordered points (next section; §3.4.2.2), coloured by the dot product of the resolved vectors (\(\cos \beta = \Omega \cdot \mathbf{T}\)).

The second of these options give a marginally cleaner presentation, and the disclinations are shown alongside the vector \(\Omega\) and \(\mathbf{T}\). This gives additional information on how \(\Omega\) varies along the loop, which can aid identification of charged loops (Chapters §4 and §5). However, for many purposes, simply visualising \(\cos \beta\) is sufficient and those visualisations use the first option.

### 3.4.2.2 Defect to ordered points

Simply calculating \(D\) and extracting \(s(r), \Omega(r)\) and \(\mathbf{T}(r)\) is sufficient for identifying and characterising the local properties of disclinations. However, we
require further steps for calculating non-local properties, such as the loop contour length $L$, or the writhe $W_r$ and twist $T_w$.

To calculate non-local properties, we build an algorithm that converts each disclination into an ordered sequence of points (an example is given in Fig. 3.6). In essence, this means that we turn a scattered set defect cells ($s > s_{\text{cut}}$) into a polymer, with the associated vectors ($\Omega$ and $T$) defined at each monomer site. Another purpose built in to this method is that the dyadic deconstruction (Eq. (3.31)) gives $\Omega$ and $T$ but does not resolve their relative sign, nor whether they are continuous along the loop. Situations can arise where the vectors are incorrectly flipped. The correct relative sign and continuity must be manually sorted by ensuring the correct sign of $\text{sgn}(\text{Tr}(D)) = \text{sgn}(\Omega \cdot T)$ via Eq. (3.31) [29].

For achieving an ordered sequence of points with smoothly-varying $\Omega$ and $T$, we apply several steps. These steps start with a single cell and recursively build a connected cluster of cells which form the defect line/loop. To do this, defect cells are given an identifier $I$, which control which cells can be iterated over and grouped into points (monomers). Cells with $I = 0$ are in the cluster and can be iterated over, $I = 1$ are in the cluster and cannot be iterated over, and $I = -1$ are not in the cluster. These steps are i) initialisation, ii) sorting, iii) points to monomer and iv) ordering monomers.

**Initialisation:** the defect cells are found and the cluster is initialised.

1. Defect cells are found as $s > s_{\text{cut}}$. All cells are assigned an identifier $I = -1$, which means that they have not been assigned to the cluster yet (Fig. 3.5a).

2. To initialise the cluster, a defect cell is chosen and assigned $I = 0$ (Fig. 3.5b).

**Sorting:** cells are iterated over to build the cluster. This step cycles through all $I = 0$ cells until there are no $I = -1$ left. Within this step, $\Omega$ and $T$ are flipped to ensure continuity and correct relative sign (Fig. 3.5c-f).

3. A $I = 0$ cell is chosen and assigned with $I = 1$. This ensures that the sorting loop doesn’t re-select the same cell. For this cell, all neighbouring cells are found. If any neighbour is not already in the cluster ($I = -1$), it is added to the cluster by assigning $I = 0$ (Fig. 3.5c).
Figure 3.5 **Schematic of steps to convert a defect to an ordered sequence of points.**

- **a.** Disclinations are constructed as cells where $s > s_{\text{cut}}$ [§3.4.2.1] and assigned an identifier $I = -1$ (orange).
- **b.** A defect cell is chosen and given identifier $I = 0$ (blue). Iteration over all $I = 0$ begins.
- **c.** The $I = 0$ cell is given $I = 1$ (dark blue). Neighbouring cells are given identifier $I = 0$.
- **d.** The selected and neighbour cells are grouped into a monomer (closed black outline).
- **e.** A new $I = 0$ cell is changed to $I = 1$. Neighbour cells are identified and changed to $I = 0$ if previously $I = -1$.
- **f.** Iteration continues and additional monomers are found for $I = 1$ and neighbour cells that are not already associated with a monomer.
- **g.** A monomer at position $r_c$ can be added to the start or end of an ordered sequence. To be added to the start of the chain, the monomer must be within 5 cells of the first point in the sequence ($r_0$) and satisfy $t_{\text{start}} \cdot T > 0$. To be added to the end of the chain, the monomer must be within 5 cells of the last point in the sequence ($r_N$) and satisfy $t_{\text{end}} \cdot T > 0$.

Here, $T$ is the tangent vector of the monomer at $r_c$, $t_{\text{start}}$ is the vector pointing from $r_c$ to $r_0$ and $t_{\text{end}}$ is the vector pointing from $r_N$ to $r_c$.

4. Corrections to $\Omega$ and $T$ are found by comparing vectors between neighbouring cells with $I = 1$ and $I = 0$. Those with $I = 1$ have already been sorted, so corrections are applied to $I = 0$. The vector signs are flipped according to:

(a) $\text{sgn}(\text{Tr}(D)) = \text{sgn}(\Omega \cdot T)$

(b) $T_0 \cdot T_1 > 0.0$, where $T_0, T_1$ are the tangent vector for $I = 0, 1$ respectively.

Here, (a) ensures the correct relative sign and (b) that the vectors are continuous throughout the cluster.
Figure 3.6  Example of a disclination loop converted into a sequence of ordered points. Left: a disclination loop is visualised as an isosurface $s = s_{cut}$. Right: the same loop is constructed as an ordered array of points. Each point has an associated rotation vector $\Omega$ (red arrows) and tangent vector $T$ (blue arrows), which smoothly vary along the loop. Simulation data from Chapter §5.

Points to monomer: clustered cells are grouped into monomers.

5. The selected cell and neighbours are grouped as a monomer if not already included in another monomer (Fig. 3.5d).

6. The composite cells are averaged over to obtain $T$ and $\Omega$ per monomer.

Ordering monomers: monomers are added to the start or end of an ordered sequence (Fig. 3.5g).

7. The monomer is checked if it lies within 5 lattice cells of the first ($|r_c - r_0| \leq 5$) or last monomer in the sequence ($|r_N - r_c| \leq 5$). Here, $r_c$ is the current monomer, $r_0$ is the start monomer and $r_N$ is the end monomer in the sequence.

8. To ensure the monomer placement is consistent with the line tangent $T$, two unit vectors are constructed $t^{end} = \frac{r_N - r_c}{|r_N - r_c|}$ and $t^{start} = \frac{r_c - r_0}{|r_c - r_0|}$. These unit vectors identify the direction of the current monomer to the end monomer $t^{end}$ and the direction of the start monomer to the current monomer $t^{start}$.

9. The monomer is added to the end of the sequence if $|r_N - r_c| \leq 5$ and $t^{end} \cdot T > 0$. The monomer is added to the start of the sequence if $|r_c - r_0| \leq 5$ and $t^{start} \cdot T > 0$. If neither condition is satisfied, the monomer is neglected.
Overall, these steps obtain an ordered sequence of points that compose the defect loop (Fig. 3.6).

### 3.4.2.3 Ribbon framing vector

In Chapter § 2.1.8.3, we described how the topological properties of purely $-1/2$ disclination loops can be inferred from the self-linking number, a topological invariant associated with ribbons [85, 86], which we will utilise to analyse the properties of disclinations accompanying nematic colloids in N-MPCD simulations. The geometric description of ribbons require two pieces of information [65, 183]:

- Information about the tangent curve of the ribbon. This requires the positions $\mathbf{r}$ that compose the ribbon, and the tangent vector $\mathbf{T}$ at each point.
- A framing vector $\mathbf{w}$ that represents the perpendicular orientation of the ribbon.

These three vectors enable the writhe $W_r$ (Eq. (2.36)) and twist $T_w$ (Eq. (2.37)) to be calculated, which combine to give the self-linking number $S_l$ (Eq. (2.35)). Of these, the position $\mathbf{r}$ and tangent vectors $\mathbf{T}$ are found from the previous section. However, obtaining the framing vector $\mathbf{w}$ requires additional steps. Here, we outline the methods used for obtaining $\mathbf{w}$ for a $-1/2$ disclination loop.

A characteristic of $-1/2$ profiles is that the local director $\mathbf{n}$ is always oriented perpendicular to $\mathbf{T}$ (§ 2.1.6.2). This is valuable in constructing $\mathbf{w}$, since all directions of $\mathbf{n}$ satisfy the ribbon requirement that $\mathbf{w} \perp \mathbf{T}$. Therefore, all that is needed is to pick one of these director orientations and to track how it varies along the loop. We choose $\mathbf{w}$ to be one of the three radially outward pointing $\mathbf{n}$. While $\mathbf{w}$ must vary continuously, it is simplest to identify all three radial orientations $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$, and then check for continuity afterwards.

To identify $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$, we must extract the local director on the plane perpendicular to $\mathbf{T}$. For identifying the local director, we construct a cube (Fig. 3.7a) of $5 \times 5 \times 5$ lattice cells centred on each of the aforementioned ordered points (§3.4.2.2). In the N-MPCD simulations, this cube size is sufficient to contain the disclination cross-section (which has a diameter of $\approx 2$ lattice cells using $s \geq s_{cut}$.
Figure 3.7  **Schematic of steps to obtain framing vector.**  

A point along the disclination line is chosen (dark blue sphere). About that point, a $5 \times 5 \times 5$ box is constructed. Cartesian directions are indicated, $\mathbf{e}_x$ (red arrow), $\mathbf{e}_y$ (green arrow), $\mathbf{e}_z$ (blue arrow). The disclination tangent vector $\mathbf{T}$ is shown as a dark blue arrow. 

**b.** A transformation is applied to the box frame so that $\mathbf{T}$ is aligned along $\mathbf{e}_z$.  

**c.** The transformed director field (silver) is resolved on the central slice of the box, oriented perpendicular to $\mathbf{T}$.  

**d.** Within the slice, a test loop is drawn (grey circle) and test vectors $\mathbf{r}_{\text{test}}$ are constructed to point radially outward from the defect core. 

**e.** One radial orientation of the $-1/2$ profile, $\mathbf{w}_1$ (orange arrow), is found as the $\mathbf{r}_{\text{test}}$ that is most aligned with the local director at a point along the test loop. 

**f.** Inverse rotation is applied to the framing vector $\mathbf{w}_1$ to return to Cartesian basis.  

**g.** The other two $-1/2$ orientations $\mathbf{w}_2$ and $\mathbf{w}_3$ are found by $2\pi/3$ rotations of $\mathbf{w}_1$ about $\mathbf{T}$.  

**h.** The framing vector (orange arrows) is chosen for each defect point as one of $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$ (orange/silver arrows) that is most closely aligned with previous point. These steps find a smoothly varying framing vector $\mathbf{w}$ along the disclination loop.

From § [3.4.2.1](#), and the director in the immediate surrounding. Next, we identify the plane perpendicular to $\mathbf{T}$. Because, $\mathbf{T}$ varies continuously along the loop, it is simplest to transform into a frame where $\mathbf{T}$ is aligned with a Cartesian axis. Therefore, a rotation matrix $\mathbf{R}$ is constructed which aligns the local disclination tangent $\mathbf{T}$ with $\mathbf{e}_z$ (Fig. 3.7b). Subsequently, the rotation transformation is applied to $\mathbf{n}$. This operation enables the radial director to be found on the transformed plane with normal vector $\mathbf{e}_z$ (Fig. 3.7c).

To find $\mathbf{w}_1, \mathbf{w}_2$ and $\mathbf{w}_3$ on the plane, we construct a test vector $\mathbf{r}_{\text{test}} = \cos \theta_{\text{test}} \mathbf{e}_x + \sin \theta_{\text{test}} \mathbf{e}_y$ centred on the core (i.e. the centre cell in the $5 \times 5 \times 5$ box; (Fig. 3.7d)). The purpose of $\mathbf{r}_{\text{test}}$ is to use as a probe for radially outwards orientation. This
works by building a circuit of points \( \mathbf{r}_l \) that surrounds the core. On these points, the test vector \( \mathbf{r}_{\text{test}} \) is compared with the local director \( \mathbf{n}(\mathbf{r}_l) \). Determined over all points \( \mathbf{r}_l \) and test orientations \( \theta_{\text{test}} \), one of the candidate framing vectors, \( \mathbf{w}_1 \), is chosen as the \( \mathbf{r}_{\text{test}} \) that maximises the absolute value \( |\mathbf{r}_{\text{test}} \cdot \mathbf{n}(\mathbf{r}_l)| \) (Fig. 3.7f). The inverse rotation transform \( R^{-1} \) is applied to \( \mathbf{w}_1 \) to revert back to the original basis (Fig. 3.7f), and \( \mathbf{w}_2, \mathbf{w}_3 \) are determined as orientations \( 2\pi/3 \) rotated relative to each other about \( \mathbf{T} \) (Fig. 3.7g).

With the three radial orientations identified, the last step is to choose one framing for each point along the loop. The framing vector is initialised as \( \mathbf{w} = \mathbf{w}_1 \) for the first point along the loop, and subsequent points choose from one of the three \( \mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3 \) orientations that minimise the rotation angle compared with \( \mathbf{w} \) from the previous point in the sequence (Fig. 3.7h). This process results in a continuously varying framing vector \( \mathbf{w} \) along the disclination loop, up to \( 2\pi/3 \) rotations at the loop endpoints (§2.1.6.2).

### 3.5 Splay-bend parameter

When studying active turbulence, we consider nematic structures beyond topological defects, such as the kinked bend walls formed by the hydrodynamic instability (§2.2.5). To identify these, the splay-bend parameter \( S_{SB} \) is employed [182]. The splay-bend parameter is constructed from derivatives of \( \mathbf{Q} \) as

\[
S_{SB} = \partial_i \partial_j Q_{ij}, \tag{3.32}
\]

with summation convention applied on repeated indices. The splay-bend parameter can be understood by constructing the tensor order parameter \( \mathbf{Q} = S \frac{1}{d-1} (\nabla \cdot \mathbf{n}) (n_i n_j - \delta_{ij}) \) with a constant scalar order \( S \). From Eq. (3.32), this finds

\[
S_{SB} = \frac{dS}{d-1} (\nabla \cdot (\mathbf{s} - \mathbf{b})), \tag{3.33}
\]

where \( d \) is the dimension, and \( \mathbf{s} = \mathbf{n} (\nabla \cdot \mathbf{n}) \) and \( \mathbf{b} = \mathbf{n} \times (\nabla \times \mathbf{n}) \) are the splay and bend vectors. This form makes it clearer than Eq. (3.32) that \( S_{SB} \) measures the divergence of the difference between splay and bend. For this reason, \( S_{SB} \) has proven useful as a visualisation parameter for inferring the local deformation structure around disclination lines/loops [27, 86], and for identifying bend walls in active-nematics [111].
3.6 Flow structures

In addition to studying nematic structures, we also identify structures in the instantaneous velocity field. This section introduces the methods we use to explore the activity-induced constraints on the organisation of topological defects and turbulent flow patterns. For many classes of fluid flows, understanding instantaneous flow patterns and spatial coherence can be explored in terms of the velocity gradient tensor $A = \nabla \mathbf{v}$ \cite{184,185}. This tensor encodes rich geometric information about the fluid motion and deformation through its $d^2$ components. The velocity gradient tensor is naturally decomposed as

$$A = E + W,$$  \hspace{1cm} (3.34)

where $E = \frac{1}{2} (A + A^T)$ is the symmetric rate-of-strain tensor, and $W = \frac{1}{2} (A - A^T)$ is the anti-symmetric rate-of-rotation (vorticity tensor). This decomposition was previously introduced in § 2.2.3.

The geometric interpretation of $A$ can be obtained by examining $E$ and $W$ separately. For clarity, we do this in two-dimensions, though discussions naturally extend to 3D. Furthermore, we assume incompressibility (Eq. (2.42)). The rate of strain tensor in 2D is

$$E = \frac{1}{2} \begin{pmatrix} e_{xx} & e_{xy} \\ e_{yx} & e_{yy} \end{pmatrix}. $$  \hspace{1cm} (3.35)

The diagonal elements of the rate of strain tensor ($e_{yy} = -e_{xx}$) describe the stretching or compressing of a fluid element and the off-diagonal elements ($e_{xy} = e_{yx}$) are the rate of shearing strain. An example of pure extensional flow is shown in Fig. 3.8a.

The rate of rotation tensor in 2D is

$$W = \frac{1}{2} \begin{pmatrix} 0 & \omega_z \\ -\omega_z & 0 \end{pmatrix}, $$  \hspace{1cm} (3.36)

with off-diagonal components dependent on the vorticity $\omega_z = (\nabla \times \mathbf{v}) \cdot \mathbf{e}_z$. This vorticity tensor contains information on the rotational motions of the fluid. An example of purely rotational flow is shown in Fig. 3.8b.

In Chapter § 6, we characterise the instantaneous structure of the streamline
Figure 3.8 *Simple flow structures.* a, Pure extensional flow (lilac arrows) with $\mathbf{E} \neq \mathbf{0}$ and $\mathbf{W} = \mathbf{0}$. b, Pure rotational flow with $\mathbf{W} \neq \mathbf{0}$ and $\mathbf{E} = \mathbf{0}$. c, Simple shear flow for $\mathbf{E} = \mathbf{W}$.

patterns using the $Q$ criterion \[186\],

$$Q = \frac{1}{2} \left( \| \mathbf{W} \|_2^2 - \| \mathbf{E} \|_2^2 \right), \quad (3.37)$$

which is the difference between the Euclidean norm squared ($\| \mathbf{A} \|_2^2 = A_{ij}A_{ij}$) of the strain and rotation rate tensors. This parameter is helpful for interpreting the local topological structure of the streamlines because it is directly equivalent to the second invariant of the velocity gradient tensor under incompressibility, $Q = \frac{1}{2} ((\nabla \cdot \mathbf{v})^2 + \| \mathbf{W} \|_2^2 - \| \mathbf{E} \|_2^2)$. Regions where vorticity dominates (elliptical streamline topology) are identified as $Q > 0$, while strain-rate dominated (hyperbolic streamlines) are found as $Q < 0$. A special case for fluid deformation occurs in the case $Q = 0$, where the strain-rate and rotation-rate balance to form simple shear $\mathbf{E} = \mathbf{W}$. Simple shear flows have velocity gradients that are perpendicular to the flow direction, so that $\mathbf{A}$ has a one-dimensional structure (Fig. 3.8c) \[187, 188\]. Regions where $Q = 0$ are referred to as viscometric \[169\].

The Okubo-Weiss parameter \[189, 190\] is equivalent to $Q$ up to a minus sign, but limited to two dimensions. The Okubo-Weiss parameter is defined as the determinant of $\mathbf{A}$. The determinant is equivalent to the second invariant in two-dimensions, but is different in three-dimensions (third invariant). Since we consider applications in three-dimensions, we use the $Q$ criterion rather than the Okubo-Weiss parameter.

Isosurfaces of $Q$ are frequently used in visualising three-dimensional vortex structures in geophysical flows \[191\], and more recently have been applied to two-dimensional biophysical flows such as microtubule-kinesin active turbulence \[122\] and confluent cell layers \[192\]. However, no prior studies have quantitatively considered the interplay of topological flow structures using $Q$ and nematic structures, as is done in Chapter §6.
Chapter 4

Mesoscale simulations of nematic colloids
4.1 Introduction

One particularly versatile form of self-organised matter arises through the addition of inclusions in passive liquid crystals. Through imposed boundary conditions (homeotropic or tangential), colloidal particles can directly tune and respond to topological and geometric features in the order parameter field, which provides a pathway to create a variety of topological composite materials, such as photonic crystals [193], cloaks and metamaterials [194], or self-quenched glasses [84].

To study colloidal inclusions in passive nematics, this chapter employs nematic Multi-Particle Collision Dynamics (N-MPCD), a mesoscale particle-based hydrodynamics solver (Chapter §3). Following the design of a boundary-method for capturing inclusion-solvent elastic interactions, we assess the suitability of the algorithm for studying topological phenomena and self-assembled dynamics. We begin by quantifying the effective anchoring strength, which is indirectly tuned via particle interactions with a boundary. In three-dimensions, topological defects form that broadly confirm the structures predicted by elastic energy minimisation [44]. A pair of surface defects, known as Boojums [195], are found for colloids with tangential anchoring. With normal anchoring, a Saturn ring and a dipolar halo are identified. The elastic-response of the N-MPCD algorithm is validated by computing the elastic force between a colloid and a wall, as well as between two colloids. Both interactions follow scaling laws in agreement with previous theoretical predictions. The numerical ability to simulate topological details and elastic forces will enable future studies to study colloidal inclusions in active and complex environments, an avenue which is not yet well explored [196].

A second purpose of this chapter is to study defect structures in an environment that has fluctuating hydrodynamics, a feature that is intrinsically ingrained in N-MPCD. Colloidal dispersions in nematics have mainly been studied with deterministic continuum models, either via free energy minimisation techniques [84, 86], or by means of hybrid lattice Boltzmann simulations [143]. However, fluctuations are non-negligible for small inclusion embedded in active bio-fluid environments. The N-MPCD topological patterns are studied, both over time and in steady state, with a single colloidal particle or a colloidal dimer. For the dimer, thermal fluctuations and boundary influences can lead to tilted and non-ideal versions of the expected entangled structures. While in steady state, disclination loops are always associated with -1/2 wedge profiles; however,
en route to equilibrium thermal noise enables metastable states with transient patterns that possess twist or localised $+1/2$ wedge profiles.
4.2 Methods

This chapter employs the N-MPCD algorithm (Chapter §3), with inclusions simulated as mobile boundaries. Throughout the results, values are given in MPCD units of cell size $a = 1$, fluid particle mass $m = 1$ and thermal energy $k_B T = 1$. From these, the unit of time is a derived quantity, $\tau = a \sqrt{m/k_B T} = 1$. Simulation time $t$ iterates with time-step size $\delta t = 0.1$. Simulations are performed in two ($d = 2$) and three ($d = 3$) dimensions with system sizes $[L_x, L_y]$ and $[L_x, L_y, L_z]$ respectively, aligned with a Cartesian basis $e_x, e_y, e_z$. The average number of particles per cell is $\langle N_c \rangle = 20$. The nematic mean free potential is set to $U = 20$, corresponding to deep in the nematic phase [146]. Other nematohydrodynamic parameters include the rotational friction $\gamma_R = 0.01$, shear susceptibility $\chi = 0.5$ and tumbling parameter $\lambda = 2$. Unless otherwise stated, colloids with radii $R = 6$ are used in three-dimensions, and $R = 10$ in two-dimensions. The effective particle rod-length is $\ell_u = 0.006$ (Eq. (3.25)). In all simulations, MPCD particles start with randomly generated positions and velocities. While the bulk fluid properties remain constant between simulations, the boundary conditions vary between studies, in addition to initial particle orientations. These initialisation parameters are specified at the start of each results section.

Defects are characterised in three-dimensions using the disclination density tensor $D = s(r) \Omega \otimes T$ (§3.4.2.1). Disclination loops are identified as isosurfaces where $s(r) \geq 0.9$. For obtaining continuous $\Omega$ and $T$ vectors along the loop, disclinations have been converted to an ordered sequence of points (§3.4.2.2). Geometric and topological analysis of disclination loops utilises the self-linking number framework introduced in §2.1.8.3. In these calculations, a ribbon framing vector $w$ is constructed using the procedure from §3.4.2.3. Disclination contour lengths are calculated by summation of bond lengths between ordered points. All visualisations in three-dimensions use the Mayavi python library (§3.3).

4.3 Anchoring strength

Anchoring strength determines the extent to which geometric features can be imprinted on the nematic director (§2.1.3.4). For $Z \gg 1$, surface anchoring can be sufficiently strong to form topological defects in the bulk liquid crystal.
In continuum free-energy or lattice-Boltzmann simulation methods, the anchoring strength and bulk elasticity are input parameters, enabling $Z$ to be tuned. In contrast, individual fluid particles carry out the anchoring conditions in N-MPCD. The particle orientation transformations are hard-set, orienting exactly with the anchoring easy-axis (Eq. (3.11)). However, since collision events and hydrodynamic fields are coarse-grained into lattice cells composed of $N_c$ particles, the effective anchoring strength is not necessarily infinite. This is because only a subset $N^*_c$ of the $N_c$ particles in a cell perform the transformation.

In this section, we characterise the effective anchoring regime that arises from the orientation transformations on the $N^*_c$ particles that violate a surface (Eq. (3.10)). One method of obtaining $Z$, is to measure the Kleman-de Gennes extrapolation length $\xi_K = K/W$ (Eq. (2.16)). Then

$$Z = \frac{R}{\xi_K},$$

is simply the ratio of lengthscales. A simple geometry for measuring the extrapolation length is a cell with hybrid anchoring conditions. Here, we measure this in two-dimensions in a hybrid-aligned nematic cell (HAN). Planar anchoring is applied on the bottom surface ($y = 0$), homeotropic on the top ($y = L_y$) and periodic boundary conditions are applied in $e_x$ (Fig. 4.1a).

To establish a prediction for $\xi_K$, the director can be written in terms of an orientation angle $\theta(y)$, which depends only on the vertical coordinate $y$ since there is translational invariance in $e_x$. Assuming a finite extrapolation length $\xi_K$ behind each boundary, the boundary conditions are $\theta(-\xi_K) = 0$ and $\theta(L_y + \xi_K) = 90^\circ$.

In the equilibrium configuration, the minimum energy solution of the Frank free energy (Eq. (2.7)) penalises nematic gradients, forming a linear relationship between $\theta$ and $y$. The resulting predicted extrapolation length is

$$\xi_K = \frac{1}{2} \left( \frac{90}{m_g} - L_y \right),$$

where $m_g$ is the gradient of the linear fit in degrees per unit length.

To obtain $\xi_K$ and $Z$ for the N-MPCD simulations, we perform 20 independent simulation runs with total timesteps $T_S = 1000$. For each simulation, 100 data points are recorded, equally spaced in time. The director is initialised with random orientations, requiring a warmup time of $T_W = 1000$ before data collection begins, to ensure the equilibrium configuration is reached.
Figure 4.1  **Extrapolation length.** a, A hybrid-aligned nematic (HAN) cell of size $L = 50$ with planar anchoring on the bottom surface, homeotropic on the top, and periodic boundaries on the sides. The director field is shown as the white line field. For finite strength anchoring, the anchoring starts an effective distance $\xi_K$ behind each surface. b, Director orientation $\langle \phi(y) \rangle$ with vertical height $y$, averaged over horizontal position $x$, time $t$, and 20 simulation runs. Red squares present orientation when only the $N^* \leq N_c$ particles that directly violate Eq. (3.10) have the anchoring conditions applied. Dark blue circles are for transformations applied to all particles within a cell $N_c$.

Measurements of $m_g$ are obtained as linear fit of $\langle \theta(y) \rangle$ against $y$ (Fig. 4.1b). Here, $\langle \cdots \rangle$ is an ensemble average over all time and $x$. This gives $m_g = 1.684 \pm 0.001$ and $\xi_K = 1.700 \pm 0.001$. For the default radii used in this study of $R = 6$ (3D) or $R = 10$ (2D), the dimensionless anchoring numbers are $Z = 3.75$ (3D) and $Z = 6.25$ (2D), using Eq. (4.1).

In Fig. 4.2a, we show the director configuration for a two-dimensional colloid with $R = 10$. Despite $Z > 1$, this does not present any singularities in the bulk director. The anchoring on the colloid is not sufficiently strong to form topological defects. Therefore, the emergent anchoring strength is not capable of studying bulk topological phenomena on suitable simulation scales.

To observe topological defects, $Z$ must be increased either by increasing $R$ or reducing $\xi_K$. We choose to increase the anchoring strength, since larger colloids would require greater system sizes. To increase the anchoring strength, the proportion of particles in a cell with orientation transformations is $N^*_c$ increased. This is done by applying the anchoring transformation (Eq. (3.11)) directly to all particles in cells that are intersected by the boundary ($N^*_c \to N_c$). This reduces mixing between particle orientations in the nematic collision, effectively
Figure 4.2  The director field around a colloidal particle with different anchoring strength.  

a, A two-dimensional colloid (circle) with \( Z = 6.25 \) only weakly deforms the surrounding director and no topological defects are observed.  
b, A colloid with \( Z = 68.0 \) forms two \(-1/2\) defects (blue trefoil symbols). The director field is shown as the white line field. Both simulations have a colloid radius \( R = 10 \) and are performed in a system size \( L_x = L_y = 50 \) with periodic boundary conditions.

increasing the anchoring strength.

When \( N_c^* \rightarrow N_c \), the gradient of the linear fit (Fig. 4.1) is found to increase to \( m_g = 1.811 \pm 0.003 \), which gives an extrapolation length \( \xi_K = 0.147 \pm 0.0002 \). The anchoring number is calculated using Eq. (4.1) to be \( Z = 40.8 \) (3D with \( R = 6 \)) or \( Z = 68.0 \) (2D with \( R = 10 \)). Thus, the new approach increases the strength by an order of magnitude and the director field now exhibits a pair of topological defects in the bulk nematic order (Fig. 4.2b; blue trefoil symbols).

For the purpose of studying elastic and topological phenomena in N-MPCD, the strong anchoring transformations are applied throughout this chapter.
4.4 Defects around a single colloid

The topological defects associated with nematic colloids are central to the organisation of self-assembled structures [73]—their strong elastic deformation forming particular long-ranged patterns and dominating relaxation kinetics [11]. For this reason as a first application of the algorithm, this section explores the three-dimensional defects accompanying isolated colloids, examining their characteristics in steady-state and when initialised out of equilibrium.

With these defect-focussed aims, a single spherical colloid is initialised within a thermal quench (randomised particle orientations) in an \( L_x = L_y = L_z = 40 \) domain with periodic boundary conditions applied on all walls. A total of 20 simulations are conducted for a colloid with homeotropic anchoring, while 5 simulations are performed for the planar configuration. The simulations are run for a duration of \( T_S = 1000 \), after an initial warmup phase of \( T_W = 400 \). During the warmup phase, particles rapidly align their orientations, forming domains of nematic alignment driven by the mean field interaction potential \( U = 20 \) (§3.2.2.2). As data collection starts, the nematic director is continuous except at disclinations, which present as loops. Over time, the loops combine and minimise in size until \( t \approx 600 \), where the nematic director field approaches configurations close to the global equilibrium. In this steady state, defects form distinctive arrangements close to the colloidal surface, with features dependent on the homeotropic or planar anchoring conditions.

For the case of planar anchoring in steady state (Fig. 4.3a), the inability for a tangential vector field to continuously coat a sphere (§2.1.7) necessitates two surface defects at the colloidal antipodes, known as Boojums [195]. These can either be hyperbolic point defects split in half by the mirror plane of the colloid, or separated into handle-shaped semi-loops that connect two \(+1/2\) closely separated surface defects [198]. Semi-loops are observed for N-MPCD simulations from a quench (Fig. 4.3a) and resemble experimental images of Boojum defects (Fig. 4.3d). Colloids with homeotropic anchoring nucleate one of two configurations, both containing an odd point charge (§2.1.8.1). The first of these is a Saturn ring—a closed \(-1/2\) disclination loop surrounding the equatorial axis [68, 69]. The local \(-1/2\) nature can be seen by the purple colouring, representing \( \cos \beta = -1 \). The second is a hyperbolic hedgehog, forming a topological dipole [67].
Figure 4.3 *Steady-state defect configurations associated with a single colloid in N-MPCD and experiments.* a, Planar anchored colloid with Boojum defects in N-MPCD. b, Homeotropic anchored colloid with a Saturn ring defect in N-MPCD. c, Homeotropic anchored colloid with a hyperbolic hedgehog opened into a halo-like ring in N-MPCD. Director field slice shown by grey rods and colloids as silver spheres. Disclinations are isosurfaces coloured by \( \cos \beta \) (colouring same as Fig. 2.6). d, Photograph of two Boojum defects obtained with bright field microscopy. Image reproduced from [5]. e, Photograph of a Saturn ring defect. f, Photograph of a hyperbolic hedgehog defect. Both e, and f, are reproduced from [2].

In N-MPCD, 17 of the 20 homeotropic simulations finished with a Saturn ring (Fig. 4.3b), which closely resemble the equatorial defect rings observed in experiments (Fig. 4.3e). The other 3 ended with an intermediate structure between a point hedgehog and Saturn ring (Fig. 4.3c) [40]. None of the simulations produced a localised point defect, which are the expected dipolar colloid-defect complex in experiments (Fig. 4.3f). In this work, we refer to this intermediate state as a dipolar halo. In experiments, topological dipoles are the stable state whenever \( Z = R/\xi_K \) is large, while Saturn rings are preferred in confinement and for smaller colloids with weaker anchoring [66]. Simulations predominantly reproduce Saturn rings [199] and this is also the case for N-MPCD.

We next show an example of the defect coarsening towards a Saturn ring. Soon after the quench, the nematic field far from the colloid has ordered, but a single
large loop remains, gradually relaxing into a Saturn ring configuration (Fig. 4.4). Away from equilibrium, the loop is free to sample disclination profiles outside of purely trefoil-like $-1/2$. This is demonstrated by colouring the disclinations with $\cos \beta = \Omega \cdot T$ (§2.1.6.2), which shows segments of twist (green/blue), while the region closest to the colloid is $-1/2$ (purple). The loop in Fig. 4.4 is charged, requiring $\Omega$ to make a full revolution \[69\]. However, the rotation is not homogeneous and $\Omega$ remains largely uniform for large segments of the disclination that are distant from the colloid. Conversely, the segments of the disclination closest to the colloidal surface support nearly the entire variation of $\Omega$. At later times ($t \approx 600$), the loop reduces in size and the anchoring constraint on the colloid forces $\Omega$ to rotate into the expected constant anti-parallel configuration $\Omega \cdot T = -1$, forming the expected Saturn ring.

This section has demonstrated that the bulk N-MPCD is capable of cleanly resolving and characterising disclination configurations around single nematic colloids. The intrinsic stochasticity of the collision operators enable relaxation pathways to be explored, a feature which is utilised in more detail for systems with two colloids in §4.7. In the next section, we verify the dynamical response of nematic colloids to long-range features of the bulk director field.

Figure 4.4  
Dynamics of a near-colloid disclination loop relaxing into a Saturn ring. The disclination rotation vector $\Omega$ (red) and tangent vector $T$ (navy blue) are shown as arrows. Each frame is shown with the corresponding simulation time $t$. Disclination loops are constructed as tubes (§3.4.2.1) and coloured by $\cos \beta$. 

\[
t = 540 \quad t = 560 \quad t = 620
\]
4.5 Elastic interactions

The nematoelastic interactions between colloids and defects allow them to self-assemble into colloid-defect complexes \[67, 73\]. These steady-state complexes with homeotropic anchoring appear either as elastic quadrupoles (Saturn ring; Fig. 4.3c) or dipoles (dipolar halo; Fig. 4.3c). In environments with multiple colloids or confining surfaces, these far-field deformations mediate elastic forces with power law forms dependent on the dominant dipole/quadrupole moment (Eq. (2.32)). This section characterises long-range power-law interactions, and angle-dependent attraction/repulsion of quadrupolar elastic forces.

4.5.1 Power-law forces

To quantify the power-law nature of nematic interactions in N-MPCD, a colloid interacting with a wall with strong homeotropic anchoring is considered. This setup is preferred over a pair of mobile colloids because it removes additional complexities arising from the relative orientation of a pair of nematic colloids (which will be considered in § 4.5.2). For separations from a single wall, the elastic force is expected to be purely repulsive, and decays with distance from the wall \[75, 79\]. To evaluate the decaying force magnitude with colloidal distances from the wall, measurements are performed in both two and three dimensions.

In two-dimensions, the system size is set at $L_x = L_y = L$ with periodic boundary conditions in $e_x$ and solid walls in $e_y$. Both upper and lower solid walls have no-slip boundary conditions, but only the lower boundary has anchoring conditions applied, with strong homeotropic alignment. Four colloid radii are sampled $R \in [6, 8, 10, 12]$, with system sizes $L \in [50, 55, 60, 80]$ respectively, to adjust for system-size effects. The director is initialised from $n = e_y$. The bulk uniaxial alignment produces a pair of near-surface point defects with $k = -1/2$ charges in 2D (Eq. (2.18)). A simulation warmup time of $T_W = 1000$ is applied, where the colloid is held fixed and the director relaxes to the equilibrium configuration. Simulations are then performed for $T_S = 30000$, with the colloid mobile and responsive to the nematic environment. A total of 40 independent simulation runs are performed for each $R$. In three-dimensions, two colloid radii are used. The first is $R = 4$ with $L_x = L_y = L_z = 30$, and the second is $R = 6$ with $L_x = L_y = 30, L_z = 35$. Simulations have periodic boundary conditions in $e_x$.
Figure 4.5 Measurements for determining the force-distance relation. 

a. Schematic of colloid (navy circle) with radius $R$, initialised within the far-field director $\mathbf{n}$, forming equatorial -1/2 defects (blue trefoil symbols). The colloid experiences an elastic repulsion force due to the wall $\mathbf{F}_{\text{wall}}$, which is probed by a gravitational-like external force $\mathbf{F}_G$. The distance $h$ between the colloid’s centre of mass and the wall is $h_{eq}$ when $\mathbf{F}_G = \mathbf{F}_{\text{wall}}$. 

b. Example of 30 colloidal trajectories (grey) for a two-dimensional colloid with radius $R = 10$. The time-dependent ensemble mean is shown by dark blue curve, that fluctuates about the time-averaged mean (red horizontal line). The red shading is the standard error about the time-averaged mean.

c. Example snapshot of a colloid interacting with the homeotropic anchored wall (black horizontal line). The white line field is the director and background colouring is the scalar order parameter $S$.

and $\mathbf{e}_y$, and impermeable no-slip walls in $\mathbf{e}_z$. Similar to two-dimensions, only the lower plate has homeotropic anchoring conditions. The director is initialised along $\mathbf{n} = \mathbf{e}_z$, which forms a quadrupolar Saturn ring. The simulations run for $T_S = 4000$ following a warmup period of $T_W = 1000$, where the colloid is held static. Statistics are generated from 30 independent measurements for each $R$. For convenience, we will refer to $\mathbf{e}_G$ as the anchoring direction on the bottom plate (i.e. $\mathbf{e}_G = \mathbf{e}_y$ in 2D and $\mathbf{e}_G = \mathbf{e}_z$ in 3D).

The decaying power-law nature of the elastic forces are determined by measuring the interaction forces of a nematic colloid at a distance $h$ away from a homeotropic anchored wall. In the proximity of the wall, the colloid experiences a strong elastic repulsive force, $\mathbf{F}_{\text{wall}}$, that decays with distance. This can be represented as a quadrupole-quadrupole interaction between the colloid and it’s mirror image on the other side of the wall \[79\]. Theoretical predictions of the elastic force is \[75, 200–202\]

$$\mathbf{F}_{\text{wall}} \sim K \frac{R^{2d}}{h^{d+3}} \mathbf{e}_G,$$  \hspace{1cm} (4.3)

in $d$ dimensions and nematic elastic constant $K$. In addition, the motion of
the colloid through the fluid experiences a drag force due to viscosity $F_{\text{drag}}$, and a fluctuating force $F_{\text{fluc}}$ that enters due to the stochasticity of the collision operators. To measure $F_{\text{wall}}$, we apply an external gravitational-like body force to the colloid

$$F_G = M_c G,$$  \hspace{1cm} (4.4)

where $M_c = \frac{4}{3} \pi R^3 \langle N_c \rangle$ is the mass of the colloid in 3D or $M_c = \pi R^2 \langle N_c \rangle$ in 2D. The constant acceleration $G = -G e_G$ is directed towards the homeotropic wall with strength $G$. The applied body force (Eq. (4.4)) probes the elastic force by introducing an equilibrium distance $h_{eq}$ at which $F_{\text{wall}} + F_G = 0$ (Fig. 4.5a). When the elastic and applied forces balance, the colloid only fluctuates about $h_{eq}$ (grey trajectories in Fig. 4.5b). Therefore, the fluctuating and drag forces can be neglected in the force measurements provided there is statistical certainty on $h_{eq}$. For this reason, the simulations are iteratively re-initialised from new start positions $h \approx h_{eq}$, so that when data collection begins, the mean of all runs at time $t > T_W$ (blue solid line) has unbiased fluctuations about the time-averaged mean (red solid line). The equilibrium position $h_{eq}$ is taken as the time-independent mean, with the standard error as the statistical uncertainty (red shading).

The results of the force measurements are presented in Fig. 4.6. Elastic forces are largest at smaller colloid separations from the wall, with magnitudes $|F_{\text{wall}}| =$

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**Figure 4.6** Elastic interaction forces between colloids of radius $R$ and a homeotropic anchored wall. **a**, Two-dimensional elastic repulsion force $F_{\text{wall}}$ measured at equilibrium colloid-wall separation distances $h_{eq}$. Distances are scaled by the colloid radius $R$. **b**, Same as **a** but for three-dimensions. The black lines, shown for comparison with the expected scaling (Eq. (4.3)), has a gradient of $-5$ (2D) and $-6$ (3D). Errorbars represent the standard error.
\( F_{\text{wall}} \approx 10 \) in 2D (Fig. 4.6a) and \( F_{\text{wall}} \approx 50 \) in 3D (Fig. 4.6b). At increasing separations, these forces rapidly decay. Comparing with predictions (Eq. (4.3); black slope), N-MPCD elastic forces decay with the expected power law in two- and three-dimensions. In two-dimensions \( F_{\text{wall}} \sim h^{-5} \) holds well for all sampled colloid radii. In three-dimensions, the repulsion matches \( F_{\text{wall}} \sim h^{-6} \) for \( R = 6 \), but experiences a smaller power law for \( R = 4 \). This indicates that N-MPCD elastic interactions are most accurately resolved for colloid radii \( R > 4 \). Overall, these force measurements demonstrate that N-MPCD is capable of forming long-range quadrupolar deformation in the bulk nematic order and that the colloids dynamically respond to elastic stresses on their surface.

### 4.5.2 Force anisotropy

While the interactions between colloids and walls are purely repulsive, the long-range interactions between pairs of quadrupolar colloids are more complicated since they can alternate between repulsive and attractive depending on relative quadrupole orientation \[11, 57, 75\]. In this section, we study the orientational nature of the elastic force. The force anisotropy measurements are performed in two-dimensions for simplicity.

The angular dependence of the interaction between two colloids is studied by fixing one colloid at \( r_1^0 = (40, 40) \), while a second mobile colloid is allowed to explore different relative configurations \( r_2^0 = (40 + \Delta x, 40 + \Delta y) \) (Fig. 4.7a). These configurations are \( \Delta x = r_s \cos \theta_s \) and \( \Delta y = r_s \sin \theta_s \) with separation magnitude \( r_s \in [40, 50, 55, 60] \) and orientation angle, of \( \theta_s \in [0^\circ, 6^\circ, 11^\circ, 17^\circ, 22^\circ, 33^\circ, 45^\circ, 56^\circ, 68^\circ, 79^\circ, 90^\circ] \). Simulations have periodic boundary conditions on all walls, with system size \( L_x = 80 + 40 \cos \theta_s \) and \( L_y = 80 + 40 \sin \theta_s \). The far-field director alignment is initialised along \( \mathbf{e}_y \), which preferentially positions two \(-1/2\) defects on either side of the colloids – establishing the same quadrupole orientation for both colloids. The simulation time is \( T_S = 3000 \) after a brief warmup time \( T_W = 5 \), which allows the defects to form without significantly altering the quadrupole direction.

Two vectors are measured to determine the attractive or repulsive dynamics of the mobile colloidal probe (Fig. 4.7a). The first is the separation vector between the colloids \( r_s^0 = r_2^0 - r_1^0 \) (blue arrow). This establishes a constant reference to measure the response of the mobile colloid. The second vector \( r_{\text{mob}}^t = r_2^t - r_2^0 \) is temporally varying, recording the displacement of the mobile colloid at time
Figure 4.7  Measurements for determining the two-dimensional attraction-repulsion between mobile and fixed colloids.  

a, Schematic with colloids (navy circles) initially separated by \( \mathbf{r}_s^0 \) with polar angle \( \theta_s \) relative to \( \mathbf{e}_x \). The far-field director is initialised along \( \mathbf{n} \), which, at short times, fixes the orientation of the \(-1/2\) defects (blue trefoil symbols) to the colloid’s equator. At time \( t \), the mobile colloid moves to a new position. The displacement vector is \( \mathbf{r}_{\text{mob}}^t \). 

b, Example trajectories for 15 simulations (grey) at a starting separation \( r_s^0 = 50 \) and angle \( \theta_s = 45^\circ \). The trajectories are measured as the projection magnitude of the mobile displacement onto the axis of the initial separation \( \mathbf{r}_s^0 \cdot \mathbf{r}_{\text{mob}}^t \). The attraction-repulsion behaviour is measured over the time interval \( t = 200 \) to \( t = 500 \), as indicated by the red shaded region. The mean is shown as the solid dark blue line, and standard error as blue shading. 

c, Snapshot of the self-assembly into a chain, which occurs if colloids are initialised with small separations and angles. Defects are shared between the colloidal disks, influencing an attractive response at small angles and separations.

\( t \) from the start position (red arrow). Individual mobile colloids are regarded to have repulsive (attractive) behaviour if the projection of \( \mathbf{r}_{\text{mob}}^t \) on the initial separation direction \( \mathbf{r}_s^0 \) is positive (negative). The individual trajectories are noisy (grey trajectories in Fig. 4.7b) and after some time the \(-1/2\) defects reorient to aid self-assembly into chains (Fig. 4.7c), which misalign the relative quadrupole orientations. Therefore, 15 simulation runs are performed, for each combination of \( r_s \) and \( \theta_s \) (for a total of 660 simulations). The response behaviours are measured from the early time dynamics \( 200 \leq t \leq 500 \) (red shading in Fig. 4.7b). The minimum time of \( t = 200 \) is chosen to establish sufficient statistical certainty on the attraction-repulsion trajectories. Ensemble averages of the projection magnitude \( \mathbf{r}_s^0 \cdot \mathbf{r}_{\text{mob}}^t \) are performed, extracting the mean \( \mu \) and standard error \( \sigma_M = \sigma / \sqrt{N} \). The nature of each colloidal site \( (r_s \cos \theta_s, r_s \sin \theta_s) \) is calculated as attractive if \( \mu \leq -\sigma_M \), repulsive if \( \mu \geq \sigma_M \) and neutral otherwise.

The N-MPCD mobile colloid does indeed exhibit regions of both repulsion and attraction. This is shown as blue (repulsive) and yellow (attractive) scatter
Figure 4.8  **Attraction-repulsion zones between two-dimensional interacting quadrupolar colloids.** One colloid is fixed at the origin (navy blue quarter circle) and a second mobile colloid probes the interaction at surrounding points. Both colloids have radius $R = 10$. The colour of each point represents attractive (orange), repulsive (blue) or neutral (black) interactions. Background shading shows the far-field expectation for interacting quadrupoles (Eq. (4.5)).

The repulsive regions are clearest for pole-to-pole orientations and exist in the far-field limit of small-angle defect-to-defect orientations. Configurations with intermediate relative angles exhibit attractive interactions. Far-field interactions between two quadrupolar colloids separated by a distance $r_s$ with a relative angle $\theta_s$ are predicted to have the form \[ F_{\text{pair}} \sim K \frac{R^4}{r_s^5} \cos(4\theta_s), \] in 2D. The sign of the force in (Eq. (4.5)) is shown as the yellow ($F_{\text{pair}} < 0$) and blue shading ($F_{\text{pair}} > 0$) in Fig. 4.8. The theoretical prediction agrees with the N-MPCD simulations, especially in the far-field.

However, some discrepancies exist between theoretical predictions and N-MPCD simulations. At moderate to large $\theta_s$, a small number of attractive points (yellow) are measured in idealised repulsive zones (blue shading), and repulsive points (blue) in attractive zones (yellow shading). These sampled point outliers can be partially attributed to the inherent stochasticity of the algorithm. Thermal fluctuations create uncertainty on the colloidal trajectories and perturb the locations of accompanying $-1/2$ defects, which misalign the quadrupoles.
from their assumed fixed orientation. In addition, the theoretical expectation (Eq. (4.5)) assumes far-field quadrupole interactions where deformations are small and linear (Eq. (2.31)). This assumption is challenged by N-MPCD, since nonlinearities influence the colloidal dynamics. These nonlinearities arise because the measurements are performed at small distances 2.5 to 6r_s/R, with non-negligible self-interactions via periodic boundary conditions, and within a thermally-fluctuating director field. The expectation also breaks down at small θ_s and r_s (Fig. 4.8). The N-MPCD algorithm produces attraction at these sampled points, in contrast with the idealised prediction of repulsion (Eq. (4.5)). This attractive behaviour can be understood by the mechanics of self-assembly. The dimer pair quickly self-assembles into a linear chain [202, 203], causing the colloids to become attractively bound (Fig. 4.7c). Unlike 3D, two-dimensional nematic colloids have a pair of −1/2 point defects (§ 2.1.5), which can be freely shared between colloids.

This section has demonstrated that elastic interactions between colloids and their environment are sufficiently resolved by N-MPCD. Resolving colloidal dynamics via impulse conservation of particle transformations (§ 3.2.4.3), captures the elastic quadrupolar nature of a Saturn ring (in 3D) or of a disk with two free -1/2 point defects (2D). The results have shown promising potential for studying inclusions in active nematic fluids, where surrounding elastic deformation will be temporally varying. With defect structures around isolated colloids and elastic interactions now resolved, the next section will explore the ability of N-MPCD to resolve details of the more exotic disclination structures between mobile colloidal pairs in 3D.
4.6 Defects around colloidal dimers

Three-dimensional systems with two or more colloids, enable a rich topological interplay between point defects and disclination loops [10, 204], facilitating a broad range of defect structures including *entangled* disclination loops that surround multiple colloids (§ 2.1.8.3). To assess the ability of N-MPCD in probing the nature of these loops, this study explores geometric and topological properties of three-dimensional defects accompanying colloidal dimers. Entangled disclinations are a well-studied problem, experimentally [3], theoretically [204] and in a wide range of simulation methods from continuum [83, 138] to mesoscopic approaches [140, 150]. However, N-MPCD brings an ideal perspective, since it is able to access rare states and explore their finite lifetimes via thermal fluctuations, and has a demonstrated ability to resolve fine details of defects geometric structure (Fig. 4.4). For this reason, this section first identifies the possible disclination structures in N-MPCD, and then characterise the topological features—in particular, probing the interplay between writhe and topological charge.

Studies of disclination states around pairs of colloids have elucidated the metastability of entangled structures. These nontrivial states can be induced by a thermal quench [83], laser manipulation [3], chiral ordering [205], or self-quenched with high colloidal volume fractions [84]. In this study, these states are reached by initialising the bulk fluid from a thermal quench. Simulations are launched with two homeotropic-anchored, mobile colloids at positions $q_1 = [20, 20, 13]$ and $q_2 = [20, 20, 27]$, in a $L_x = L_y = L_z = 40$ domain with periodic boundary conditions on all walls. Simulations run for the duration $T_S = 1000$. During a warmup phase ($T_W = 200$), nematic order forms and no data is collected.

Eight disclination states are observed from the N-MPCD simulations with either one or two $-1/2$ disclination loops (Fig. 4.9). Of these, the two states that are not considered entangled are extensions of the single colloid case, with either two Saturn rings (Fig. 4.9a) or two dipolar halos that assemble into a chain (Fig. 4.9b). The others are entangled, featuring a disclination loop that wraps around the colloidal dimers. Five of these entangled configurations are well-documented [206] and have illustrative names that describe the shape of their disclinations [11]. The figure-of-theta (Fig. 4.9c) has two loops ($n = 2$): one large ring that encircles both colloids, and another smaller ring positioned between them. Taken together, the disclinations resemble the Greek letter ‘θ’. The figure-of-omega (Fig. 4.9d) and
Figure 4.9  *Defect states accompanying colloidal dimers.*  

- **a**, Saturn rings.  
- **b**, Dipolar halos.  
- **c**, Figure-of-theta.  
- **d**, Figure-of-omega.  
- **e**, Figure-of-eight.  
- **f**, Tilted-figure-of-theta.  
- **g**, Tilted-figure-of-omega.  
- **h**, Tilted-figure-of-eight.  

Disclinations are visualised as in Fig. 4.3, confirming each configuration is associated with $-1/2$ disclination loops (purple).

Figure 4.9 shows a variety of defect states that can occur in colloidal dimers. These states include:

- **a**, Saturn rings: These are rings of colloids that are aligned in a specific pattern, resembling Saturn’s rings in the solar system.
- **b**, Dipolar halos: These are halos with dipolar symmetry, likely formed due to the interaction between the colloids.
- **c**, Figure-of-theta: This configuration resembles a figure-of-eight, where the colloids are arranged in a specific geometric pattern.
- **d**, Figure-of-omega: Similar to **c**, but with a different orientation or symmetry.
- **e**, Figure-of-eight: These are single loop entanglements ($n = 1$), which shape similar to the letter ‘Ω’ and number ‘8’ respectively. Additionally, the N-MPCD algorithm reveals the existence of tilted analogues of the figure-of-theta (Fig. 4.9f), figure-of-omega (Fig. 4.9g) and figure-of-eight (Fig. 4.9h). These are tilted with respect to the axis the colloids reside in. While rare, tilted entanglements emerge when the director field does not form a uniform alignment axis away from the colloids (Fig. 4.10). When it does so, it generates modulated order that cannot relax to the ground state. In these simulations, the combination of colloids, periodic boundary conditions and quenched disorder are able to trap these tilted states.

With the disclination states identified, we next characterise their topological and geometric properties. To obtain these, we utilise the self-linking number framework for $-1/2$ disclinations (§2.1.8.3), which we summarise here. Colloidal...
anchoring enforces a constraint for the local director to lie in a plane perpendicular to the line tangent $T$ ($\cos \beta = -1$ in purple). This in-plane constraint enables the disclination to be treated as a ribbon. A framing vector $w$ is assigned (Fig. 4.11), which tracks the $-1/2$ orientation along the loop ($\S$ 3.4.2.3). The framing vector enables the topological properties of the $-1/2$ disclination to be found via the self-linking number $S_I$, which counts the number of times the framing turns around the tangent on traversing the loop. Due to the three-fold symmetry of $-1/2$ profiles, $S_I$ takes third-integer values $S_I \in i/3$ for $i \in \mathbb{Z}$. The $S_I$ is calculated from the writhe $W_r$ (Eq. (2.36)) and twist $T_w$ (Eq. (2.37)) using the Călugăreanu-White-Fuller theorem $S_I = W_r + T_w$ (Eq. (2.35)). From the self-linking number, the topological classification $\nu$ is found by Eq. (2.34). The disclination charge is inferred as $\nu = 0$ then $p = \text{even}$ or if $\nu = 2$ then $p = \text{odd}$. To compare properties between each state in Fig. 4.9 $W_r, T_w, S_I$ and $p$ are presented in Table 4.1 in addition to the number of loops $n$.

First, we examine the properties for the entangled single loop ($n = 1$) states. For the figure-of-eight, figure-of-omega and their tilted analogues, the self-linking number is found to be $S_I \approx \pm 2/3$ (Table 4.1). Additionally, the $S_I \approx \pm 2/3$ can be visualised for the two figure-of-eight states by tracking the orientation of the $-1/2$ profile (Fig. 4.12a). In choosing a reference and tracking the profile rotations along the loop (orange curve), the orientation is rotated by $\pm 2\pi/3$ over the entire

Figure 4.10  **Director field slices around standard and tilted colloidal-dimer states.**  

- **a.** Figure-of-eight structures are associated with a uniaxial far-field director field.  
- **b.** Tilted-figure-of-eight has a director field that modulates away from the dimer. The director is shown in grey. Disclinations coloured by $\cos \beta$. 

![Figure-of-eight](image1.png)  
![Tilted-figure-of-eight](image2.png)
Figure 4.11  Framing and tangent vectors for calculating the Wr and Tw. Example shown for the figure-of-eight state with framing \( w \) (orange arrows) and disclination tangent \( T \) (blue arrows). Disclination loops coloured by \( \cos \beta \).

contour of the loop. For each \( n = 1 \) state, the Sl is composed entirely from writhe, while the twist remains essentially zero in each state (Table 4.1). Self-linkings composed entirely of writhe were previously observed for the figure-of-eight and figure-of-omega \([85]\), since the strong radial constraint on the disclination profile penalises twisting of the orientation. We show the same writhe/twist balance also hold when the disclinations are in tilted conformations. The \( \pm \) sign on the Sl relates only to the chirality of the conformation and does not influence the topological classification of the loop. Indeed, mapping to the disclination loop index reveals that all four states are topologically trivial \( \nu = 0 \) (uncharged with \( p = \text{even} \)). The \( n = 1 \) disclination line balances the two point charges provided by the colloids (modulo 2). Therefore, each \( n = 1 \) state is topologically equivalent.

We next examine the disclination states with \( n = 2 \). Each state has a self-linking of \( \text{Sl} \approx 0 \) (Table 4.1). This is the case for the individual rings (Saturn rings and dipolar halos), and the entangled figure-of-theta structures, each presenting \( \text{Wr} \approx 0 \) and \( \text{Tw} \approx 0 \). We visualise the ribbon (orange curve) for the two figure-of-theta states in Fig. 4.12b, which confirm the calculated properties. The reference orientation smoothly connects to the final orientation, with no local (or global) twisting or coiling over the circuit. The \( \text{Sl} = 0 \) properties indicate that each loop carries a hedgehog charge \( p = \text{odd} \) (Eq. 2.34), balancing the global charge neutrality between the two loops (modulo 2). These results show that each \( n = 2 \) state is topologically equivalent with identical geometric decomposition into \( \text{Wr} = 0 \) and \( \text{Tw} = 0 \). Therefore, the tilted states are simply smooth transformations of their non-tilted counterparts.
Table 4.1 **Classification of each of the eight identified nematic disclination states (Fig. 4.9)** in terms of topological and geometric information. Disclination properties include the writhe (Wr) and twist (Tw), which combine to give the topologically-protected self-linking number $Sl = Wr + Tw$. Topological point charge $p$ associated with colloidal dimers combine to give a trivial nematic texture (even), allowing even contributions from each $n = 1$ or two odd contributions for states with $n = 2$ loops. The properties are calculated directly for the frames shown in (Fig. 4.9).

<table>
<thead>
<tr>
<th>Disclination State</th>
<th>$n$</th>
<th>Wr</th>
<th>Tw</th>
<th>Sl</th>
<th>$p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saturn rings</td>
<td>2</td>
<td>0.014</td>
<td>0.001</td>
<td>0.029</td>
<td>odd</td>
</tr>
<tr>
<td>Dipolar halos</td>
<td>2</td>
<td>0.009</td>
<td>0.003</td>
<td>0.023</td>
<td>odd</td>
</tr>
<tr>
<td>Figure-of-Theta</td>
<td>2</td>
<td>0.035</td>
<td>0.002</td>
<td>0.025</td>
<td>odd</td>
</tr>
<tr>
<td>Figure-of-Eight</td>
<td>1</td>
<td>0.699</td>
<td>-0.027</td>
<td>0.672</td>
<td>even</td>
</tr>
<tr>
<td>Figure-of-Omega</td>
<td>1</td>
<td>0.652</td>
<td>0.009</td>
<td>0.661</td>
<td>even</td>
</tr>
<tr>
<td>Tilted-Figure-of-Theta</td>
<td>2</td>
<td>0.005</td>
<td>0.005</td>
<td>-0.008</td>
<td>odd</td>
</tr>
<tr>
<td>Tilted-Figure-of-Eight</td>
<td>1</td>
<td>-0.705</td>
<td>0.051</td>
<td>-0.654</td>
<td>even</td>
</tr>
<tr>
<td>Tilted-Figure-of-Omega</td>
<td>1</td>
<td>0.618</td>
<td>0.065</td>
<td>0.683</td>
<td>even</td>
</tr>
</tbody>
</table>

This section has demonstrated that N-MPCD is able to simulate the expected disclination structures associated with colloidal dimers, and found tilted defect analogues of the entangled states. The tilted states are formed by non-uniformities of the surrounding director. Analysing N-MPCD defects using the self-linking number framework confirmed the topological equivalence between all -1/2 disclination loop, which are only distinguishable between $n = 1$ or $n = 2$ configurations. For all states, $Tw = 0$, since the radial anchoring penalises torsion. To maintain $Sl$, the defect cancels topological charge by generating net writhe $Wr$. The emergence and ability to calculate these properties using N-MPCD, demonstrates that the algorithm can be fruitfully employed to extract fundamental properties of disclination loops.

### 4.7 Entanglement kinetics

With each of the disclination states identified and characterised, we study the relaxation pathways that lead to the formation of these states. Since N-MPCD simulates fluctuating nematohydrodynamics, the simulations stochastically sample states as they relax towards accessible lower free energy configurations. This section studies instances of these pathways and elucidates the finite lifetimes of metastable entangled states. These pathways are explored via the contour lengths $L$, which generally decrease as the system relaxes from thermal disorder (Fig. 4.4). These simulations use the same parameters and starting conditions as
§ 4.6

Four examples of the contour length evolution are shown in Fig. 4.13. The first of these (Fig. 4.13a) shows a relaxation passing through a figure-of-theta structure. At early times (Fig. 4.13a.1), a small loop exists, sandwiched between the colloids with a contour length $L$ comparable-to-but-less-than the circumference of the colloids. Simultaneously, a large disclination loop rapidly collapses around the colloids, forming the figure-of-theta state (Fig. 4.13a.2). The number of loops is $n = 2$ throughout. In N-MPCD, the figure-of-theta is only sampled transiently, passing rapidly through loop-reconnections to form two Saturn ring colloids (Fig. 4.13a.3). Despite strong transitions in the individual loop lengths (Fig. 4.13a and Table 4.1), the total contour length has a negligible change between the two states—with two equal-sized Saturn rings that sum to the total disclination length of the two figure-of-theta loops.

Another kinetic trajectory observed in N-MPCD is a single ($n = 1$) quenched
disclination loop (Fig. 4.13b.1) that collapses to form a figure-of-omega state (Fig. 4.13b.2). The figure-of-omega entangled state is found to be metastable with a constant contour length for \( t \approx 100 \), after which time the dimer transitions to two Saturn rings (Fig. 4.13b.3). Unlike the transition from the figure-of-theta state in Fig. 4.13a, the transition from the figure-of-omega state involves a topological conversion from \( SL \approx 2/3 \) to two rings with \( SL \approx 0 \) (Table 4.1). Equivalently, this corresponds to a transition from a single uncharged loop, to two charged loops.

The tilted entanglements can show somewhat different trajectories because of their non-uniform global director alignment (Fig. 4.13c). The tilted state arises because the disclination collapses at an off-set to the colloidal axis (Fig. 4.13c.1), passing into the tilted-figure-of-theta (Fig. 4.13c.2). The tilted figure-of-theta state endures for an extended time with minimal changes to the conformation, until a segment of the disclination line reconnects into a fleetingly brief tilted-figure-of-omega state (Fig. 4.13c.3). Finally, the disclination divides into two dipolar halos with orientations tilted with respect to each other (Fig. 4.13c.4).

An \( n = 1 \) tilted relaxation trajectory can also occur, starting with a larger loop (Fig. 4.13d.1) that encloses the colloid pair to form the tilted-figure-of-omega state (Fig. 4.13d.2). As in Fig. 4.13c, this tilted-figure-of-omega state is short lived and in this case transitions to the tilted-figure-of-eight (Fig. 4.13d.3) without transitioning through \( n = 2 \). Interestingly, the tilted-figure-of-eight is observed to be the most stable of any of the entangled states observed in N-MPCD simulations, remaining in the same configuration for the entire simulation, with minimal variation in contour length. This parallels experimental observations [207], albeit for different states and surrounding order, where chirality or modulated order can offer protection from reaching the global free energy minimum [82]. In addition, figure-of-eights have been associated with the greatest stability of all entangled structures [3]. Despite the intrinsic stochasticity of the numerical approach, the tilted-figure-of-eight was not observed to relax into states with \( n = 2 \) rings.

Infrequently, less conventional entangled-dimer relaxation dynamics are revealed by N-MPCD, such as the situation shown in Fig. 4.14. Similar to the tilted structures, this trajectory eventually relaxes into a modulated global director field (Fig. 4.10). However, at early times, an unexpected entangled state emerged in which the disclination loop had a localised segment with a +1/2 wedge profile (Fig. 4.14b). The +1/2 profile is smoothly connected by fleeting twist to a
majority $-1/2$ loop. This wedge-twist state necessarily contains $p = 0$ to balance the charges of the dimers. Generally, such $+1/2$ wedge profiles are discouraged since the global director alignment cannot coexist with the low-symmetry of the $+1/2$ wedge and out-of-plane twist is penalised by the radial colloidal anchoring. The penalty against twist is resolved by a rapid reorientation of the rotation vector $\Omega$, which rotates by $\pi$ relative to the global basis over a small segment of the disclinations (Fig. 4.14a). The $+1/2$ segment of the disclination gradually approaches the colloids (Fig. 4.14b.2) until it combines with a $-1/2$ profile, facilitating a topological transition from a single loop ($n = 1$) to a state with a pair of $-1/2$ dipolar halos (Fig. 4.14b.3).

These results demonstrate that the fluctuating-hydrodynamics of N-MPCD is suitable for studying relaxation dynamics from thermalised initial conditions. The study found that loops reduce in length to find lower energy configurations, and topological transitions preserve total contour length. Fig. 4.13 also indicates that disclination recombination events, that retain the same number $n$, cannot be identified from loop number, length or topological/geometric properties of loops, and require further measures for a full statistical analysis of topological transitions. One benefit of N-MPCD is that the intrinsic thermal noise allows energetically unfavourable states to occur albeit with small probability, uncovering that entangled states do not strictly require $-1/2$ disclination loops.
Figure 4.13  Relaxation pathways for dimer-associated disclination loops following a thermal quench, as measured via the disclination contour lengths \( L \) scaled by colloid radius \( R = 6 \).

a, Figure-of-theta transitioning to Saturn rings.  
b, Figure-of-omega transitioning to Saturn rings.  
c, Tilted figure-of-theta transitioning to dipolar-halo pair, passing briefly through a tilted figure-of-omega state.  
d, Tilted figure-of-omega transitioning to tilted figure-of-eight.  
In each panel, topological transitions via loop reconnection or splitting events are indicated by vertical dashed lines.  
The time \( t = 0 \) corresponds to the first recorded timestep for which the largest disclination loop is entirely contained within the periodic system.  
Circular scatter points denote a single loop (\( n = 1 \)) and two loops (\( n = 2 \)) are shown as square markers, while the total contour length is shown as the navy blue line.  
Example snapshots are shown directly below each panel.
Figure 4.14 Quenched disorder can sample out-of-equilibrium disclination configurations. 

(a) Early-time snapshot of a charge-neutral disclination with a localised $+1/2$ profile (yellow segment), visualised as in Fig. 4.4. 

(b) Relaxation trajectory of the normalised contour length $L/R$ with time $t$. Markers, lines and colouring the same as Fig. 4.13.

4.8 Conclusion

In assessing the suitability of nematic Multi-Particle Collision Dynamics (N-MPCD) for studying colloids in complex and out-of-equilibrium situations, this work explored defect structures and elastic forces associated with an embedded colloid in a passive nematic fluid. The intrinsic stochasticity of the algorithm uncovered properties of topological disclination loops both in and out of equilibrium (by relaxing from a thermal quench).

Applying N-MPCD to isolated colloids in three-dimensions reproduces the predicted colloid-disclination complexes. These simulations found quadrupolar Saturn rings and dipolar halos for homeotropic anchoring, as well as quadrupolar Boojums defects shaped into antipodal handles for planar anchoring. The elastic interactions between mobile quadrupolar colloids were studied and confirmed to decay with the expected power-laws in two- and three-dimensions at separations from a homeotropic anchored wall. Further, the force anisotropy of two-dimensional interacting quadrupolar disks is demonstrated, showcasing angular attraction and repulsion behaviors.

Finally, this work studied the quenched and steady-state structures of disclination
loops entangling colloidal dimers. Despite being a noisily fluctuating algorithm, N-MPCD not only simulates the expected disclination states, but also could resolve details of defect topology and geometrical structure with fine precision. Analysing disclinations as ribbons demonstrated the intriguing interplay between loop coiling (net writhe) and topological charge. Writhed configurations enable the disclination loop to visit all director orientations (on a unit sphere \( \mathbb{S}^2 \)) twice, forming a neutral point charge (modulo 2). This allows a single \( n = 1 \) loop to balance the point charges of two inclusions. These results show that the writhed charge-neutral loops can exist in non-ideal and tilted disclination structures. Allowing the algorithm to explore relaxation from a quench uncovered that total loop contour lengths is preserved in topological transitions (i.e. re-connection and splitting). Disclination states sample configurations that minimise their contour length. Entangled states are demonstrated to be unstable, eventually transitioning to the expected Saturn ring or dipolar halo configurations. However, the tilted configurations have a stronger degree of stability, reaching the dipolar-ring configurations at long times, or remaining in the tilted-figure-of-eight configuration for the entirety of the simulation.

While these results are obtained for \( Z = 40 \) and periodic boundary conditions, N-MPCD could be utilised to simulate the possible defect structures and relaxation pathways within other settings. For instance, N-MPCD could be used to study the stability of entangled states confined in planar-anchored nematic cells. This is the preferred geometry used in experiments [208], which have reported that quadrupolar structures are favoured over dipolar in tight confinement [11]. A thorough investigation of the stability of disclination states with varied confinement and \( Z \) could be performed, which may guide the design of soft materials. With twisted nematic cells, N-MPCD could be utilised to study obscure disclination states such as twisted entangled loops [207] and escaped rings [82]. The coarse-grained efficiency of the algorithm makes it a suitable method for the study of self-quenched colloid-nematic gels (Fig. 2.9c), which may be able to unpick the topological features of the percolated -1/2 disclination loops that wrap around colloidal clusters [84]. The ease of control over complex surfaces could be used to explore colloids in complex geometries, including the possibility of assembly in constructed, non-trivial knotted fields [62].

In the context of inclusions in active nematic fluids, the implementations could be used to study how colloids may themselves order flow states, through screening the hydrodynamic instability, or how one might harness microfluidic control of
colloidal trajectories with pressure-driven flows and varying micro-channel wall curvature \[209\]. For alternative choices of framing vectors, it might be possible to analyse disclinations using the ribbon framework in active nematic fluids (AN-MPCD) \[153\], which may reveal further relationships between loop geometry, and topological invariants of charged disclinations loops. Overall, this numerical approach is well-suited to study the relationship between topology and rheological properties.
Chapter 5

Active nematic multiple emulsions
5.1 Introduction

The previous chapter (§ 4) began the topic of topologically-induced constraints through exploration of elastic interactions and disclination structures associated with colloidal particles in a passive nematic. One of the demonstrations of this work was that inducing topological charge constraints, by adding radial hedgehogs via each colloid addition, can establish particularly rich self-organised disclination conformations in the quench-induced relaxation to equilibrium. Anchoring-favoured pure -1/2 disclination loops entangle pairs of colloids in such a way that topological charge is cancelled via writhe.

In this chapter, we turn to another example of self-organisation under topologically induced constraints, but now also with the addition of activity. A particularly interesting geometry for exploring this theme is double (or multiple) emulsions, in which one or more passive isotropic droplets (or cores) are embedded in a larger active liquid crystalline droplet. Experimentally, these systems can be created by water-oil-water emulsions produced by microfluidic techniques [210]. These active droplets and double emulsions provide a remarkable example of tunable 3D topological active matter. A globally non-trivial ($p \neq 0$) nematic fluid can be created via a homeotropically anchored confining sphere (or large droplet). If inner isotropic droplets with homeotropic anchoring are added, then a variety of disclination patterns can be generated that conserve the difference between the global constraint and the internal charges modulo 2. Therefore, the number of inner droplets can be used to control the topology of the emerging patterns in a simple way.

Tuning topology in this way is interesting because the nematic features can couple with activity to generate complex flow patterns, morphologies [46, 135], and droplet motility [17]. These confining geometries have mostly been studied as droplets or thin shells. In many of these studies, topological defects have been identified to dominate self-organisation processes [211, 212]. For instance, in active droplets with planar anchoring, disclination lines have been associated with the formation of finger-like protrusions, surface wrinkles and droplet invagination [135]. Alternatively, for droplets with homeotropic anchoring, disclination loops dominate the internal structures, featuring regimes of loop rotation and dynamical recombination and annihilation interactions [27]. The topological defects are altered in the case of planar-anchored thin shells. These quasi-two-dimensional surfaces require a total winding of $k = 2$. Experiments and
simulations have observed dynamical regimes where four $+1/2$ orbit counter-rotating vortices at the poles of the shell $[213–215]$. Therefore, confined active nematics offer a playground for testing the relationship between topology and active pattern formation.

Here, we numerically study the spatiotemporal dynamics and morphology of multiple active emulsions with homeotropic anchoring. Our analysis characterises how the emulsion topology combines with activity to form self-organised flow states. Focussing on the cases of extensile activity in the large outer droplet and a single or a pair of passive inner droplets, we find rich physical behaviour, encompassing controllable nonequilibrium spatiotemporal motility patterns, and nontrivial disclination topologies. First, we find that an emulsion with a single passive inner droplet within a larger active droplet can become self-motile in a defect-free configuration, with an activity-driven transition between a translating and a rotating regime. Second, an emulsion with two passive cores induces a charged disclination loop that behaves as a self-assembled spinner at low activity. On the other hand, the internal flow loses coherence and chaotic dynamics ensue at large activity. Corresponding to this transition, the disclination line in the system significantly stretches and writhes, continually supporting topologically-protected self-recombination. This yields states with odd numbers of charged disclination loops, and integer numbers of neutral loops. These results report a rich selection of topologically equivalent charged loops ($\nu = 2$), with director patterns that extend beyond the pure $-1/2$ disclination loops associated with passive nematic colloids (Chapter §[4]).
5.2 Methods

5.2.0.1 Simulation details and parameters

The hydrodynamic modelling used for the liquid crystal double emulsions are described in terms of the coarse-grained quantities: (i) global fluid velocity $\mathbf{v}(\mathbf{r}, t)$, (ii) a set of passive scalar phase fields $\phi_i(\mathbf{r}, t)$ and (iii) a tensor order parameter $\mathbf{Q}(\mathbf{r}, t)$. The droplet phase indices are $i = 1, 2$ for a single core, and $i = 1, 2, 3$ for a double core. The equations of motion for each field are detailed in §2.2.3. This solves the Cahn-Hilliard equation (Eq. (2.46)), and $\mathbf{Q}$ evolution (Eq. (2.39)) via a finite difference scheme, while the incompressible Navier-Stokes (Eq. (2.43)) and incompressibility equation (Eq. (2.42)) are solved by a standard lattice-Boltzmann approach [42, 216, 217].

The model parameters and results are given in terms of simulation units. These are $A_0 = 1.2 \times 10^{-1}, a = 10^{-2}, k_\phi = 0.14, M_\phi = 10^{-1}, \Gamma_Q = 1, \xi = 0.7, K = 0.065$ and $W_\phi = -0.05$. A mapping to physical units can be obtained by fixing the length, time and force scales respectively given by $l_s = 10\text{nm}, t_s = 1\text{ms}, f_s = 1\mu\text{N}$, which are set to 1 in lattice units (see for example [46]). Simulations are performed on 3D square lattices with size $L_x = L_y = L_z = 128$. Periodic boundary conditions are applied on all walls.

The simulations have three defined regions. An outer droplet, one or two inner droplets (cores), and an outside region. The outer droplet is simulated as an active nematic, while the cores and the surrounding outer region are isotropic passive fluids. Defining the regions using phase fields will use $\phi_i = \phi_0$ and $\phi_i = 0$, which are the two coexisting minimas of Eq. (2.10), and $r$, the radial distance from the centre of the initialised core/droplet.

- Single inner emulsion: A fluid droplet of radius $R_1$ (core) is encapsulated within another droplet of radius $R_2$, with $R_1 < R_2$. Two separate phase fields are used $\phi_1$ and $\phi_2$. For the core: $\phi_1 = \phi_0 = 2$ for $r \leq R_1$ and $\phi_1 = 0$ for $r > R_1$. The outside region is: $\phi_2 = \phi_0 = 2$ for $r \geq R_2$ and $\phi_2 = 0$ for $r < R_2$. The outer droplet has all $\phi_1 = 0, \phi_2 = 0$ for $r < R_2$ and $r > R_1$. In the outer droplet, $\mathbf{Q}$ is randomly initialised ($\mathbf{Q}^2 \ll 1$). In the outside region and inner core, $\mathbf{Q}$ is zero. Extensile activity values are provided with the results and range between $\zeta \in [0, 0.055]$. In all simulations $R_2 = 32$. The inner core radius is $R_1 = 16$, except for the low activities ($\S$ 5.4.1) where...
$R_1 = 24$.

- Double inner emulsion: Two fluid droplets of radius $R_1$ and $R_2$ (with $R_1 = R_2$) are embedded in a larger droplet with radius $R_3$ (with $R_3 > R_1, R_2$). Three separate phase fields are used $\phi_1, \phi_2, \phi_3$. For one core, $\phi_1 = \phi_0 = 2$ for $r \leq R_1$ and $\phi_1 = 0$ for $r > R_1$. The other core has $\phi_2 = \phi_0 = 2$ for $r \leq R_2$ and $\phi_2 = 0$ for $r > R_2$. The outside region is $\phi_3 = \phi_0 = 2$ for $r \geq R_3$ and $\phi_3 = 0$ for $r < R_3$. The outer droplet has all $\phi_1 = 0, \phi_2 = 0, \phi_3 = 0$ for $r < R_3$ and $r > R_1, R_2$. In the outer droplet, $Q$ is randomly initialised ($Q^2 \ll 1$). In the outside region and both inner cores, $Q$ is zero. Extensile activity values use $\zeta \in [0, 0.2, 0.4, 0.8]$. In all simulations $R_3 = 32$ and $R_1 = R_2 = 8$. A schematic of the phase fields is shown in Fig. 5.1.

### 5.2.0.2 Defect analysis

Disclination loops are analysed using the disclination density tensor ($\S$ 3.4.2.1). We identify defects as isosurfaces where $s(r) = 0.033$, and further identify $\Omega$ and $T$ by constructing an ordered sequence of points that compose the disclination ($\S$ 3.4.2.2). The contour lengths are calculated by a summation of the bond lengths between points. All visualisations use the Mayavi library ($\S$ 3.3).
Figure 5.1  Double inner core emulsion in terms of phase fields. The nematic emulsion is a large droplet (closed blue surface), with two inner cores inside (smaller blue spheres). The phase fields values are visualised by a horizontal slice of the total phase field $\bar{\phi} = \sum_{i=1}^{3} \phi_i$, where $i$ is the phase index. The slice is coloured yellow for $\bar{\phi} = \phi_0 = 2$ and blue $\bar{\phi} = 0$. Labels are provided for the individual phase fields $\phi_1, \phi_2, \phi_3$ in each of the four regions (two cores, droplet, outside). The radius of the droplet is $R_3$ and of the cores are $R_1$ and $R_2$. 
Figure 5.2 Equilibrium structures of passive double emulsions with homeotropic anchoring. a, Single-core double emulsion. b, Two-core double emulsion. Grey lines represent the director field. Defect loop is visualised an isosurface \( s = 0.033 \) and coloured according to \( \cos \beta \) (Fig. 2.6). This allows for the identification of local director profiles, such as twist-type \( (\cos \beta = 0) \), \( +1/2 \) comet-shaped \( (\cos \beta = 1) \) and \( -1/2 \) trefoil-shaped \( (\cos \beta = -1) \).

5.3 Passive emulsion

Before activity is applied, the system is equilibriated as a passive nematic emulsion. The phase fields \( \phi_i \) and \( Q \) relax to equilibrium values that minimise the free energy \( F_{\phi} \) (Eq. (2.12)). In this section, we present the equilibrium states for single and double inner cores.

For a single inner emulsion, the equilibrium state enforces the inner core to reside directly at the centre of the nematic droplet (Fig. 5.2a). This state is free of topological defects, since the inner emulsion creates a hedgehog that satisfies the confinement-induced constraint of \( p = 1 \). By the complementary homeotropic boundary conditions, the nematic forms a radial, pure-splay texture.

When a second inner emulsion is added, it contributes another \( p = 1 \) and so the global charge constraint cannot be satisfied by a continuous director field. A static charged disclination loop is nucleated in the bulk fluid (Fig. 5.2b). The loop is found at the centre of the outer droplet, between the pair of inner droplets in the lateral plane. Further, an inspection of the geometric features of the loop, through analysis of \( \cos \beta = \Omega \cdot T \) (§ 2.1.6.2), reveals an interesting structure. The loop has two \(-1/2\) defect profiles (purple segments) that are closest to the inner droplet interfaces. These near-droplet \(-1/2\) segments are bridged by two.
+1/2 profiles (yellow segments). The −1/2 and +1/2 sections smoothly convert by means of intermediate twist defects (green segments). As a shorthand, we will refer to this disclination pattern as +-+-.

This loop geometry contrasts with the steady-state loops associated with nematic colloids in the previous chapter (Chapter §4), which are pure -1/2 disclinations (purple). Additionally, this loop contrasts with the famous experiments of Poulin et al. in 1997, which had a similar set up of an inverted passive nematic emulsion with inner isotropic emulsions [67]. Those experiments observed that dipolar linear chains of multiple inner droplets are connected by hyperbolic hedgehog defects (Fig. 2.5b). We attribute these differences to two reasons. Firstly, compared to Poulin et al., point hedgehogs are associated with large $Z$ (Eq. (2.30)). This suggests that anchoring strength is weaker here. Further, simulations are less likely to observe point defects than experiments, even for comparable $Z$ (§4.4). Secondly, the loop is different from the charged -1/2 ring that forms between colloidal dimers (Fig. 4.9b,c,f), while here, a loop is situated perpendicular to the two cores. In the case here, confinement encourages the inner cores to be separated with the disclination laterally between them. The +1/2 segments, residing in the bulk, are not subjected to the strong anchoring constraint that favours −1/2 disclinations (§2.1.8.3). The differences between these charged loops are important to note since the active dynamics build directly from the equilibrium states and loop profiles influence active backflows (§2.1.6).

Throughout the rest of this chapter, we will explore how the equilibrium picture changes when activity is applied.
5.4 Single inner emulsion

In this section, we explore how activity influences the droplet dynamics and flow states for a single inner emulsion. A variety of extensile activity values are applied, in the range $\zeta \in [0, 0.06]$, which exhibit three distinct dynamical behaviours. We refer to these regimes as low, medium and high activity.

One convention to note, is that this section uses the symbol $\omega$ to represent the angular velocity. In §3.6 and Chapter §6, the same symbol is used for the vorticity.

5.4.1 Low activity: translational regime

At the lowest activities ($\zeta \in [0.0, 0.002]$), the inner droplet is at rest and unable to overcome the bulk elastic restoring forces (Fig. 5.3a). However, beyond this limit, the emulsion acquires spontaneous motion along a rectilinear trajectory. Spontaneous motility can be observed in Fig. 5.3a, where the inner emulsion velocity magnitude $|v|$ is non-zero at $\zeta \sim 0.002$.

The mechanism of spontaneous motility arises from the interplay between anchoring-induced deformation patterns and active flow coupling. However, it differs subtly from the typical hydrodynamic instability observed for bend fluctuations in extensile active fluids (§2.2.5), since the director deformation is...
primarily splay-type (Fig. 5.3b). If the internal core is exactly at the centre of the active droplet, this state is quiescent and the double emulsion is non-motile. On the other hand, an initial perturbation of the core breaks the ideal splay pattern, and, correspondingly, the isotropy of active stress. The polarisation direction of active stress is in the direction of the displaced core, which can overcome restoring elastic forces for sufficiently high activity. This renders the core self-motile along the initial displacement with two primary vortices trailing the inner core.

Another way of quantifying this instability is through the activity number $A$ (Eq. (2.51)), which quantifies the ratio of active stresses to elastic restoring forces. With the parameter values given in § 5.2.0.1 and lengthscale $R_1 = 16$, the transition from rest to spontaneous motion occurs at $A \sim 1$. Therefore, the dimensionless number $A$ predicts spontaneous self-propulsion to occur when active forces exceed passive restoring forces. Throughout the rest of this chapter, we provide $A$ alongside the activity $\zeta$ (given in simulation units) to guide experimental validation.

### 5.4.2 Medium activity: rotating regime

Further increasing the activity to $\zeta = 0.045$ ($A = 13$) generates a new self-motility regime. Beyond an initial warmup period of $t \sim 250000$, the encapsulated core is found to display a persistent periodic motion along a circular trajectory (Fig. 5.4a). The periodicity of the dynamics can be observed by measuring the inner emulsion centre of mass velocity $V$ (Fig. 5.4b) and angular velocity $\omega$ (Fig. 5.4c), which modulate sinusoidally with time. An additional detail is that the droplet motion lies only in a single rotation plane, which is spontaneously chosen. This can be seen by $V_z \approx 0$ and $V_x \approx V_y \neq 0$ and $\omega_x, \omega_y \approx 0$ and $\omega_z > 0$. The rotation plane has a normal vector (with normal vector $e_z$) with a well-defined handedness.

To understand the source of the rotational motion, we turn to the director and flow field, which are visualised in the panels (Fig. 5.4d). The circular droplet motion is complemented by the emergent flow patterns, which have transformed from a previously dipolar vortex pair (Fig. 5.3b for $\zeta = 0.01$) into a single vortex with the same fixed rotation axis along $e_z$ and handedness as the motion of the inner core. The inner droplet motion is complementary with the emergence of a bend streak, which coincides with strong parallel-directed flows (yellow velocity arrows). The bend streak, and strong flows, are oriented
in the azimuthal direction of the droplet enforcing the handedness of the droplet
dynamics. In comparison to the low activity case, where deformation was confined
to a single axis, this flow state illustrates that activity supports the breaking of
axial symmetry by allowing director deformation to overcome the elastic restoring
forces.

5.4.3 High activity: meandering regime

At the largest activity considered (ζ = 0.06; A = 15), chaotic-like trajectories of
the inner emulsion emerge (Fig. 5.5a). Unlike the medium activity case, which
was coherent and confined to a single plane, the core dynamics are now fully
three-dimensional and noisy. The greater active stresses lead to a greater speed
of the core (Fig. 5.5b) which is approximately twice as large as for ζ = 4.5 × 10^{-2}.
The angular velocity ω (Fig. 5.5c) is comparable in magnitude to before, albeit
irregular since the flows are not coherent. Therefore, the droplet dynamics are a
signature of the turbulent-like chaotic flows that are typical in the limit of large
Figure 5.5  Meandering motion of single inner emulsion at high extensile activity. Same as Fig. 5.4 but with $\zeta = 0.06$.

activity number $A$ (Eq. (2.51)).

5.4.4  Discussion

This section revealed the emergent flow patterns and core dynamics for a topologically trivial system with a single inner droplet (where no defects are required). Increasing activity leads to different motility regimes in which the spontaneous flow exhibits three well-defined structures: a double vortex in the low-activity translational regime, a single vortex in the intermediate-activity rotating regime and a chaotic structure in the high-activity meandering regime.
5.5 Double inner emulsion

In this section, we consider the case in which the fluid of the inverted emulsion is imposed to be topologically nontrivial. This is done by embedding two inner cores in the outer droplet. This builds from the equilibrium picture in Fig. 5.2b, where a topologically charged loop resides laterally between two inner cores, presenting a +-+- pattern. While in the defect-free single emulsion case we studied primarily the motion of the inner cores, here we will pay particular attention to the dynamics and geometry of the disclination loop—which is predicted to couple strongly to active flows (§2.2.6.2). We separate this study into low, medium and high activity cases, for three selected activity values ($\zeta = 0.02, 0.04, 0.08$) that are seen to form distinct dynamical regimes.

5.5.1 Low activity: uniform rotor

At low activity ($\zeta = 0.02; A = 4$), the interplay of active flows and nematic topological features unveil an intriguing dynamical response, forming a coherently revolving disclination loop (Fig. 5.6). The loop rotates in a rotor-like manner about an axis that connects the two cores, where each core remains stationary near the interface of the confining emulsion. Complementing the loop’s rotation...
Figure 5.7  **Topological patterns and local flows of double inner emulsion at low extensile activity.** Disclination loop from Fig. 5.6a now shown with the rotation vector $\Omega$ (red arrows) and $\mathbf{T}$ (large blue arrows). At the centre of each $\pm 1/2$ wedge profile ($\Omega \cdot \mathbf{T} = \pm 1$), a circular disk provides the local director (black lines) and flows (coloured arrows).

is a single emergent vortex in the flow-field (Fig. 5.6c), which persists over time and adopts the same rotation axis and sense as the loop. In time, the loop retains an approximately constant contour length $L/R_1 \approx 9.6$ (Fig. 5.8a).

To unpick the relationship between the coexistent dynamics of the vortex and disclination, the topological director patterns, and their local flows, are explored. This study centres on the simulation snapshot (Fig. 5.7). The topological patterns are first considered, which we present using two formats. The first of these is the disclination colouring by $\cos \beta$. This shows that the loop alternates twice between $-1/2$ profiles nearest the cores (purple; $\cos \beta = -1$), and $+1/2$ equidistant between them. Twist-type (green) smoothly connect the wedge profiles. This director pattern is the +++ loop.

Further topological information is stored in $\Omega$ and $\mathbf{T}$, which are shown as red and blue arrows (Fig. 5.7). The relative orientation of these arrows complements the profile description ($\cos \beta = \Omega \cdot \mathbf{T}$). Additionally, viewing $\Omega$ in isolation highlights that the loop is topologically charged. By performing a double transformation between $+1/2$ and $-1/2$, $\Omega$ is able to make a full $2\pi$ winding.

However, the topological patterns alone are not mappable to dynamical features, so we also identify the orientational features of the disclination patterns, and connect these to local flow patterns. For simplicitly, only wedge-type orientations
are considered. To obtain these, a small circular disk is constructed at the centre of each of the four $\pm 1/2$ segments. Each disk has a radius of 5 lattice cells and is oriented with normal vector parallel to the local $\mathbf{T}$. The local director is mapped to the inside of the disk, while the velocity field is provided on the perimeter.

First examining the $-1/2$ profiles in Fig. 5.7, the director highlights three-fold director symmetry, with one of the radial orientations pinned to the core. The magnitude of the local flows are weak, as evident by the purple colouring, which is a quarter of the magnitude of the strongest flows (colour bar as in Fig. 5.6).

Examining the $+1/2$ profiles in Fig. 5.7, the bend-side of the polar orientation is directed azimuthally with respect to the confining droplet. Strikingly, the local flows are aligned parallel to the $+1/2$ orientation and have the largest velocity magnitude compared to the rest of the droplet (yellow). These local flow characteristics are consistent with the theoretical predictions for an isolated profile (§ 2.2.6.2). Therefore, the figure paints the picture that, despite additional nematic deformation sources, the $+1/2$ profiles are dominant in generating and tailoring the active flows to form the coherent vortex structure.

Why do the $+1/2$ profiles orient azimuthally at all? One explanation arises from considering the geometric constraints formed by the homeotropic anchoring
Figure 5.9  *Transition from uniform to chiral rotating loop for double inner emulsion at moderate extensile activity.*  

**a-d.** Uniform rotor.  

- **a-c.** Same as Fig. 5.7 but for $\zeta = 0.04$ and times $t = 4 \times 10^5$ and $t = 4.5 \times 10^5$.  
- **d.** Same configuration as a but visualised as Fig. 5.7.  

**e-h.** Chiral rotor. Presented the same as a-d but for $t = 5 \times 10^5$ and $t = 5.5 \times 10^5$.

conditions on the inner emulsions and confining interface. Since $+1/2$ defects self-propel in the direction of bend, their orientation is geometrically incompatible with the radially-enforced (splay) at the boundaries. Therefore, azimuthal orientations are the only compatible configuration for self-motile bend deformations that do not violate the anchoring constraints.

### 5.5.2 Medium activity: transition to chiral rotor

Increasing the activity to $\zeta = 0.04$ ($A = 6$) further strengthens the active stresses in comparison to the elastic restoring forces. The loop retains the rotor-like dynamics with $-1/2$ pinned to cores and $+1/2$ constrained to azimuthal motions. The rotor dynamics are complementary with a single coherent vortex (Fig. 5.9a-c), which is driven by $+1/2$ profile active backflows. This can be seen since the velocity magnitude is strongest at the core of the $+1/2$ defect (Fig. 5.9c), and flows are directed parallel to the bend side of the $+1/2$ orientation direction (Fig. 5.9d). These dynamical features are equivalent to the low activity case ($\zeta = 0.02$; Fig. 5.6). However, a new loop configuration arises for this activity. The $-1/2$ segments coil around each core, forming an ‘s’ shape. A consequence
of the ‘s’ shaped coiling is that the loop shape departs from the simple circle or ellipse shape (Fig. 5.2b and Fig. 5.6) that lies entirely in a plane. These two ‘s’-shaped regions continuously revolve with the flows, but their axial pinning to the cores retains the rotation axis for the loop and flows.

With the +1/2 profiles located equidistant between the two inner cores, the flow state is achiral. However, this symmetry is unstable and eventually transitions into a chiral pattern (Fig. 5.9e-h). In this transition, the activity is sufficient to break the core-imposed anchoring constraint that suppresses bend, and the two +1/2 profiles each skew towards one of the inner emulsions (Fig. 5.9). Another indication of this transition can be observed in the contour length (Fig. 5.8d), which transitions from $L/R_1 \approx 19$ (achiral; $t < 40000$) to $L/R_1 \approx 17.4$ (chiral; $t > 40000$).

The flow states in Fig. 5.9e-g show there is a central vortex that maintains the loop rotation, but this periodically revolves the rotation axis. Correspondingly, the -1/2 disclination segments transition from an ‘s’ shape to a ‘c’-shaped conformation, which forms close to a full -1/2 circle from the side view (Fig. 5.9g). We call this flow state a chiral rotor since the disclination has broken mirror symmetry about the lateral plane, and maintains a periodic loop rotation.

### 5.5.3 High activity: chaotic dynamics

At yet larger activity ($\zeta = 0.08$; $A = 9$), the emergence of chaotic dynamics contributes rich dynamical and topological states (Fig. 5.10) that resemble active living polymers [218]. Active living polymers, have dynamical conformations that regularly stretch, break and recombine. Likewise, the charged disclination loop, changes form from the simple +-+- pattern and simple shapes formed at low and intermediate activities. At high activities, the loop continuously stretches (Fig. 5.8c) and writhes into complex conformations. The -1/2 segments of the loop now display stronger coiling around the passive cores (purple), and hairpin-like sudden reversals of the tangent $T$ emerge in bulk associated with +1/2 segments (yellow). The higher activity enables the charged loop to depart from the +- pattern. Examples can be seen with three +1/2 profiles (Fig. 5.10b-d), that locally ‘pinch’ and drive the disclination loop dynamics. The association of +1/2 profiles and strong loop curvature has been formerly reported in [4], and coincides with the self-motile nature of +1/2 active backflows (§ 2.1.6).
As the loop continues to stretch and writhe, the surrounding flow states continuously vary, inducing unsteady bulk flows, which in-turn couple to the configuration of the disclination loop. The chaotic dynamics eventually cause the loop to undergo splitting and recombination dynamics, leading to multiple loops (Fig. 5.10e-h). This can be seen by Fig. 5.8, which predominantly shows one ($n = 1$) disclination, but episodes of $n = 2$ or $n = 3$ can be observed. However, topological constraints restrict the number and nature of possible loop combinations. Since the two-core emulsions must adhere to an odd bulk charge, configurations with 3-charged loops can be observed (Fig. 5.10e). This can be visually inspected by the two -1/2 disclination loops that form an intermediate Saturn ring/dipolar halo like pattern (purple), that are associated with charged loops accompanying colloidal particles ($\S 2.1.8$). To obey the global charge requirement, the third loop is implied to be charged, with two +1/2 and two twist profiles. However, while the number of charged loops is constrained to odd numbers, the number of neutral loops have no constraints on their number, and examples can be observed with one (Fig. 5.10g-h) or two (Fig. 5.10f) trivial loops.
Types of disclination loops found in two-core emulsions. a, Saturn ring \(-1/2\) disclination loop constrained to inner cores. b, \(+--+\) charged loop. c, Plus half-twist charged loop. d, Wedge-twist neutral loop. e-f, Writhed charged loops. Loops selected from \(\zeta = 0.08\) configurations, except for b with \(\zeta = 0.02\). Loops coloured by \(\cos \beta\) and constructed as tubes (same as Fig. 4.4). Rotation vector \(\Omega\) shown as red arrows and tangent vector \(T\) as blue arrows.

accompanying the odd charged loop. For example in Fig. 5.10f, a \(+--+\) charged ring is accompanied by two charge neutral wedge-twist disclinations (Fig. 2.6b). In Fig. 5.10g, a neutral wedge-twist loop coexists with a dipolar halo. Finally in Fig. 5.10h, a \(+--+\) is shared between the two cores with a single wedge-twist loop. In each case, loops are always observed to have \(-1/2\) disclination profiles pinned to the passive cores, demonstrating that geometric constraints are crucial to the self-assembled defect organisation in these confined topological environments.

### 5.5.4 Profiles of disclination loop

The topological patterns of charged disclination loops, created by the active environment, are unlike the predominantly \(-1/2\) cases for passive nematics (Chapter § 4). Here, we summarise and characterise the possible disclination loops that are observed in these double inner emulsion states.

First, we review the simple cases of topologically \textit{charged} and elliptical-shaped loops \((\nu = 2)\). For low activity, only \(+--+\) loops are observed Fig. 5.6. This is
favoured since the emulsions each pin the two immotile -1/2 profiles, and +1/2 avoid boundaries due to geometric incompatibility with the radial anchoring. In the high activity regime, splitting and recombination dynamics can lead to a variety of possible loops. These can be pure -1/2 disclination loops constrained to single cores (Fig. 5.10e,g) or bulk +1/2-twist charged loops (Fig. 5.10e). Each of these three loops are associated with topological charge.

To understand why these are charged, we turn to the vector decomposition $\Omega$ and $T$. A $2\pi$ winding of $\Omega$ allows the director to sample all orientations on the unit sphere, and carry a hedgehog charge. However, the topological patterns ($\cos \beta$) are also dependent on the relationship between $\Omega$ and $T$. Three examples of loops found in double emulsions are presented in Fig. 5.11. In each case, the loop is oriented so that $T$ points, and winds, in an anticlockwise circuit. We first consider the Saturn ring loop (Fig. 5.11a). Pure $-1/2$ profiles are formed when $\Omega$ is antiparallel to $T$. Therefore, $\Omega$ winds in the same anticlockwise sense as $T$, but with an opposite relative orientation. Conversely, the +++- loop can alternate between two $+1/2$ and $-1/2$ orientations if $\Omega$ winds in an opposite direction to $T$ in a clockwise sense (Fig. 5.11b). Finally, the double $+1/2$-twist loop is particularly interesting because $\Omega$ winds in the perpendicular plane to the $T$ rotations (Fig. 5.11c). Ideal representations of each of these loops are shown in Fig. 5.12 with the winding plane indicated by the black arrows. This figure highlights the conclusions of the analysis on simple charged loops. Each loop is topologically equivalent, carrying a hedgehog charge and classified by $\nu = 2$.

However, these loops are geometrically distinct. Charged loops can be smoothly transformed into each other through a transformation of the winding plane of $\Omega$.

More complex examples of charged loops ($\nu = 2$) emerge at high activity when motile $+1/2$ profile segments are able to ‘pinch’ loop segments. The orientations of $\Omega$ along the disclination are shown in Fig. 5.11e-g. Alike to the quench-driven nematic colloids in § 4.1, the topological charge is not evenly distributed over the loop and $\Omega$ most sharply varies around cores. However, because there is a much wider variety of conformations and topological patterns, we do not explore their nature further.

Finally, the high activity regime also observes neutral loops ($\nu = 0$). However, in contrast to bulk active turbulence of extensile active nematics, which tend to observe twist-type disclinations (Fig. 2.6c, § 2.6.2), the loops here are wedge-twist (Fig. 5.11d, Fig. 5.10f-h). Wedge-twist disclinations have a uniform $\Omega$ across the loop (Fig. 2.6b).
5.5.5 Discussion

This section studied the dynamics of charged disclination loops in an imposed topologically non-trivial bulk environment. These charged loops are unlike the -1/2 charged loops observed in near-equilibrium passive liquid crystals (§ 2.1.8 and Chapter § 4). The results show that, while topology creates a stable charged loop, geometry subtly tunes the possible defect profile patterns. In the presence of activity, these geometric details are crucial to determining the emergent motility and loop dynamics. In particular, +1/2 profiles are motile and drive loop dynamics in the direction of their orientation. In contrast, −1/2 profiles are passively anchored to the inclusions. The combination of these profile-specific dynamics and geometric constraints, via homeotropic anchoring, allow a rich variety of possible dynamical states. These states are spatiotemporally ordered for low to middle activity with rotor-like dynamics accompanied by a single vortex. However, at high activity flow states lose coherence. The emergent chaotic-loop dynamics resemble living polymers with stretching, writhing, splitting and recombination dynamics. Additionally, activity is shown to drive a rich variety of topologically equivalent charged loops, which differ in geometric features, and correspondingly motility dynamics.
5.6 Conclusion

This chapter centred on exploring how imposed topological constraints can influence the dynamical features of trivial (uncharged bulk) and non-trivial (charged bulk) active nematic fluids. These emulsions consist of a large active nematic droplet containing a number of smaller passive droplets (cores) in its interior. In each case, anchoring is homeotropic — imprinting topological hedgehog charges into the bulk fluid, rather than the surface. Therefore, the number of cores determines the global topology of the director field.

In the case of the topologically trivial single-core emulsion, low activity renders the system self-motile, whilst remaining defect-free. The steady-state motility patterns are notable, because they encompass a transition between translational and rotational motion at higher activity. This transition was not previously observed in single 3D active nematic droplets. In previous studies, tangential anchoring leads to only rotation, while helical trajectories are only observed when including chiral contributions, either in the free energy [46, 219] or in the stress tensor [220]. As further increasing activity yields chaotic dynamics, this double emulsion provides a remarkable example of a simple active matter system with a particularly rich dynamical behaviour.

When there are two internal passive cores, the double emulsion is topologically nontrivial, because the normal anchoring at all surfaces induces the bulk liquid crystal pattern to have an odd topological charge. This two-core emulsion can spontaneously rotate, either regularly or in a chaotic fashion, according to the value of the activity. In the regularly rotating regime, the steady state involves formation of a large, essentially planar, charged disclination loop. This loop has an interesting geometry, where two local $+1/2$ defect profiles coexist with two other local $-1/2$ profiles. This charged loop is geometrically different from those in an active nematic droplet without passive cores [27], which is also a topologically non-trivial system but where the local defect profile is more commonly twist [4]. In our case, the $-1/2$ profile appears in the vicinity of the colloidal cores, in analogy with the profiles associated with Saturn rings around passive colloidal particles in nematics (§4.3).

These results suggest that the combination of active flows, plus inclusion-induced topological constraints and confinement-induced geometric constraints, can be utilised to design target disclination patterns and corresponding flow states.
Geometric constraints allow control over the orientation of the rotation vector in the case of simple elliptic charged loops. Systems with further numbers of inner emulsions may find higher order winding profiles of simple loops, and establish additional constraints to the chaotic conformational dynamics of writhed charged loops.

Besides representing a novel type of topological active material and providing a rich playground for testing theories linking topology and pattern formation, active double emulsions also have value biomimetically, as a toy model for a cell with a single centrosome or nucleus (a single-core emulsion), or dividing cells with a mitotic spindle pushing on two centrosomes (a two-core emulsion). Within this context, it would be of interest to study the minimal ingredients leading to “cell motility” [221], “nuclear rotation” [222] and “cell division” [20], which may provide a route for future research aimed at self-assembling minimal cells [223]. Here, we have considered extensile activity (e.g., due to microtubule and kinesin) and normal anchoring; we expect that addressing these questions on biomimetic systems will require extending our study to contractile activity, which is more appropriate for modelling actomyosin. At low activity, contractile is expected to produce similar behaviours as extensile, such as self-propulsion and rotation of single cores [224] and motile $+1/2$ disclination segments [20], although these dynamics are in the reverse direction. Future studies could explore the influence of the splay-type hydrodynamic instability on inner core and defect loop dynamics, and identify how the instability is different when the anchoring is varied from a predominantly splay type geometry (homeotropic boundary conditions at droplet surface) to bend type (planar anchoring).
Chapter 6

Spontaneous self-constraint in active nematics flows
6.1 Introduction

In the last two chapters, we studied the self-organised dynamics of passive and active nematic liquid crystals with imposed constraints, tuning trivial and nontrivial topologies via inclusions and confinement. In the active case, the interplay between topological nematic features and extensile active flow coupling form an interesting selection of flow states. One feature that arose, is the case of a charged disclination loop, performing rotor- and chaotic-like morphological dynamics. The dynamics of the loop and the imprinted features on the flow field could be understood through the self-motility of $+1/2$ profiles, which drive rotation, and anchoring of $-1/2$ profiles to inclusions, which pin the rotation axis.

In fact, understanding pattern formation [17] and biological functionality [225], as driven by topological defects has been a particularly successful approach in the literature. This has been most well studied in the two-dimensional active nematic films — both in spatio-temporally ordered confinement [146] and in active turbulence (§2.2.4). In §2.2.6.1 we discussed that defects are often viewed as controlling their own dynamical evolution, with only perturbations – either due to local deformations or neighbouring defects – causing deviations from their ideal trajectories. However, the dynamics of topological defects with respect to features of the flow field are not yet fully understood. Therefore, this chapter is about activity-induced self-constraints that emerge through the coupling between these two fields.

In this chapter, we reveal that the non-linear coupling between flow and orientational fields in active nematics leads to a strong, two-way, self-constraint. On the one hand, we report that self-motile topological defects are tightly constrained to specific flow boundaries, while, on the other hand, these surfaces are driven by mesoscale defect-associated nematic deformations. Specifically, our results demonstrate that self-motile $+1/2$ defects are found solely on specific isosurfaces of flow boundaries identified as viscometric surfaces — contours where vorticity and strain-rate balance. These surfaces dictate evolution of the self-motile topological defects, which align with and move along the contours since there is no deformation of the streamlines along these paths. We uncover how this causes the defects to break their ideally predicted mirror symmetry and be classified according to their instantaneous handedness. However, the spontaneous self-constraint is a co-dependency and we find that the viscometric surfaces, in turn, follows the mesoscopic deformation network of the orientational field. While
we focus on 2D extensile active nematic turbulence, we present evidence that our conclusions hold whenever activity couples to plus half-integer topological defects. The generality of these novel perspectives may provide greater insight into a more universal understanding of fluidic systems with non-linear field couplings and topologically protected states, as well as suggest a mechanism by which biological morphology could be dynamically protected.
6.2 Methods

To explore the relationship between active nematic defects and flow structures, data produced by experiments and simulations are utilised. Here, we outline the methods and analysis used.

The experiments in this study were provided by Claire Doré and Teresa López-León, based on the microtubule-kinesin experiments in [17]. An active nematic film is created by self-assembling filamentous microtubule bundles at an oil-water interface with kinesin motor clusters. The kinesin motors act as cross-linkers and hydrolyse ATP suspended in the aqueous phase, fueling extensile active stresses in the microtubule film. Microtubule bundles are imaged via confocal fluorescence microscopy, which allows the nematic tensor order parameter $Q$ (Eq. 2.3) to be inferred through coherence-enhanced diffusion filtering [226], and the velocity field $v$ using an optical flow method [227]. The active film is studied in two situations: firstly in bulk active turbulence and secondly in channel confinement. The unconfined active nematic layer was prepared in a closed observation chamber (3 mm×22 mm). For confinement, photoresist platforms were placed on top of the observation chamber, trapping the active nematic inside rectangular channels (thickness 100 μm) [228].

To simulate active turbulence, the continuum active nematohydrodynamic equations for mass Eq. (2.41), momentum Eq. (2.43), and orientation Eq. (2.39) are solved using a hybrid lattice-Boltzmann approach [42]. This chapter focusses on extensile, flow aligning, two-dimensional active turbulence, but the results and conclusions are tested more generally across active nematic systems, which includes studying other regimes of active turbulence, confinement, friction, and three-dimensions.

Except where otherwise stated, the 2D extensile active nematic simulations use the parameters (in lattice Boltzmann units): density $\rho = 1$, rotational diffusivity $\Gamma_Q = 0.3375$, flow-aligning parameter $\lambda = 1$, bulk energy density scale $A_0 = 1$, distance from the isotropic-nematic transition $\gamma = 3$, dynamic viscosity $\eta = 4/3$, Frank elasticity $K = 0.05$ and extensile activity $\zeta = 0.1$. Periodic boundary conditions are used in a system size of $L_x = L_y = 80$. The velocity and director fields are randomly initialized. A warmup time of $T_W = 1 \times 10^4$ is used before data is collected for $T_S = 2 \times 10^4$ lattice Boltzmann time steps.
Defects are characterised in two-dimensions using the topological charge density (Eq. (3.28)). To identify defects, a charge density cutoff \( q_{\text{cut}} \) is applied (§ 3.4.1.1).

In the experiments, \( q_{\text{cut}} = 1.5 \), while for the simulations \( q_{\text{cut}} = 4 \). This is chosen via visual inspection as the strongest parameters that identify the most defects correctly. The orientations of 2D point defects are found using Eq. (3.29). In three-dimensions, defects are characterised using the disclination density tensor (Eq. (3.30)). Disclination lines and loops, in bulk and channel flow states, are identified as isosurfaces where \( s(\mathbf{r}) \geq 0.1 \).

We use the \( Q \) criterion (Eq. (3.37)) to characterise the instantaneous flow fields structures. Two-dimensional isosurfaces of \( Q \) are identified using the skimage Python library [229]. Vortices are identified as closed regions where \( Q > 0 \). In visualisations of two-dimensional active flow structures, we calculate the circulation (vortex strength) as

\[
\Gamma = \oint_c \mathbf{v} \cdot d\mathbf{l} = \oint \mathbf{\omega} \cdot d\mathbf{S},
\]

(6.1)

where \( c \) is the closed \( Q = 0 \) isosurface. We employ the area integral definition to simplify the handling of non-zero genus vortices. Here, the area element \( d\mathbf{S} \) is in terms of lattice Boltzmann nodes. Vortex regions are identified by a clustering algorithm that connects neighbouring nodes satisfying \( Q > 0 \).

The active lengthscale is calculated in two-dimensions as \( \ell_\zeta = \sigma^{-1/2} \), where the defect number density is \( \sigma = (N_{+1/2} + N_{-1/2}) / (TL^2) \) for \( N_{\pm1/2} \) nematic defects over total timesteps \( T_S \) and system size \( L \). In three-dimensions, we measure the director autocorrelation function

\[
C_{nn}(|\mathbf{r} - \mathbf{r}'|) = \frac{\langle \mathbf{n}(\mathbf{r}; t) \cdot \mathbf{n}(\mathbf{r}'; t) \rangle}{\langle \mathbf{n}(\mathbf{r}; t) \cdot \mathbf{n}(\mathbf{r}; t) \rangle},
\]

(6.2)

where \( \mathbf{r} \) and \( \mathbf{r}' \) are two field points and \( t \) is time. The average \( \langle \cdots \rangle \) is over all points in space and time. The active lengthscale is selected as the fit of the decaying exponential.
Figure 6.1 *Plus-half topological defects reside on isolines of $Q = 0$. a,* Scanning confocal microscopy of experimental active film. Plus-half defects marked as green comet-shaped symbols and minus-half defects by dark blue trefoil-shaped symbols. Zero-isolines of $Q$-criterion are shown as solid lines, coloured by the handedness of the enclosed vortex—red for clockwise and blue for anti-clockwise. Scale bar: 100 µm. *b,* Numerical simulation of active turbulence. Circulation of each vortex coloured representing the vortex strength. Nematic director field plotted as grey line field.

### 6.3 Constraint on topological defects

The interplay of topological defects and the $Q$-criterion is investigated by partitioning domains of vorticity dominated ($Q > 0$) and strain-rate dominated ($Q < 0$) flows. The boundaries between these two domains are isosurfaces of simple-shear ($Q = 0$), which enclose vortices ($Q > 0$). In overlaying nematic topological defects, we report a striking finding. Previous studies have qualitatively observed $+1/2$ defects to be found near the edge of vortices [122, 230], however isolines of $Q = 0$ demonstrate that $+1/2$ defects reside directly on this boundary (Fig. 6.1). This colocation is remarkably strong, with experiments (Fig. 6.1a) and simulations (Fig. 6.1b) showing the probability of finding a $+1/2$ defect decays exponentially with distance from the isoline, decreasing orders of magnitude over a fraction of the active lengthscale (Fig. 6.2). Because of the tight connection between $+1/2$ and $Q = 0$ surfaces, we refer to this pinning of $+1/2$ disclinations to $Q = 0$ as a *self-constraint* throughout this chapter. On the contrary, the snapshots (Fig. 6.1a,b) and slower decay of distances from $Q$ (Fig. 6.2), reveal that this constraint does not extend to $−1/2$ disclinations. While defect pair creation/annihilation events occur on $Q = 0$ (Fig. 6.3), with
Figure 6.2 *Probability distribution function (PDF) of nearest distances of ±1/2 defects to \( Q = 0 \) boundary.* Shown for experiments (triangle markers) and simulations (circle markers), with colour representing +1/2 (green) and −1/2 defects (blue). The distance \( d \) is scaled by the active lengthscale \( \ell_\zeta \).

the +1/2 defect pinned to the isoline throughout the process, the -1/2 defects instead unbind over time and can thereafter be associated with any streamline topology.

Often, active flow states are visualised by their vorticity field [121, 230]. In two-dimensions, the vorticity pseudovector \( \omega \) has only one non-zero component, which enables the rotational component of the flow field to be visualised as a scalar field \( \omega(\mathbf{r}) = \mathbf{\omega}(\mathbf{r}) \cdot \mathbf{e}_z \). Isosurfaces of \( \omega = 0 \) separate flow domains with left or right-handed rotation. By visualising defects alongside \( \omega = 0 \) contours, most but not all, +1/2 defects fall on these isosurfaces (Fig. 6.4a; dash-dotted lines). This is further verified by comparing the distribution of distances of +1/2 defects to contours of \( Q = 0 \) and \( \omega = 0 \) (Fig. 6.4b). The wider distribution of \( \omega = 0 \) distances, relative to \( Q = 0 \), demonstrates that vorticity isolines do not strictly constrain the defect paths. Therefore, +1/2 defects are constrained not to where the vorticity is zero but rather where the vorticity and strain rate balance.

Constructing \( Q \) from the theoretical expectations of the active flow fields generated by isolated +1/2 or −1/2 disclination profiles (Eq. (2.59) and Eq. (2.60)), Fig. 6.5a shows that vortices reside laterally about the +1/2 defect (\( Q > 0 \)) with strain-rate dominated flow in front and behind (\( Q < 0 \)). The separatrix (\( Q = 0 \)) between these domains present two lines that are degenerate only at the core of the defect. In contrast, the expectation for −1/2 disclinations
(Fig. 6.5b) is more complicated. At the centre of the defect, the flows are strain-rate dominated, while six vortices of alternating handedness form away from the core. Despite the $Q < 0$ prediction, all signs of $Q$ are observed in practice (Fig. 6.6). Because $-1/2$ defects do not satisfy the self-constraint, this chapter does not consider them further. While this idealised theoretical picture successfully captures some aspects of the self-constraint, we see in the next section that it is unable to predict important features of the isosurface/defect dynamics.
Figure 6.4  Plus-half topological defects and isolines of zero vorticity.

a, Same snapshot as Fig. 6.1b, but vorticity field $\omega$ is coloured and grey arrows for the velocity field. Zero-vorticity contours are shown as lilac dash-dot lines. Left: Examples where the vorticity is non-zero (top) and zero (bottom) at the $+1/2$ defect position.  
b, Distribution (PDF) of $+1/2$ defect distances $d$ from $\omega = 0$ (lilac) in experiments (triangle markers) and simulations (circle markers). The $+1/2$ PDF of distance from $Q = 0$ (Fig. 6.2) are shown in green. Distances scaled by characteristic active length $\ell_\zeta$. 
6.4 Subclasses of defects

Thus far, we have revealed that +1/2 defects are located on \( Q = 0 \). These isosurfaces represent flow structures of simple shear and define the closed borders of vortices (\( Q > 0 \)). How do defects arrange themselves along \( Q = 0 \)? Fig. 6.1a,b illustrates that defect/viscometric surface complexes exist in two distinct configurations: either a +1/2 defect is positioned at an intersection of viscometric lines, or a defect lies parallel to a single \( Q = 0 \) line. In the first case (Fig. 6.7a), a +1/2 defect is positioned at a cross-road between two viscometric lines and has two equally strong counter-rotating vortex regions on either side of the defect axis. The flow directly in front and behind is strain-rate dominated. Thus, the defect has mirror symmetry along its head-tail axis. This corresponds to the ideal picture of a solitary defect (Fig. 6.5a), which is tacitly the expectation of flows around defects in active turbulence [20]. At the defect core, flows are directed parallel to the defect orientation (self-propulsion direction). However, although the ideal model predicts vortices on either side of the defect, vortices have zero velocity at their core (Fig. 6.5a). Thus, the self-consistency of vortices propulsively moving alongside motile defects is necessarily challenged.

Instead, the ideally expected mirror symmetry around the isolines is broken (Fig. 6.7b,c). Many of the defects in these states orient parallel to a single viscometric line, with vorticity dominating on one side and strain rate dominating
Figure 6.6  *Minus-half topological defects are not constrained to isolines of* $Q = 0$. Simulation snapshot of the flow geometry around $\pm \frac{1}{2}$ nematic defects. While the $\pm \frac{1}{2}$ defect (green marker) is constrained to $Q = 0$, $-\frac{1}{2}$ defects (navy blue trefoils) can be found anywhere. In this snapshot, one $-\frac{1}{2}$ defect is in a strain-dominated region (top left), one in a vorticity-dominated region (right) and one on a $Q = 0$ border (bottom left). Visualisation same as Fig. 6.1.

on the other. This spontaneous handedness of a subpopulation of defects is not predicted by the ideal model for a solitary defect; however, defects with this configuration persist for long durations and are observed to be the majority (Fig. 6.1a,b). This is because a motile defect can persistently move along the $Q = 0$ line, circulating around a single neighboring vortex. As a result, local chirality spontaneously emerges in this globally achiral system. This spontaneous handedness is necessarily erased when ensemble averaging fields around defect cores.

To obtain a statistical description of the flow field structure, we modify the standard ensemble average over all $\pm \frac{1}{2}$ defects [231] to account for each chiral/achiral subclasses. We calculate $\langle Q \rangle_{\Delta r^2}$ as the average $Q$ in a small region $\Delta r^2$. Here, $\Delta r^2$ is set to be a rectangle of seven by six lattice units on either side of the orientation axis of the defect. Taken over all $\pm \frac{1}{2}$ defects, the difference between the right and left side $\langle Q \rangle_{\Delta r^2}^{\text{diff}} = \langle Q \rangle_{\Delta r^2}^{\text{right}} - \langle Q \rangle_{\Delta r^2}^{\text{left}}$ is computed. From the distribution of $\langle Q \rangle_{\Delta r^2}^{\text{diff}}$, the three defect subclasses (clockwise-handed, symmetric, anticlockwise-handed) are identified. Anticlockwise-handed cases with a vortex on the left-side correspond to strongly negative $\langle Q \rangle_{\Delta r^2}^{\text{diff}}$ and are identified as the lowest 10% of the distribution. Likewise, the clockwise cases have a vortex on
Figure 6.7 Subclasses of plus half topological defects, identified by their local flow structure. a-c, Simulation snapshots of +1/2 defects, for the cases of a mirror symmetric, b mirror-symmetry-broken with clockwise vortex, and c anticlockwise vortex. d-f, Time and ensemble averaged director fields and Q-criterion around +1/2 defects sorted by handedness. d, Mirror-symmetric state, e clockwise-handed state and f anticlockwise-handed state. The Q = 0 isoline is shown by solid lines. The ensemble averaged vorticity field is clockwise (red) and anticlockwise (blue). Averaged director with black lines and velocity field with purple arrows.

the right-hand-side and are identified as 90% and above. The mirror symmetric subclass is assigned to between 10% and 90%. From defects in these bins, the local flows are averaged.

The flow-averaged profiles are shown in Fig. 6.7d-f. The flows of the two non-symmetric cases (Fig. 6.7e,f) are distinct from the mirror-symmetric case (Fig. 6.7d). In the mirror-symmetric case, the streamlines are parallel to the defect orientation, supported by the two lateral vortices. However, the streamlines are curved in the mirror-symmetry broken cases, enclosing a single vortex. Despite a clear handedness, Q = 0 still represents simple shear. This is because the velocity gradients are everywhere orthogonal along the isosurface. The presence of the handed subclass implies that Fig. 6.5a must be reinterpreted as an idealisation rather than expectation.
We quantify the nature of these defect/viscometric surface complexes via the distribution of alignment angles $\theta$ between the $+1/2$ defect axis and the $Q = 0$ boundary tangent (Fig. 6.8). In experiments and simulations, the most likely alignment is directly parallel. The distribution decays steadily with angle so that the least likely alignment is perpendicular. The parallel alignments are associated with the handed configurations (Fig. 6.7b-c,e-f). To compare with the likelihood of observing a mirror-symmetric defect, we consider two models of a solitary defect and their predictions for $\theta$.

The first of these models uses the solution for the active flow around a solitary $+1/2$ (Eq. (2.59)). Constructing the velocity gradients and using Eq. (3.37) gives

$$Q = \left( \frac{\zeta}{6\eta} \right)^2 (3 \sin^2 \phi - 1),$$

(6.3)

where $\phi$ is the polar angle defined from $e_x$. Since the $+1/2$ defect is oriented with $e_x$, the alignment angle $\theta = \phi$. Therefore, solutions to $3 \sin^2 \theta = 1$ find the ideal alignment between the $+1/2$ orientation and $Q = 0$ to be $\theta = 35.26^\circ$. The second model is even simpler: it is made by approximating the parallel force field in Eq. (2.56) as a localised point $f$. For a point force oriented along $e_x$, solving the Oseen tensor Eq. (2.58) and constructing the $Q$ criterion gives

$$Q = \left( \frac{f}{4\pi\eta|\mathbf{r}|} \right)^2 (2 \sin^2 \phi - 1).$$

(6.4)

Solving $Q = 0$ finds that $2 \sin^2 \theta = 1$ and so this point force aligns at an angle of $45^\circ$ relative to the viscometric contours. While the point-force model predicts a quantitatively different angle, it qualitatively does a satisfactory job modelling the $Q = 0$ isolines.

These ideal $\theta$ predictions are indicated by the dashed lines in Fig. 6.8. Comparing these lines to the distribution from experiments and simulations highlights that the measured angle tends to be smaller than the ideal models. The mirror-symmetry-broken configurations are preferred to the symmetric configuration predicted by the ideal solitary-defect theory.

We next explore the relevance of the subclasses on defect dynamics. To do this, we construct defect trajectories that are distinguished by handed and mirror-symmetric categories. The longest resolved trajectories ($> 9$ points) are shown in Fig. 6.9, accompanied by a scatter symbol that records whether the defect is in
Figure 6.8 *Probability distribution function (PDF) of alignment angles* $\theta$ *between the defect orientation and the tangent of the associated viscometric* ($Q = 0$) *line.* The vertical blue dash-dot line indicates the ideally expected alignment from Eq. (6.3) and the grey dashed line indicates the alignment angle for a point active force from Eq. (6.3).

the handed or mirror-symmetric subclass, as determined by the flows through $\langle Q \rangle^{\text{diff}}_{\Delta r^2}$. Defects weave between curved and straight trajectories (Fig. 6.9a). When the trajectories curve, defects are associated with the handed subclass, and the handedness of the defect trajectory matches the associated vortex. This is quantified by a scatter plot of trajectory curvature with defect velocity (for all defect trajectories).

Overall, these trajectories reveal that defect subclasses, associated with one (handed) or two (mirror-symmetric) vortices, offer a more direct perspective on the rotational influences of self-propelled disclinations. This provides a more mechanistic view of defect trajectories over the current hydrodynamic models, which assume these influences are driven by coarse-grained active torques mediated by interactions between quasiparticles (§ 2.2.6.1).

This section has shown that defects are not only constrained in their dynamics to particular flow isolines, but intermittently transform between the mirror-symmetric and broken-mirror-symmetry cases as they navigate the borders of vortices. In the next section, we uncover that the prevalence of the chiral subclass in extensile active turbulence is a consequence of the hydrodynamic instability.
Figure 6.9 *Instantaneous handedness of a plus half defect dictates its future trajectory.* **a.** Defect trajectories in active turbulence (simulations). The symbols are coloured by the associated defect/vortex symmetry subclass—clockwise (red triangle), anticlockwise (blue triangle), or mirror symmetric (white circles). The initial point of each trajectory is represented by a green +1/2 defect symbol. Separate trajectories with > 9 resolved points are overlain. **b.** Scatter plot of the +1/2 defect velocity and instantaneous curvature of the trajectory. The +1/2 defect velocity $|u_+|$ is the distance between separated points in the trajectory divided by time. The velocity is scaled by $u_0$, the peak velocity from a distribution of all +1/2 defects. Crosses (with colors of the three defect/vortex subclasses) are centred on the average curvature and velocity, with errorbars indicating standard deviation. The negative trajectory curvature represents anti-clockwise defect dynamics, and positive curvature shows clockwise trajectories. Curvature is shown in units of inverse active length scale $\ell_\zeta$. 

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Figure 6.10  **Viscometric surfaces generated by bend walls.**  Left: Same snapshot as Fig. 6.1b with colourmap corresponding to the scalar splay-bend parameter $S_{SB}$ (Eq. (3.32)). Narrow lines of strong negative $S_{SB}$ are interpreted as bend walls. Middle and right panels are the next two snapshots in time.

### 6.5 Role of bend walls

To understand the emergence of the subclasses of $+1/2$ defects and the pinning mechanism of the self-constraint, it is crucial to note that defects are point singularities in the director field (§ 2.1.5) but are not localised singularities in the solutions for the active force. As seen by the continuum equations (Eq. (2.56)), the integral curves of the force density are smooth and directed parallel with the $+1/2$ orientation at the core of the defect (Fig. 2.15a). The magnitude of the force decays with distance $1/r$ from the isolated defect core. However, more generally, active force is generated from any deformation of the orientation field. In active turbulence, deformations do not only conform to isolated sources and so active force is not limited to regions in the immediate vicinity of defects. In particular, bend walls are a signature of the hydrodynamic bend instability in wet extensile active nematics (§ 2.2.5). Bend walls are narrow lines of sharp kinked bend deformation between nematic domains. As extended structures of highly localised deformations, bend walls generate strong active forcing and bend constricts into system-spanning narrow kink lines [124]. Defect pairs unbind along these walls (Fig. 2.14) and the self-motile $+1/2$ defect unzips the bend wall as it advances [19]. It is then presumed that significant forces only occur in the immediate vicinity of defects. However, in practice this is not observed in experiments or simulations. Rather, the hydrodynamic instability is incessantly constricting bend into sharp kink walls (Fig. 6.10), as demonstrated by the splay-bend parameter $S_{SB}$ (Eq. (3.32)).
The strongly negative values of $S_{SB}$ highlight an interconnected network of lines (bend-walls) that frequently terminate or fork at point defects (Fig. 6.10). This network is not static; instead, it dynamically exchanges connections between points and branches in new directions. Through visualising $S_{SB}$ alongside the $Q = 0$ contours, one can observe that the bend walls strongly correlate with the viscometric lines. The timeseries (Fig. 6.10) illustrates that bend walls and $Q = 0$ mutually shape each other, which guides the paths that defect follow. This interdependence of bend walls and $Q = 0$ is quantified by the $S_{SB}$ distribution in Fig. 6.11. The $S_{SB}$ is skewed more towards negative (bend) values than for the system as a whole (Fig. 6.11).

The extended concurrence of bend walls and $Q = 0$ lines suggests that interpreting the self-constraint should factor in bend walls. In light of this, we construct a series of models that first interpret the flow generation around bend walls, and second build upon the idealised view of defects as solitary points to incorporate broader extended structures. The first two models construct example bend-wall director configurations and solve for the active flows and $Q$ criterion. The last set of models considers defects and bend walls together via a simplified force model. In these, the flows and $Q$ are obtained by numerically solving the Stokes equation (Eq. (2.53)). These simple steps demonstrate that defects cannot be treated as isolated points but must be considered in conjunction...
with mesoscale defect/kink-wall structures, explaining the interdependence of viscometric contours and handedness of bound +1/2 defects arising in active nematics.

### 6.5.1 Linear bend wall

For the first model, we explore the flow patterns generated by an infinite uniaxial bend wall. An example director field is constructed, \( \mathbf{n} = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y \), in terms of the orientation angle

\[
\theta(y; \lambda) = \pi \cos^2 \left( \frac{y}{\lambda} \right). \tag{6.5}
\]

This director is chosen because a central band of bend is created when constraining \( \theta(y; \lambda) \) within the boundaries \( y = -\lambda/2 \) and \( y = \lambda/2 \), where \( \lambda \) is the modulation wavelength (Fig. 6.12). At \( y = 0 \), bend \( \mathbf{b} = \mathbf{n} \times (\nabla \times \mathbf{n}) \) is oriented along \( -\mathbf{e}_x \).

The active force density generated by \( \theta(y; \lambda) \) is calculated. Assuming \( S \) is constant, the active forcing \( \mathbf{f}^c = -\zeta \nabla \cdot (\mathbf{n} \otimes \mathbf{n}) \) is found to be

\[
\mathbf{f}^c = \zeta \frac{\pi}{\lambda} \sin \frac{2y}{\lambda} (\cos 2\theta \mathbf{e}_x + \sin 2\theta \mathbf{e}_y). \tag{6.6}
\]
This profile of active force is shown in Fig. 6.12a, showing that the force is strongest, and unidirectionally aligned along \( \mathbf{b} \) at \( y = 0 \). Away from \( y = 0 \), the force gradually reverses orientation and the magnitude diminishes to zero at the boundaries \( y = \pm \lambda/2 \).

In determining the corresponding flow structure, we work with the Stokes equation (Eq. (2.53)) under the assumption that active stresses dominate elastic stresses. To solve this, the pressure gradients \( \nabla p(\mathbf{r}) \) must be obtained. While the active forces are local, the pressure is non-local and adjusts itself to changes in the flow field so that the fluid is everywhere divergence free (Eq. (2.42)). We take the divergence of Eq. (2.53) and apply the incompressibility condition Eq. (2.42). This obtains a Poisson equation for the pressure

\[
\nabla^2 p = \nabla \cdot \mathbf{f}_\zeta
= \zeta S_{SB}.
\] (6.7)

Here, we applied Eq. (3.32) with constant \( S \) to write the Laplacian in terms of the \( S_{SB} \) (§ 3.5). The right-hand side of Eq. (6.7) reveals that the pressure sources are directly controlled by \( S_{SB} \) and tuned in strength by the activity. Therefore, for extensile active nematics (\( \zeta > 0 \)), regions of positive \( S_{SB} \) act as pressure sources and negative \( S_{SB} \) are pressure sinks. With the interpretation \( S_{SB} \sim \nabla \cdot (\mathbf{s} - \mathbf{b}) \) (Eq. (3.33)), bend walls are associated with strongly negative values of \( S_{SB} \), owing to localised bend. Interpreting Eq. (6.7) with \( S_{SB} \) in this way suggests that the bend walls constitute a line-like continuum of pressure sinks.

For the example bend wall, we can now solve for the pressure gradients. Since the director (Eq. (6.5)), and active force (Eq. (6.6)), have translational symmetry in \( \mathbf{e}_x \), all derivatives with respect to \( x \) are zero. The pressure gradient forces can be simply obtained by integrating Eq. (6.7)

\[
\mathbf{f}^p = -\frac{\partial p}{\partial y} \mathbf{e}_y = -\zeta \frac{\pi}{\lambda} \sin \frac{2y}{\lambda} \sin 2\theta \mathbf{e}_y.
\] (6.8)

In Fig. 6.12b, the pressure gradient forces (Eq. (6.8)) can be visualised as force arrows directed inwards, everywhere perpendicular to the line tangent of the bend wall. These inward force arrows demonstrate the pressure-sink nature of bend walls.
By determining the net force contributed by Eq. (6.6) and Eq. (6.8)

\[ \mathbf{f}^\kappa + \mathbf{f}^p = \zeta \frac{\pi}{\lambda} \sin \frac{2y}{\lambda} \cos 2\theta \mathbf{e}_x, \]

(6.9)

the pressure gradients are revealed to everywhere balance the \( y \)-components of the active forces, leaving a resultant force oriented parallel to \( \mathbf{e}_x \) (Fig. 6.12c). To maintain force balance (Eq. (2.53)),

\[ \eta \nabla^2 \mathbf{v} = -\zeta \frac{\pi}{\lambda} \sin \frac{2y}{\lambda} \cos 2\theta \mathbf{e}_x \]

(6.10)

Therefore, the source of the flows \( \mathbf{v} \) stem from the resultant active/pressure force density in Eq. (6.9). These flows are necessarily directed parallel to the axis of the bend wall (\( \mathbf{e}_x \)), due to the balanced force in \( \mathbf{e}_y \).

Finally, we determine the structure of the activity-driven flow field formed by the bend wall. By integrating Eq. (6.10) with respect to \( y \), the velocity gradient is

\[ \mathbf{A} = -\zeta \frac{\sin(\pi \cos(2y/\lambda))}{2\eta} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \]

(6.11)

which is upper diagonal and demonstrates simple horizontal shear flow (§3.6). Here, the one-dimensional structure of \( \mathbf{A} \) prevents closed streamlines, and hence no domains of vorticity or strain-rate dominated flow are formed. The \( \mathcal{Q} \) criterion is zero everywhere, rather than just at the core of the bend wall. Therefore, this entirely simple shear flow pattern is insufficient to explain the colocation of bend walls and \( \mathcal{Q} = 0 \) (Fig. 6.10).

This study of a uniaxial bend wall has indicated the internal mechanisms that form simple shear flows. Deformation generates active forces, which self-preserve incompressibility by creating pressure gradient forces. Together, these forces balance to form simple shear flows. However, in order to generate flow structures that are not strictly \( \mathcal{Q} = 0 \) everywhere, the invariance along the bend wall must be broken.

### 6.5.2 Wavy bend wall

In this second example, \( x \)-invariance is broken by introducing bend wall curvature. The linear example (§6.5.1) is perturbed into infinitely long sinusoidal waves. The director is constructed once again of the form \( \mathbf{n} = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y \).
Figure 6.13  Model of an infinitely long, repeating wavy bend wall.  

a, Initial splay-bend parameter ($S_{SB}$) field with repeating model bend walls in purple, with same colourbar as Fig. 6.10a.  
b, Resulting $Q$ of steady-state active flows due to fixed $S_{SB}$ from a. The circulation colouring is the same as Fig. 6.1b.  
c, Resulting steady-state $S_{SB}$ due to fixed flows from b.  
d, Resulting steady-state flows due to fixed $S_{SB}$ from c. Director field is shown as black lines, the velocity field as grey arrows and $Q = 0$ contours as solid lines.

but with an angle chosen to be

$$\theta(x, y; \lambda) = \pi \cos^2 \left( \frac{x}{4\lambda} \right) + \frac{\pi y}{\lambda}. \quad (6.12)$$

This director field generates a periodic sequence of bend and splay walls that modulate sinusoidally about slices of $y$ (Fig. 6.13a). Colouring by $S_{SB}$, Fig. 6.13 shows that the director alternates between wavy walls of bend (purple) and splay (green). Analytically obtaining the generated flow structure is too advanced for this example bend wall since $x$–invariance doesn’t hold. Therefore, to make progress in understanding the coupling between bend walls and the $Q$ criterion, we turn to numerical solutions.
This numerical study is split into two parts. First, we numerically solve Eq. (2.43) to obtain the velocity field. This provides insight on the flow structures generated by the bend/splay walls and their relationship with \( Q \). Second, we probe the two-way coupling between bend walls and flow structures. The influence of flows on nematic structure is usually neglected \([20]\), but is essential for understanding cross-field constraints. Thus, for understanding this interplay, we will fix the velocity field and evolve \( Q \) using Eq. (2.39).

In Fig. 6.13a, we show the bend walls alongside the \( Q = 0 \) isolines (solid lines). This shows that \( Q = 0 \) is formed along backbone of the bend walls. This is also observed for splay walls. Further, the director modulation breaks the pure simple shear flow patterns (§ 6.5.1) into regions of \( Q > 0 \) and \( Q < 0 \) surrounding the bend wall. The isolines enclose vortices \( (Q > 0) \), which are coloured by their circulation (Fig. 6.13b). The vortices collect at the peaks and troughs of the bend/splay walls with alternating handedness. The circulation handedness is determined by the cross product of the tangent curve of active forcing and the normal to the curve (concave direction). Outside of the pattern of vortices, rate-of-strain dominates the velocity gradients (shown as white).

As a test of the feedback between the bend wall director structure and \( Q = 0 \) isolines, the velocity field is held fixed and the director is able to evolve in time (Fig. 6.13c). Compared to the starting configuration (Fig. 6.13a), the bend deformation is tightly localised, as evident by the strongly negative \( S_{SB} \) that forms a thin wave. In contrast, the splay-type deformation has nearly vanished (shown in white). The accentuation of bend at the expense of the splay, is in line with expectations from the hydrodynamic instability—where bend is the unstable mode for extensile activity (§ 2.2.5). Here, the instability is demonstrated through the feedback of active flows and director configurations rather than using wavelength analysis \([124]\).

As a final test of the cross-field coupling, the flow structure is solved for the director configuration in Fig. 6.13c. This shows that the \( Q = 0 \) once again coincides with the bend wall (Fig. 6.13d). One difference between the flows before the director evolution (Fig. 6.13b) and after (Fig. 6.13d), is that vortices have merged. Despite the instability, an important finding is that the only preserved structures in (Fig. 6.13) are the backbone of the bend wall, and \( Q = 0 \) along these walls.

This wavy bend wall model has successfully demonstrated the colocation of bend
Figure 6.14  

$Q$-criterion and velocity field predicted by Stokesian line force model of bend walls. Red and blue shading indicate clockwise and anti-clockwise vorticity-dominated regions, while the white regions are strain-rate dominated. The $Q = 0$ contours are solid lines. The unit-vector velocity field is shown with grey arrows. The line force is shown as a solid purple line with the direction of forcing indicated by the purple arrows. The start and end points of the force line are represented by green and blue circles, respectively. Forces are constructed as: a, point source, b, straight finite line and c, circular arc.

We found that not only do bend walls generate $Q = 0$ along their backbone, but that $Q = 0$ also preserves the structure of bend-walls. This simple model further highlights the important role that bend-walls play in shaping active flow structures. In contrast to the tacit assumption that defects are responsible for establishing the flow structure, this idealised modulated director example shows that vortices can be formed without nematic singularities.

6.5.3 Stokesian force model

One missing piece of these bend wall models is that these idealised line-like structures are continuous and omit topological defects. Motivated by the interconnected network of $S_{SB}$ that links bend walls and defects together (Fig. 6.10), we advance our model to account for both defects and bend walls.

We choose to bypass the director details and instead compose a model directly in terms of active force. The simplest model of the force generated by these structures is a line of force with end points; the line being the bend wall and end points being the defects. This qualitatively captures the localised active forcing associated with these structures.

We calculate the velocity field and $Q = 0$ contours for the following force cases:
(i) an isolated point, (ii) a finite straight line, (iii) a curved line (Fig. 6.14a-c). For each case, the Stokes equation (Eq. (2.53)) is solved, but with the active force replaced with a generalised force density $f$. These solutions are performed in two-dimensions with a system size of $L_x = L_y = 1000$. Each point on the discretised line contributes to the overall velocity field through the two-dimensional Oseen tensor (Eq. (2.58)).

(i) Consider a simple point-force model of a solitary defect. A single point force is oriented in the positive $e_x$ direction (Fig. 6.14a). In agreement with the ideal analytical solution of a solitary $+1/2$ defect (Fig. 6.5a), modeling defects as simple point-forces is sufficient to qualitatively predict the mirror-symmetric configuration at intersections, as was shown in Eq. (6.4). However, viewing a defect in isolation is not capable of predicting the handed configurations (Fig. 6.7b-c), nor the observed distribution of intersection angles (Fig. 6.8) because defects are associated with narrow kink walls, even in steady-state turbulence (Fig. 6.10a).

(ii) To account for bend walls as simply as possible, we now present a model that recognises that deformations and associated force density localises along the narrow bend walls, and treats defect/bend-wall complexes as finitely long, straight force lines. For this, 500 point sources are arranged across 500 horizontal lattice points, oriented in the positive $e_x$ direction (Fig. 6.14b). This model predicts a more acute angle between the $Q = 0$ contours and the defect axis, improving on case (i) but not resolving the essential inability to predict handed configurations.

(iii) One additional complication is required: kink walls do not remain straight. Due to the inherently unstable nature of extensile active nematics, bend walls continuously curve (Fig. 6.10). We introduce curvature to the force model by considering a circular arc of active forcing, parameterised in terms of $s$. Positions on the arc are $r'(s) = R(\cos s e_x + \sin s e_y)$. To construct the force, 500 point sources are placed between $s = 5\pi/8$ and $s = 3\pi/8$ with a total arclength of 500. The force direction points parallel to the line tangent $f'(s) = f(\sin se_x - \cos se_y)$ with $f = 1$ (Fig. 6.14c) . This model results in the upper, anti-clockwise $Q = 0$ contour separating from the bend wall, while lower, left-handed $Q = 0$ isoline colocalises along the bend wall. Hence, defects modelled as the singular ends of finitely long, curved kink-walls produce the symmetry broken case with vorticity-dominated flows on one side and strain-rate dominated on the outside of the bend wall.
Figure 6.15  **Pair-creation events occur where viscometric surfaces converge on bend walls.** A long bend wall drives viscometric flow along much of its backbone. A pair creation event occurs where the bend wall and the two viscometric surfaces converge to meet at a point. Black arrow indicates the arrow of time. Colourmap identifies line-like bend walls through the strongly-negative $S_B$ (same as Fig. 6.10). Zero-isolines of the $Q$-criterion are shown as solid lines, coloured in red for clockwise and blue for anti-clockwise. Nematic $+1/2$ defects marked by green comet-shaped symbols and minus-half defects by dark blue-trefoil shaped symbols.

The combination of these simple models illustrate that bend walls are important to the interdependence of defect dynamics and viscometric surfaces. First, bend-wall constriction via the hydrodynamic instability causes active forces to be localised along narrow lines, resulting in shearing flows that neither stretch nor elongate streamlines. Self-motile $+1/2$ defects unzip these narrow bend walls as they preferentially move along them and thus are elastically constrained to $Q = 0$. Finally, the finite length and curvature of the bend walls cause the mirror-symmetry-broken case, demonstrating that the broken symmetry is not simply due to random interactions and torques from the isotropic active turbulence.

### 6.5.4 Creation events

Although simple, the above models allow us to make novel predictions about defect dynamics. For instance, it has long been noticed that pair creation events occur somewhere along extended bend walls \cite{19, 129} but predicting the creation site has not previously been possible. However, the $Q$ criterion framework immediately allows one to identify where along bend walls to predict pair-creation events—creation events occur along $S_B$ lines where $Q = 0$ isolines converge (Fig. 6.15).
6.5.5 Discussion

This section has unveiled that the dynamics of defects are contingent upon extended nematic structures associated with the hydrodynamic instability of wet active nematics. Curved kink walls not only preferentially support $Q = 0$, guiding the paths that motile $+1/2$ follow, but also organise defects into achiral and chiral subclasses associated with one or two vortices respectively. Our models predict that the latter subclass is supported by bend walls directly, and imply that active nematic fluids with suppressed instabilities would fall under the mirror symmetric configuration. In the next section, we explore the universality of the constraint and provide interpretations of defect dynamics more generally across active nematic systems.
Figure 6.16 The spontaneous self-constraint between motile $+1/2$ defects and viscometric surfaces holds for other regimes of active turbulence. 

**a.** Active extensile turbulence with an alignment parameter in the flow-tumbling regime ($\lambda = 0.3$). Same visualisation as Fig. 6.1b. **b.** Contractile active turbulence ($\zeta = -0.1$) in an operating regime with rare instances of bound $+1/2$ defect pairs creating effective $+1$ defects, which do not need to be on $Q = 0$. Snapshot shown for system size $L_x = L_y = 160$ and same visualisation as Fig. 6.10a. **c.** Comparison of distance from $Q = 0$ for different tumbling parameters $\lambda$ in the shear-aligning ($\lambda = 1$), flow-tumbling ($\lambda = 0.3$) and intermediate ($\lambda = 0.6$) regimes.

6.6 Generalising the self-constraint

So far, this chapter has illustrated a spontaneous self-constraint between defects and flow structures in extensile, 2D active turbulence, but this phenomenon is substantially more general, apparently holding whenever $+1/2$ topological defects are moving within active nematics. This section will focus on showing this in two-dimensional active nematics, but the final section will explore the generality of the self-constraint in three-dimensions §6.7. Simulation parameters are the same as previous sections except where specifically stated.

6.6.1 Other active turbulence regimes

The conclusions arrived at for flow-aligning ($\lambda = 1$) active turbulence also hold in the flow-tumbling ($\lambda = 0.3$; Fig. 6.16a) and intermediate ($\lambda = 0.6$) regimes, with no change to the likelihood of finding $+1/2$ defects away from $Q = 0$ isolines (Fig. 6.16c). Once again, defects reside on viscometric contours, and either travel along a single vortex boundary or transiently cross an intersection. The interdependence strongly resembles the flow-aligning regime, which is consistent with the expectation that active turbulence in flow-aligning and flow-tumbling
behaves similarly. Furthermore, the conclusions likewise hold for contractile activity ($\zeta = -0.1$; Fig. 6.16b). Minus-half defects are still non-motile and are not constrained to viscometric lines. Motile +1/2 defects now chase their tail and unzip splay walls; yet, they are still mostly constrained to be found self-propulsively moving where $Q = 0$. However, in flow-aligning contractile systems, there is an intriguing exception: In a narrow parameter regime, a pair of similarly charged +1/2 defects can temporarily form metastable +1 complexes [232]. These effectively immotile +1 complexes produce a flow profile that does not necessitate $Q = 0$ and, thus, these compounds do not reside where $Q = 0$, allowing them to briefly elude the confinement condition. Therefore, the motility of +1/2 defects, actively unzipping deformation walls, is central to the reported interdependence.

### 6.6.2 Confinement

The introduction of a confining lengthscale $L$ can tune active flow states from turbulent-like dynamics to spatiotemporally ordered (§ 2.2.3.1). An experimentally feasible [228, 233] method of introducing $L$ is to confine the active nematic film in a channel. In channel simulations, the Ceilidh dynamics state arises; +1/2 disclinations are observed to ‘dance’ around vortices, while -1/2 disclinations are constrained to the impermeable no-slip walls [133].

In Fig. 6.17, snapshots of channel-confined 2D active nematics in simulations (Fig. 6.17a,b) and experiments (Fig. 6.17d) are presented. The channel has $L_x = 130$, $L_y = 25$, with periodic boundary conditions in the $x$–direction and no-slip walls with planar anchoring energy $W_1 = W_2 = 0.3$ (Eq. (2.15)). In each case, the resulting vortex lattice can be identified by a periodic array of central vortices (closed red and blue contours) with vortex diameter approximately matching the channel width. The +1/2 disclinations (green) reside directly on the $Q = 0$ contours, while −1/2 are at the boundary away from the vortex perimeter. Further, the handed and mirror-symmetric configurations are clear (Fig. 6.17a,b) and have definitive roles in the +1/2 defect dynamics. The +1/2 defects orient parallel to the viscometric line when traversing a vortex (Fig. 6.17b), and are able to cross to neighbouring vortices by passing through the fleeting $Q = 0$ intersection (Fig. 6.17a).

The dance-like transition between these two subclasses is further highlighted in Fig. 6.17c. Defects periodically pass through the channel centre ($y = 0$) to vortices with an opposite handedness. At these intersections, two defects are
Figure 6.17 **Self constraint and defect dynamics in channel confinement.** **a-b,** Dancing defect dynamics in 2D confining channel, with +1/2 defects switching between $Q = 0$ intersections (**a**) and vortices (**b**). Same visualisation as Fig. 6.10a. **c,** Defect dynamics and circulation evolution in simulations. The pink shaded region identifies the time periods in which at least one defect resides on two vortices of alternate handedness simultaneously. (top) Average absolute +1/2 defect displacement, $y$, from the channel centre, scaled by the channel height $L_y$. Green shaded region represents the standard deviation of the defect height. (middle) Ensemble average of the circulation, $\Gamma$, contained inside the central clockwise (red) and anti-clockwise (blue) vortices. Shading represents the standard deviation for each of the clockwise (red shading) and anti-clockwise (blue shading) vortices. (bottom) Total number of +1/2 defects, $N_{+1/2}$, associated with the central clockwise (red) and anti-clockwise (blue) vortices. **d,** Experimental verification that the spontaneous self-constraint is retained in a channel confinement. Scale bar: 100µm.

simultaneously associated with each vortex (pink shading). Following the crossover (white background), defects traverse a single vortex (white background). At a given time, the defects only traverse vortices of a single handedness. Accordingly, the occupied vortex is accompanied by an injection of circulation (middle panel). The other vortices minimise the circulation in the absence of defects. This indicates that +1/2 defects contribute to the maintenance of vortices by generating lateral rotational flows (Fig. 6.5k).

Therefore, these channel confinement examples are not only consistent with disclinations tracing $Q = 0$, but also highlight the usefulness of identifying the subclasses of defects in describing defect transport. Defects may only circulate a
Figure 6.18  **Numerically simulated, two-dimensional active nematics with friction.**  

- **a**, Intermediate isotropic friction ($\kappa = 0.009$) still exhibits a subset of handed defects.  
- **b**, Snapshot of an ordered defect lattice for high friction ($\kappa = 0.015$), solely exhibiting mirror symmetric state $+1/2$ defects.  
- **c**, Lanes of alternating circulation form with anisotropic friction in the flow-aligning regime. Anisotropic friction is strong in the $x$–direction and zero in the $y$–direction. Dashed lines show the director field, solid lines are $Q = 0$ contours and enclosed area is coloured by circulation (same as Fig. 6.1b).

single vortex unless an intersection is made possible, where it can be transported to a vortex of opposite handedness.

### 6.6.3 Friction

In the presence of friction, the instability cannot grow to large wavelengths, which reduces the formation of sharp bend-kink walls. Homogeneous friction, for example, can modify the properties of active turbulence, tuning the flow structures into ordered arrangements of defects and vortices [234, 235]. Friction is added to Eq. (2.43) as $f_E = -\kappa \cdot v$ with isotropic friction tensor $\kappa = \kappa I$ and $\kappa \in [0.009, 0.015]$ (parameters same as [236]). By examining these flow states through the $Q = 0$ framework, it is evident that this transition to ordered flow states mirrors the interchange of defects from predominantly handed (Fig. 6.18a) to entirely mirror-symmetric (Fig. 6.18b) on increasing friction from $\kappa = 0.009$ to $\kappa = 0.015$.

A further interesting situation arises in the case of anisotropic friction [111, 237], which creates an easy flow axis. Here, $\kappa = [[0.015, 0], [0, 0]]$ and the parameters are the same as [111]. The $Q = 0$ isolines act as lanes, separating regions of distinct circulation handedness, and dictating straight defect paths through
enforcing the mirror-symmetric case. On occasion, defects may pass to a different lane, which occur through a handed interaction with a vortex, maintaining the $Q = 0$ self-constraint throughout. These cases show that viscometric surfaces offer a framework to reinterpret existing studies of defect dynamics [234, 237, 238] by identifying constraints on the paths that defects follow and categorising the subclasses of defect-vortex interactions. This may aid efforts in controlling active nematic dynamics, through tuning the geometry of the flow field.

6.7 Three-dimensional self-constraint

Understanding three-dimensional active nematics is only in its infancy, but attention is turning in this direction [28] now that these systems are experimentally viable (§ 2.2.6.2). As opposed to two-dimensions, where defects are point singularities, three-dimensional topological defects are significantly more complex, with non-local disclination lines and loops.

As a step towards interpreting the interplay of three-dimensional defects and emergent flow structures, we present three examples of 3D defect dynamics viewed within our viscometric surface framework. Two of the examples are spatiotemporally ordered flow states in confinement: i) a channel, ii) low activity regime of a multiple emulsion. The final example will show iii) bulk active turbulence.

6.7.1 Channel confinement

In similarity with two-dimensions (§ 6.6.2), confinement supports the formation of three-dimensional spatiotemporal flow states when $\ell_\zeta \approx L$. One such state is the vortex lattice [239, 240], which exists in a planar-anchored 3D duct. Here, $L_x = 130$, $L_y = L_z = 25$, with periodic boundary conditions in the $x$–direction and no-slip planar degenerate walls in $y$ and $z$ with $W_1 = W_2 = 0.3$ (Eq. (2.15)). In this state, a periodic array of vortices form (Fig. 6.19). Previous studies have noted that coherent flows coexist with disclination lines that connect channel walls [240]. Here, we reveal that these lines have two types of topological patterns with distinctive dynamics. At the walls, pure $-1/2$ disclination lines are stationary ($\cos \beta = -1$; purple). Towards the channel centre, disclination lines smoothly connect $+1/2$ at the centre ($\cos \beta = +1$; yellow) and twist at the walls ($\cos \beta =$
Defect lines move along viscometric surfaces in the three-dimensional vortex lattice. 

a. Counter-rotating vortices are shown by velocity arrows and coloured by transverse vorticity component. 
b-d. Successive snapshots of $+1/2$ disclination segments traversing the edges of vorticity-dominated regions ($Q > 0$ in grey). White is where strain-rate dominates ($Q < 0$). Pure $-1/2$ defect lines are static near walls (purple). Defect lines are visualised same as Fig. 4.3 but with isosurfaces $s_{\text{cut}} = 0.1$.

Furthermore, positive winding disclination segments are self-motile (Fig. 6.19b-d).

In Fig. 6.19b-d, we visualise the disclination lines alongside $Q = 0$ contours (grey), which are isosurfaces in 3D, as opposed to the isolines they were in previous 2D cases. Importantly, we discover that the motile disclination segments are always pinned directly to these isosurfaces. In fact, the motion of the disclinations closely resemble the two-dimensional Ceilidh dynamics state. Disclinations traverse the boundaries of vortices and pass through a $Q = 0$ intersection to transfer to the next vortex. This reveals that the viscometric framework can be used to interpret the transport of disclination lines.
6.7.2 Multiple emulsion

We next return to the rotating charged loop that forms for the low activity double core multiple emulsions (§5.4.1).

The snapshot in Fig. 6.20 reveals that +1/2 profiles, once again coincide exactly with $Q = 0$. This is insightful, because it adds another piece of information to understanding the mechanism of the rotor-like motion. The defect loops are subject to three contraints: i) A topological charge constraint, which forms a +−+− disclination pattern. ii) Geometric constraints on the director. As a consequence of radial anchoring, the −1/2 profiles are pinned to the passive cores while +1/2 profiles are located away from radial surfaces. iii) A cross-field self constraint. The viscometric surfaces constrain +1/2 disclination profiles in their trajectories and their azimuthal orientations.

6.7.3 Bulk turbulence

The confined environment of the (low activity) active double emulsions form a topologically-imposed charged disclination loop. However, in bulk turbulence,
Figure 6.21  *Defect loops reside on viscometric surfaces in three-dimensional bulk active turbulence.*  

**a.** Snapshot of the disclination network in bulk active turbulence. The $Q$ criterion is shown on two horizontal slices. Purple is vorticity dominated ($Q > 0$) and grey is strain-rate dominated ($Q < 0$).  

**b.** Distances $d$ of points on the disclination line to the nearest $Q = 0$ surface are scaled by the active lengthscale $\ell_\zeta$. Distributions constructed for defect cells with twist angle $\cos \beta \in [0, 1]$ (green curve), $\cos \beta \in [-0.1, 0.1]$ (blue) and $\cos \beta \in [-1, -0.8]$ (purple).

Activity-induced charge neutral disclination loops can be system spanning and form complex configurations (§ 2.2.6.2). In Fig. 6.21, we present a snapshot of three-dimensional active nematic turbulence. Periodic boundary conditions are applied in a system $L_x = L_y = L_z = 80$ and activity $\zeta = 0.05$. The disclination loop patterns are coloured by $\cos \beta$, which demonstrate that the most dominant disclination profile is twist-type. Predominantly twist-type profiles are in agreement with previous studies of extensile active turbulence [24, 133, 134].

Because of the chaotic flows and larger system sizes, visualising $Q$ as isosurfaces can be challenging to interpret. For this reason, we construct two horizontal slices. On these planes, $Q > 0$ is shown in purple and $Q < 0$ as silver. The snapshot illustrates that disclinations intersect the viscometric surfaces, therefore indicating that the three-dimensional self-constraint holds in bulk active turbulence. By constructing the distances of the disclination profile to the nearest $Q = 0$ surface, the sharp decay of distances over a fraction of the active lengthscale can be observed. Interestingly here, the sharp decay is strongest for the $+1/2$ profiles, but also decays rapidly for the twist and $-1/2$ profiles. One possibility for this apparent constraint on $-1/2$ and twist could be because of the smooth connection between defect profiles on the same loop. However, future work is required to understand the three-dimensional self-constraint, and to confirm this.
6.7.4 Discussion

The last two sections revealed that the cross-field self-constraint between topological defects and flow structures holds more generally than just extensile 2D active nematic turbulence. In two-dimensions (§ 6.6), defects are found to reside on $Q = 0$ for other types of bulk active turbulence, including flow tumbling, and contractile activity. Simulations and experiments of channel-confined active nematics tame the chaotic nature of flow states into a periodic lattice of vortices. These ordered flow states illustrate the significance of defect subclasses. Defects are transported from one vortex to another via a $Q = 0$ intersection (mirror symmetric subclass); otherwise, defects simply travel along the edge of a single vortex (handed subclass). Finally, the self-constraint is found to hold in the case of isotropic and anisotropic friction. Strong isotropic friction enforces mirror-symmetric defects. This demonstrates the fact that strong friction screens the hydrodynamic instability and subsequently limits the formation of bend walls, which are necessary to form the handed subclass (§ 6.5). For anisotropic friction, an easy flow axis is created which guides mirror-symmetric defects along straight paths.

In three-dimensions (§ 6.7), $+1/2$ segments of disclination lines and loops reside on viscometric surfaces. This is found in channel-confined active nematics, where disclination lines with positive winding numbers trace $Q = 0$ surfaces, while weaving between counter-rotating vortices. The motion of $+1/2$ profiles is analogous to motile defects in two-dimensional channel confinement. The interdependence between $+1/2$ profiles and $Q = 0$ isosurfaces is further demonstrated in double core multiple emulsions at low activity (§ 5.5). A charged defect loop rotates with an axis fixed by $-1/2$ profiles and motion driven by $+1/2$ profiles. The $+1/2$ segments orbit a central vortex through contact with $Q = 0$. Bulk active turbulence also highlights the essential relationship between $+1/2$ disclination segments and $Q = 0$. The generality of the self-constraint in active nematic fluids suggests that examining defects alongside viscometric surfaces provides a valuable framework for understanding the complex relationship between topology and flow structures in two- and three-dimensions.
6.8 Conclusion

In conclusion, we have identified and explained a spontaneously arising constraint between defect dynamics and viscometric surfaces, where vorticity and strain-rate balance. Though previous studies noted that defects tend to be found near the edge of vortices [122], these results quantify this not as a tendency but as a fundamental spontaneous self-constraint between defects and coherent flow structures—not just in active turbulence but in any defect-laden active nematic system. This work challenges the idea that nematic defects are solely responsible for their own dynamics—ultimately, neither defects nor hydrodynamics alone govern the multi-field dynamics that spontaneously arise in active nematics; rather, they are intrinsically interdependent. Identifying this spontaneous self-constraint revealed that viewing solitary self-motile defects as generating pairs of mirror-symmetric vortices that stay at their sides (§ 2.2.6.1) must be contextualised as an idealisation that corresponds to a subset of plus-half defects over a limited duration rather than the expectation for all defects at all times. Instead, motile defects more often move along a single viscometric surface, where there is no stretching nor elongation of the fluid, a fact that appears to hold for all motile defects in active nematics and not only 2D extensile active turbulence. This shows that defects can be classified into subclasses based on local handedness with respect to their viscometric surface surroundings. Until now, this distinction, together with any difference in emerging dynamical behaviour, has been neglected. Not only do the hydrodynamics not force the plus-half defects off these contours, but they coincide with the very bend walls that these defects are unzipping—the field dynamics are codependent. These results underscore the continual role of bend wall constriction and unzipping in steady-state dynamics—active nematic defects cannot be viewed as points but are one component of mesoscale nematic structures, highlighting the centrality of mesoscale structure in collective dynamics, providing a mechanism to manipulate the degree of orderly dynamics in a system, potential new avenues for exploring topological entropy and an imperative fact for hydrodynamic descriptions of active defect gases (§ 2.2.6.1).
Chapter 7

Discussion
In this thesis, we explored how nematic topological defects self-organise under constraints. Specifically, we exploited topological charge conservation laws to induce stable defects and studied how defects constrain their dynamics through coupling to active flows. This section will summarise (§7.1) this work, and provide an outlook (§7.2) for avenues of research that can build on these results.

7.1 Summary

The first exploration of imposed topological constraints focussed on the topology and dynamics of nematic colloids embedded in a passive nematic liquid crystal. To study this system, we extended a nematic Multi-Particle Collision Dynamics algorithm (N-MPCD) to simulate colloids that are responsive to nematohydrodynamics fields. We demonstrated that these implementations successfully reproduce the defect structures and elastic interactions expected by literature. We utilised N-MPCD to study the coarsening dynamics of defect loops around pairs of colloids. We showed that disclinations pass through a variety of entangled disclination states en route to equilibrium. These states continue to shrink and undergo transitions that preferentially form two-loop states. In this process, we revealed a variety of non-ideal configurations which are permitted by the algorithm’s thermal stochasticity. Disclinations can transiently form localised $+\frac{1}{2}$ segments or settle into $-\frac{1}{2}$ tilted configurations. For all observed $-\frac{1}{2}$ disclinations, we characterised their topological properties using the self-linking number framework. This showed that single loop entanglements cancel the imposed topological charge by forming writhed configurations. On the other hand, two loop states are charged and have zero writhe. These results demonstrate that N-MPCD can cleanly resolve the topological properties of defects, even though the algorithm is noisy. Overall, this work contributes to, and highlights, N-MPCD as a versatile algorithm for studying topological phenomena and self-assembled dynamics.

The second study focussed on how imposed topological constraints couple with activity to form dynamical flow states. For this, we utilised an extensile active nematic multiple emulsion. A tunable number of passive isotropic droplets (cores) were placed inside a larger active nematic droplet, which altered the global topological charge. For a single core, a defect-free state emerged, while the addition of a second core induced a charged defect loop. As activity increased, we found that the defect-free state exhibited core dynamics that transitioned
from self-propelled, to chiral paths, and finally to chaotic trajectories. For
the charged defect loop, we showed that increasing activity drives disclination
dynamics that resemble a rotor, chiral rotor and chaotic oscillator. We revealed
that the controlled rotational dynamics emerge because of the topological patterns
of the charged loop. The double alternation of +1/2 and -1/2 profiles establish
distinct motility behaviours. Minus half profiles are pinned to the static cores
and fix the loop’s rotation axis. In contrast, plus half profiles power the
rotation by driving strong flows parallel to their local orientation. In the
high activity limit, we showed that disclinations can depart from circular rings
to form complex conformations which continuously undergo reconnection and
recombination dynamics. We demonstrated that topological charge constraints
govern the allowed loop configurations—with odd numbers of charged loops
and integer numbers of neutral loops observed. An interesting finding of this
study is that activity reveals topological patterns that have not formerly been
observed in passive nematic environments. We showed that these patterns vary
by transformations of the winding plane of the disclination rotation vector. This
work highlights how disclination profiles can be tuned through topology and
surface geometry, which can be harnessed to design active flow states and defect
morphologies.

In the final study, we discovered an activity-induced self-constraint on +1/2
defects. Analysing two-dimensional experimental and numerical data, we showed
that these defects are pinned to viscometric surfaces, which are isolines of simple
shear. Under this constraint, we found that +1/2 defects either align parallel to a
viscometric surface or can straddle an intersection of two isolines. We showed that
the handed case is the most likely configuration in extensile active turbulence,
despite expectations that +1/2 defects associate with mirror symmetric local
flows. We found that these subclasses are helpful for predicting defect dynamics.
Defects persistently travel along the single isoline, with a chiral trajectory that
matches the handedness of the enclosed vortex. Otherwise, defects at visometric
cross-sections tend to follow straight paths. This led us to explore why the handed
case emerges. Following an initial observation that defects form an interconnected
network with bend walls, we constructed a series of models to understand how
defects, bend walls and active flows couple. Our models uncovered that bend walls
generate viscometric surfaces along their backbone. These surfaces smoothly
connect with the isolines associated with +1/2 defects. Bend walls therefore
guide and shape the viscometric paths of +1/2 defects as they unzip these
walls. We further showed that if defects are attached to curved bend walls,
then mirror-symmetry broken flows are formed. Therefore, defect motion is not accurately represented by isolated quasi-particle models since their dynamics are interdependent on an extended network of strong bend deformation. An important finding of this work is that the self-constraint is found across active nematic systems. We demonstrated the generality in a variety of two-dimensional systems, such as with friction and in confinement. Finally, we presented evidence that the self-constraint holds in three-dimensions, observing that defect lines and loops reside on viscometric surfaces. Overall this research discovered a cross-talk between nematic topological structure and activity-induced flows. The results of this work may help to understand how orientationally ordered biological fluids self-constrain their own dynamics, or could provide insight on designing flow states through tuning one of the two coupled fields.

These chapters paint a collective view of how constraints shape self-organised dynamics. Primarily, topological defects must maintain charge conservation laws, but the manner in which this occurs is tuned by director features and geometric constraints. We showed two ways that defect loops satisfy their charge constraints are through their topological patterns or shapes. Further, disclination conformations, topological patterns, and local defect orientations are tuned by anchoring constraints and director geometric compatibility. This is how defects self-organise in a passive or near equilibrium setting.

In the presence of activity, these passive nematic constraints still hold but are complicated by the generation of collective flows. Literature has identified that defects generate active backflows which are dependent on the local disclination profile and orientation. We showed that profile-driven local flows are helpful for qualitatively understanding the dynamics of non-local disclination loop topologies. However, our results also contribute two additional viewpoints to active self-organisation. One of these is that defect profiles should not be treated as isolated points—structures of extended nematic deformation influence the flow structure that form around topological defects. Our other contribution is the discovery of a cross-field self-constraint. Therefore, self-organised dynamics can be understood through the combination of nematic topological, geometric, and activity-induced self-constraints.
7.2 Outlook

Our results have proposed that three constraints dominate the self-organised dynamics of topological defects in active nematic fluids. Here, we outline several avenues for future work that could directly follow from our findings.

We showed that homeotropic-anchored inclusions establish geometrical constraints that strongly favour $-1/2$ disclination profiles. In an active setting, we found that these constraints regulate disclination loop dynamics by forming a stable rotation axis. Therefore, using surface geometry to design topological patterns and motility features is an interesting topic to explore further.

An ideal numerical method for exploring this question is N-MPCD. This is because N-MPCD can be simply extended to active nematic fluids by introducing a dipolar activity contribution to the collision operator [153, 154]. Further, a particular strength of the algorithm is the ease of implementing complex environments. For instance, three-dimensional nematic fluids with many inclusions can be simulated. Our results suggest that colloidal clusters would form a multitude of $-1/2$ profile pinning sites. With activity, it would be interesting to explore if entangled defects with localised $+1/2$ profiles might mediate dynamical self-assembly. Another direction would be to modulate channel confinement to imprint curvature on the director [170, 209, 241]. Geometries with curvature are expected to enforce constraints on $-1/2$ and $+1/2$ profiles [242]. Therefore, studies such as these would be valuable in understanding geometric constraints, and could inform the design of three-dimensional micro-devices powered by motile defect lines and loops.

Another direction for future work is to explore the three-dimensional self-constraint in more depth. The discovery of the cross-field constraint focussed on two-dimensions, where the dynamics of $+1/2$ point defects are interdependent on line-like structures in the director (bend walls) and flow field (isolines of zero $Q$). Our preliminary analysis in three-dimensions found that defect line/loop $+1/2$ profiles are constrained to two-dimensional surfaces of zero $Q$. However, there are several complexities that are unique to three-dimensions that require attention to understand the mechanisms of the constraint.

One such question is how nematic topological defects interrelate with the three invariants of the velocity gradient tensor, which classify the topology of three-
dimensional flow patterns [184]. These are the trace, $Q$, and the determinant. It would be valuable to establish whether the determinant imposes any constraints on nematic structure, or if the self-constraint is altered in compressible flows where the trace is non-zero.

In addition to flow structures, insight may be gained by establishing the nature of extended mesoscale deformation structures that are formed by the three-dimensional hydrodynamic instability. An exploration of these continuous nematic structures (i.e. not topological defects) has not yet been carried out. However, the unstable modes are bend and twist for extensile active nematics [230, 243]. Consequently, we might expect emergent nematic structures, such as spontaneous helicity. To reveal the existence of such structures, additional scalar parameters are needed to capture twist-type order since the splay-bend parameter only captures nematic deformation with a polarity. By employing these tools, one could study cross-field constraints by connecting the formation and evolution of mesoscale deformations in terms of velocity gradient invariants.

With a broader understanding of the three-dimensional self-constraint, new perspectives could be obtained on the dynamics of defect lines and loops. For instance, we discovered that the creation sites of $\pm 1/2$ defect pairs occur where viscometric intersection meet a bend wall in two-dimensions. In three-dimensions, an analogous mechanism might underpin the creation sites of disclination loops. Understanding the complex dynamics of defect loops, including splitting and recombination, could involve analysing defect profiles as they traverse zero $Q$ isosurfaces.

This work has centred on understanding the physics of the constraints that connect topology and self-organised dynamics. Given the prevalence of topological defects in biological systems—such as microbial communities, cell monolayers, and morphogenesis—it would be valuable to investigate the nature of these constraints in living settings.
Bibliography


type of active polar gels: a paradigm for cytoskeletal dynamics. *EPJE*,


[97] John Toner and Yuhai Tu. Long-range order in a two-dimensional

[98] Hugues Chaté, Francesco Ginelli, and Raúl Montagne. Simple model for

[99] Fernando Peruani, Andreas Deutsch, and Markus Bär. Nonequilibrium

[100] H. Gruler, U. Dewald, and M. Eberhardt. Nematic liquid crystals formed

[101] O. J. Meacock, A. Doostmohammadi, K. R. Foster, J. M. Yeomans, and
W. M. Durham. Bacteria solve the problem of crowding by moving slowly.

[102] Yonit Maroudas-Sacks, Liora Garion, Lital Shani-Zerbib, Anton Livshits,
Erez Braun, and Kinneret Keren. Topological defects in the nematic order

[103] Thuan Beng Saw, Amin Doostmohammadi, Vincent Nier, Leyla Kocegozlu,
Sumesh Thampi, Yusuke Toyama, Philippe Marcq, Chwee Teck Lim,
Julia M. Yeomans, and Benoit Ladoux. Topological defects in epithelia


[105] Todd Thoresen, Martin Lenz, and Margaret L. Gardel. Reconstitution of

[106] H Hess and Jennifer L Ross. Non-equilibrium assembly of microtubules:


