Chapter 5

Diffusive scaling and defect morphology in the spinodal kinetics of nematics

This chapter discusses topological defects in uniaxial and biaxial nematic liquid crystals in two and three dimensions. We suggest a novel way to identify and visualize such defects, which relies on the non-trivial variation of the amplitude of the order parameter at the defect core with respect to its bulk value. Our visualization methods provide insights into the intercommutation of defects in uniaxial and biaxial systems. We also resolve a controversy concerning the growth exponent in coarsening nematics, using large-scale simulations to access the asymptotic scaling regime.

We begin with a discussion of defect classes predicted by homotopy theory. We discuss the phase ordering of uniaxial nematics in two dimensions, describing how the visualization technique developed and discussed in Chapter 3 can be applied to locate defects in a far more transparent way than currently popular methodologies. We then discuss dynamical scaling laws and growth exponents at different stages of the kinetics. We discuss the core structure of point defects in the uniaxial phase. We describe how string defects in three dimensions may be visualized. We observe defect intercommutation events in our simulations of the coarsening uniaxial nematic. Our visualization methods enable us to describe in some detail the variation of the order parameter structure across such intercommutation events, including the variation of uniaxial and biaxial order parameters across the overlap region. We conclude our study of uniaxial nematics with a discussion of the effects of thermal fluctuations.

We then repeat these studies in the case of phase ordering in biaxial nematic phases. In contrast to predictions of defect entanglement from a group theoretical analysis, we see no such entanglement in our simulations. We discuss the structure of the core in two classes of stable defects in biaxial systems. Finally, we settle an old controversy concerning the observation of non-universal exponents in spinodal decomposition in biaxial nematics, observing that these observations are as a consequence of a long crossover to ultimately diffusive i.e. $L(t) \sim t^{1/2}$ behavior.
5.1 Introduction

Nematic systems, as a consequence of a broken continuous symmetry, exhibit fascinating topological defects and complex defect interactions [24]. Their study constitutes a challenging ground for theories, whether of phase ordering kinetics [12, 77], of homotopy theory [49] or the Kibble mechanism in cosmology [37, 21].

A brief summary of prior work on phase ordering in uniaxial and biaxial systems is the following: Zapotocky, Goldbart and Goldenfeld studied the coarsening of both uniaxial and biaxial systems in two dimensions (the order parameter space is three-dimensional whereas the spatial dimension is two-dimensional), using a cell-dynamical scheme (CDS) [77]. They found that, for uniaxial nematics: (a) the growing correlation length characterizing the sizes of domains increases as a power law in time with \( L(t) \sim t^{\phi_{\text{cor}}} \), with \( \phi_{\text{cor}} \simeq 0.40 \). In contrast, (b) the length scale characterizing the separation of topological defects increases with time as \( L_{\text{def}}(t) \sim t^{\phi_{\text{def}}} \), with \( \phi_{\text{def}} \simeq 0.374 \). The discrepancy between these growing length scales was interpreted as a break-down of dynamical scaling. Also, (c) these exponents, in addition to the exponent describing the decay of the energy density are very different from 0.5, the value predicted by naive scaling. For biaxial nematic systems, these authors find an exponent \( \phi_{\text{cor}} \simeq 0.39 \), as well as a discrepancy between the scaling exponents for growth as well as for the defect separation, suggesting that dynamical scaling may break down here as well.

Bray, Puri, Blundell and Somoza study spinodal decomposition in quenched uniaxial nematics, finding a growth exponent \( \phi_{\text{cor}} \simeq 0.45 \) and a good fit to \( S(k) \) at large \( k \) of \( S(k) \sim 1/k^5 \), i.e. indicating a Porod exponent of 5 [14]. These authors also comment on the discrepancy between the 0.45 they obtain in numerics and the expected 0.5, noting that they cannot say whether this indicates a real discrepancy or whether the data are not yet in the right asymptotic regime. These authors use a methodology in which, as in the CDS simulations, amplitude fluctuations are ignored.

Priezjev and Pelcovits have studied the dynamics of two and three-dimensional biaxial nematic crystals using a Langevin dynamics for the orientation of the frame constituted by the eigenvectors of the order parameter tensor, in an effort to understand the effects of the complex defect structures in these systems [58]. Again, these simulations assume that amplitude order is saturated. Previous work by Kobdaj and Thomas provided a justification for the observation of Zapotocky et al. of the dominance of only two types of topological defects (both corresponding to half-integer charge) at late times, by showing that, within the one-constant approximation, one class of half-integer defects is always unstable to the other class [39]. Priezjev and Pelcovits point out that the relative values of the elastic constants, beyond the one-constant approximation, can yield rich coarsening behaviour, including the formation of junction points where defect lines meet. Priezjev and Pelcovits observe no line crossings or entanglements in their coarsening sequences.

Analytically, calculations of defect structure and properties in biaxial nematics are complex because of the underlying tensorial form of the order parameter and a sixth order nonlinear term in the free energy functional. The order parameter dynamics is governed through a set of coupled nonlinear PDE characterizing the five independent components of the tensor [10]. Numerically, finding defect-antidefect pairs is hard although not impossible,
although complicated algorithms must be used to visualize tensorial data through the extensively used techniques of Müller and Westin metrics [8, 15]. On the other hand, lattice algorithms are computationally expensive because topological circuits must be constructed at each node of the lattice and the angular variation in the director and co-director performed along these circuits to identify and classify the defects. Such algorithms for tracking defects from all different classes arising in a bulk nematic system have been reported [77, 69]. An operator method for counting defect line segments is also reported [40].

Topological defects represent a non-continuity of the order parameter along regions of reduced dimensionality. At such defects, the direction of ordering is ill-defined. Such defects can be points in two dimensions and lines in three dimensions. A topologically stable defect cannot be eliminated through a continuous transformation of the order parameter. A defect is assigned an invariant quantity, the topological charge. The classification of defects lie in the map of the order parameter from physical space to a geometrical space \( R \) and defining the homotopy group \( \pi_i(R) \) where \( i = d_{sp} - d_{def} - 1; d_{sp}, d_{def} \) are the physical and the defect dimension of the problem.

The uniaxial nematic order parameter is invariant under a local transformation \( n \to -n \). Thus, the order parameter space is a sphere with antipodal points identified, termed as \( S^2/\mathbb{Z}_2 \) \(^1\) or more generically the projective plane \( \mathbb{RP}_2 \). In \( \mathcal{R} \), the circular contours, which can be contracted to a point, correspond to the topologically unstable disclinations of integer strength, as this can be eliminated from the system by making the director escape in the third dimension, as in the case of an uniaxial nematic phase. The contours terminating at the antipodal points correspond to the stable class of half integer charge defects. As the contours corresponding to \(+1/2\) defects can be continuously transformed to that of \(-1/2\) defects, there is only one topologically stable class of defect. The order parameter space is identified as the first homotopy group \( \pi_1(\mathbb{RP}_2) \) which is the two element group \( \mathbb{Z}_2 \). The conservation laws of topological charge are \( 1/2 + 0 = 1/2 \) and \( 1/2 + 1/2 = 0 \) respectively.

The biaxial nematic order parameter is invariant under a local transformation of the triad \( n \equiv -n, l \equiv -l \) and \( m \equiv -m \). The order parameter space is the group of full rotations of the triad with the antipodal points identified, termed as \( S^3/D_2^2 \) \(^2\) or more generically the projective plane \( \mathbb{RP}^3 \). The first homotopy group of the order parameter is identified as the non-Abelian eight-element group under multiplication of quaternions \( \mathbb{Q} \), whose elements are represented with \( \{I, -I, \sigma, -\sigma\} \) where \( I \) and \( \sigma \) denote the identity and Pauli matrices. The elements of the group form five conjugacy classes, \( C_{0} = \{I\}, C_{0} = \{-I\}, C_{x} = \{i\sigma_{x}, -i\sigma_{x}\}, C_{y} = \{i\sigma_{y}, -i\sigma_{y}\} \) and \( C_{z} = \{i\sigma_{z}, -i\sigma_{z}\} \) respectively.

There are a total of five stable class of defects corresponding to these conjugacy classes. \( C_{x}, C_{y} \) and \( C_{z} \) class correspond to a \( \pi \) rotation of the director about the defect core representing to a half integer charge defect whereas \( C_{0} \) correspond to \( 2\pi \) rotation so as a stable integer charge defect, which cannot be removed by a continuous transformation unlike the uniaxial nematic phase. The topologically unstable (or trivial) class correspond to a \( 4\pi \)

\(^1\)Sphere \( S^2 = SO(3)/SO(2) \) is the factorization of \( SO(3) \) with \( SO(2) \). \( S^2 \) is again factored out with \( \mathbb{Z}_2 \), which consist of two elements 0 and 1.

\(^2\)\( S^3 \) is the three dimensional sphere in four dimensions. It is factored by the four element Dihedral group \( D_2 \).
rotation of the director. The pairing and breaking of defects depend on the multiplication rule specific to a particular conjugacy class and also on the energetics. Multiplication to the same class yields either a trivial class $C_0$ or $\bar{C}_0$, but this joining-up strongly depends on the path of joining with other defects from other classes, because of the non-Abelian nature of the group $Q$ [49].

We suggest a simple algorithm to locate all classes of defects, thus simplifying such calculations considerably. We propose that the calculation of the uniaxial and biaxial degree of alignment $S(x, t)$ and $T(x, t)$ suffices to locate the defect pair from all the classes. At the core of the defect, these scalar quantities differ from their equilibrium values in the uniform state. The topological charges are found from Schlieren textures, which represent the intensity of the transmitted light through a nematic film sandwiched between crossed polarizers. As the isotropic phase coarsens into the nematic phase, both integer and half integer charged defects are found at an early stage of the dynamics, whereas at the late stage only half integer charges are stable. These defect-antidefect pairs coalesce and disappear from the system, resulting in an equilibrium defect-free nematic phase [77, 20]. Our defect finding technique clearly locates the stream-tubes in three dimensions following a quench into the nematic phase.

Such a methodology cannot be implemented in approaches where order parameter amplitudes are assumed to be a priori saturated, as in the frame-based methods of Priezjev and Pelcovits. In contrast to the CDS methods, which replace the equations of motion by an equivalent discrete map, the full equations of motion are solved here, permitting access to the detailed structure of the core in both uniaxial and biaxial nematics.

The first two sections of this chapter are devoted to the description of the phase ordering

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**Table 5.1:** Numerical parameters in the Landau-de Gennes theory used for the computer experiments in spinodal kinetics presented in this chapter.

<table>
<thead>
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<th>Figure</th>
<th>$A$</th>
<th>$B$</th>
<th>$C$</th>
<th>$E'$</th>
<th>$L_1$</th>
<th>$\kappa$</th>
<th>$\Gamma$</th>
<th>$k_B T$</th>
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<td>0</td>
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<td>0</td>
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<td>1/10</td>
<td>10$^{-4}$</td>
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<td>128$^3$</td>
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</table>
5.1. Introduction

Figure 5.1: Uniaxial degree of alignment $S$ and the nematic director field $n$ on top of that and the corresponding Schlieren textures in a coarsening nematic from the isotropic phase. Topological defects of integer and half-integer charge are clearly observed, as seen in the coloured frames of $S$ in (a)-(c) and the textures in (d)-(f). (a) Shows the formation of defects with coalesce of domains after quench from a random configuration. (c) and (f) show the defects at an early and late stage of the dynamics. The integration is performed over $6 \times 10^4$ MOL steps with unit step length.
5.2 Phase ordering in uniaxial nematics

5.2.1 Point defects: core structure and dynamics

For a quench below the spinodal temperature, the isotropic phase becomes locally unstable to a nematic perturbation and the system proceeds spontaneously to the nematic phase through spinodal kinetics. Coherent regions of local nematic order develop in time, with a distinct axis of order in each of these domains. Topological defects form at the intersections of these differently ordered domains. Coarsening proceeds through the annihilation of topological defects, increasing the correlation length of local orientational order. In two dimensions\(^3\), the defects are points while line defects appear in three dimensions.

To study coarsening kinetics, we start from a random initial configuration where we draw the order parameters $S$ and $T$ randomly from a normal distribution with zero mean and variance proportional to $F_c$, ensuring the condition, $0 < T < S$. We obtain $\cos \theta$ from an uniform distribution between -1 and 1, and choose $\phi$ similarly between 0 and $2\pi$ to gen-

\(^3\)In a 2D nematic film, the space variations are only in 2 Cartesian directions, while the spin dimension is retained to 3 i.e. all of the Cartesian directions accessible by the director to orient.
5.2. Phase ordering in uniaxial nematics

Figure 5.3: Data collapse of the direct correlation function \( C(r) \) with scaled distance \( r/L(t) \) for different times. The symbol \( \Delta \) depicts the Bray-Puri function \([13]\) for the O(2) vector model:
\[
f_{BP}(x) = B^2(0.5, 1.5) F[0.5, 0.5, 2; \exp(-x^2)] \exp(-x^2/2)/\pi.\]
The inset shows the unscaled correlation function at different times.

The director and codirector. The joint normal is obtained through the Gram-Schmidt orthogonalization technique. We then relax the system from this initial isotropic state at a temperature below the supercooling spinodal temperature. The data presented below is averaged over \(10^2\) different initial conditions for a \(256^2\) system with periodic boundary conditions. From the coarsening simulations we obtain the strength of uniaxial and biaxial order \( S \) and \( T \), and the director \( n \). Fig.[5.1(a-c)] shows \( S \) in false colours with \( n \) embedded on top of that. The director is used to construct the schlieren plots shown in Fig.[5.1(d-f)]. These plots are constructed by first projecting the director into the \( x-y \) plane, finding the angle \( \chi \) made by this projection with an arbitrary axis (say \( x \)-axis) and then computing \( \sin^2(2\chi) \). The presence of both integer and half-integer defects is clearly visible in these plots as the meeting points of four and two dark brushes, respectively. In the corresponding plots for the strength of ordering, the defects are clearly visible as localized regions where \( S \) rapidly decreases. This is the core region of the topological defect, shown in Fig.(5.2). We confirm the surprising finding that there is strong biaxial ordering inside the defect core \([63]\). These results are in perfect qualitative agreement with both theoretical predictions and previous numerical results \([63]\).

5.2.2 Dynamical scaling in two dimensions

To make a quantitative comparison with previous work, we compare results for the time-development of correlation functions during coarsening. Theoretical predictions and analytical work have verified that the correlation functions defined in Eq.(2.9-2.10) have a scaling
Figure 5.4: Data collapse of the structure function $S(k, t)$ at different times. The dash-dot line has a slope of $-4$ indicating the validity of generalized Porod’s law for $O(n)$ vector systems, with $n = d = 2$. The departure from Porod’s law at high $k$ is due to amplitude variation across the finite core size of the defects as discussed in the text. The inset shows the time dependence of the correlation length $L(t)$. The length grows as a power law with an exponent of 0.5. The maximum value of the correlation length is approximately $1/4$-th the system size, ensuring the absence of finite-size artefacts.

form $C(r, t) = F[r/L(t)]$, and $S(k, t) = L^d(t)G[kL(t)]$ [12]. Here, $C(r, t) = \sum_{|r|=r} C(r, t)$ and $S(k, t) = \sum_{|k|=k} S(k, t)$ are angular averages of the correlation functions in real and Fourier space respectively. The length $L(t)$ is extracted from the real-space correlation function using the implicit condition $C(r = L(t), t) = 1/2$. In Fig.(5.3) we confirm that the real-space correlation function does indeed scale as expected.

Our numerical data for the scaling function are in close agreement with an analytical calculation for a two-component vector model due to Bray and Puri [13], although the symmetry of this model is not the same as the tensorial symmetry of the nematic problem. A similar comparison has been made in [26]. In Fig.(5.4) we show the corresponding scaling of the Fourier space correlation function. The wavenumber $\langle k \rangle$ is the root of the second moment of the $S(k, t)$ defined by

$$\langle k \rangle^2 = L(t)^{-2} = \frac{\sum_k k^2 S(k, t)}{\sum_k S(k, t)}.$$  \hspace{1cm} (5.1)

The inset of Fig.(5.4) shows the growth of the length scale as a function of time. Theoretically, this is expected to grow as a power $L(t) \sim t^\alpha$. Our estimate for this exponent is $\alpha = 0.5 \pm 0.005$. Our results are consistent with both analytical predictions and an earlier numerical simulation. The Fourier space correlation function is expected to exhibit a short-wavelength scaling $S(k, t) \sim k^{-4}$, known as a generalized Porod law [12]. We see a clear range of
5.2. Phase ordering in uniaxial nematics

Figure 5.5: Time evolution of uniaxial degree of alignment [frames 5.5(a)-5.5(d)] in a coarsening 3D uniaxial nematic, plotted at an isosurface value 0.054 and volume rendered in false colours.
wavenumbers where Porod scaling is obtained. At very short wavelengths, corresponding to the size of the defect core where order parameter amplitude variations are important, such Porod scaling should breaks down. We see evidence for this as well, where the very highest wavenumbers in Fig.\((5.4)\) corresponding to the size less than the size of a defect core show deviations from the Porod scaling. Our numerical results for spinodal decomposition, then, agree both qualitatively and quantitatively with theoretical results and previous numerical work \[25]\.

5.2.3 Intercommutation, loop formation of line defects in three dimensions

Defects in two dimension are points, while they can be linear in one higher dimension. A uniaxial nematic phase in two dimensions coarsens through successive production and annihilation of point defect-antidefect pairs. In three dimensions, a coarsening nematic proceeds through the initial creation of line defect-antidefect pairs. The pair annihilates by inter-commutation of the line segments to form a closed loop. Different loops pass through each other to form distinct loops which finally contract and eventually disappear from the system in the late stage of the kinetics.

Fig.\((5.5)\) shows the corresponding uniaxial scalar field \(S\) at successive time steps after a uniaxial nematic quench from isotropic phase. An inter-commutation of line disclination is clearly noticeable, which can be seen in the south-west corner of the first three frames \[5.5(a)-5.5(c)\]. Last frame \[5.5(d)\] shows a loop formed at a late stage of the phase ordering kinetics where only a few defects exist. Superimposed with the scalar field \(S\), change of the director field conformation on the surface of the stream tubes of \(S\) is shown in Fig.\([5.6(a)-5.6(c)]\) while an inter-commutation event of defect line segments take place.

In Fig.\((5.7)\), we show the data collapse of the structure function as well as the uncollapsed data in the inset. However, accurate estimations of the growth exponent have not been carried out due to lack of sufficient data for statistical averages to be meaningful.
5.3 Fluctuating defect kinetics

The dynamics of defects is greatly influenced by the presence of fluctuating thermal forces. To illustrate the role of fluctuations, we calculate the time evolution of the number density of defects. This is achieved through calculating the number of field values below a certain threshold value at a particular instant of time. For our numerics we set this value to be half the value of the maximum attainable value of the field for each and every instant in time.

We calculate the total number of defects at a particular time defined as

\[ N_d(t) = \int \rho(x, t) dx \]  \hspace{1cm} (5.2)

where, \( \rho(x, t) = \sum_i q_i \delta^d(x - x_i) \) is the defect density, \( q^i \) is the winding number of the topological defect at the \( i^{th} \) space point.

Fig.(5.8) shows the variation of the defect density with time in the presence and absence of fluctuation. The initial slope in both the cases correspond to the early time diffusive scaling regime while the degree of uniaxiality saturates to their equilibrium values. In the presence of thermal fluctuation, the diffusive scaling regime is reduced in comparison to the non-fluctuating case. The fact that the slopes are equal in both cases suggests that the fluctuating force does not play any significant role in generating defect pairs, apart from speeding up the defect kinetics considerably. At the late stage of the dynamics, while a few defects diffuse in the saturated uniaxial nematic medium, the defect-anti defect pair annihilation process becomes faster than the zero temperature case, as shown in the inset of Fig.(5.8).
Figure 5.8: Effect of thermal fluctuations on the density of point defects with time is plotted. On a 256² lattice, time is iterated upto $5 \times 10^4$ steps with unit step length and averaged over 20 different initial configurations for both the cases with and without thermal fluctuation.

### 5.4 Phase ordering in biaxial nematics

#### 5.4.1 Point defects: core structure and dynamics

Our study of the biaxial nematic incorporates the space variation of the triad $\mathbf{n}$, $\mathbf{l}$ and $\mathbf{m}$ as well of the amplitude degrees of freedom $S$ and $T$, unlike previous work [77]. As the system equilibrates after the biaxial quench, the magnitude of the order parameter converges to its equilibrium value.

Defects of all homotopy classes can be found after the extraction of the uniaxial and biaxial scalar order from the $\mathbf{Q}$ tensor. The homotopy classes are classified through the variation of the director configuration around the defect, by construction of topological circuits capturing the local minima. $C_x$ ($\mathbf{n}$ rotates by $\pm \pi$, $\mathbf{l}$ does not rotate) and $C_y$ ($\mathbf{n}$ does not rotate but $\mathbf{l}$ rotates by $\pm \pi$) class of defects are found, whereas no stable $C_z$ (both $\mathbf{n}$ and $\mathbf{l}$ rotate by $\pm \pi$) class of defects are seen, consistent with the earlier analytical prediction [39] and numerical result [77].

Fig.(5.9) shows the uniaxial and biaxial order and the Schlieren textures at the indicated time steps after a biaxial nematic quench from an initial isotropic phase. In the Schlieren texture, both integer defects {four brushes at slightly north from the center of the frame [5.9(h)]} and half integer defects {two brushes in all of the three frames [5.9(g)-5.9(i)]} are seen at the early stage of the dynamics. Only half integer defects are present at the late stages of the dynamics, as indicated by two brushes in the texture frame [5.9(i)]. Although different class of defects are found in the texture, interestingly, signatures of all defect locations arising in the phase cannot be tracked only through the texture study, although they can be clearly
Figure 5.9: Panel [(a)-(c)] shows the time evolution of the uniaxial degree of alignment, [(d)-(f)] the biaxial degree of alignment and [(g)-(i)] the Schlieren texture in a coarsening biaxial nematic.
located in the uniaxial and biaxial scalar order. This also signifies those classes of defects where the deformation is solely embedded in the scalar order $S$ and $T$ and not in the vectorial order $n$. We also note that the integer defects are purely due to deformation in the vector order $n$ and no signature of deformation of $S$ or $T$ is noticeable in the field plots in Fig.5.9(a)-(f) at the place of texture with four brushes. Thus, our defect finding scheme, reported for the first time, is successful in locating all of the half-integer defect locations belonging to different classes, which cannot be tracked only from the study of Schlieren textures based on $n$.

Fig.5.10 shows the variation of $S$ and $T$ along the biaxial defect core located with our mentioned algorithm. In the $C_x$ class of defects, though both uniaxial and biaxial order are reduced from their equilibrium values, biaxial order drops more significantly than the uniaxial order. In the $C_y$ class of defects, while uniaxial order drops significantly from the equilibrium value inside the core, the biaxial order peaks. Thus the defect cores of the latter class behaves qualitatively like a half-integer defect-core in a uniaxial nematic.

5.4.2 Dynamical scaling in two dimensions: separation of time scale

To make a quantitative analysis of the dynamics of defects discussed in the previous subsection, we calculate the dynamical scaling exponent. In Fig.5.11 we confirm the scaling of the direct correlation function and the structure function for a long period of time.

The length $L(t)$ is extracted from the real-space correlation function using the implicit condition $C(r = L(t), t) = 1/2$ as in the case of uniaxial quench discussed in the previous
5.4. Phase ordering in biaxial nematics

Figure 5.11: (a) Data collapse of the direct correlation function $C(r, t)$ with the scaled distance $r/L(t)$ for different times. The inset depicts the unscaled correlator at different times. (b) Data collapse of the structure factor $S(k, t)$ with the scaled Fourier modes at different times. The depicted straight line with a slope of $-4$ indicates to the validity of generalized Porod’s law for $O(n)$ vector model systems, with $n = d = 2$. The inset shows the unscaled correlator at different times.

Figure 5.12: Growth of length scale with time in a biaxial quench. The time integration is done upto $5 \times 10^4$ steps with unit step length.
Fig. 5.12 shows the growth of the length scale as a function of time at different stages of the phase ordering kinetics. Theoretically, the length scales with time as $L(t) \sim t^\alpha$. At an early stage of the kinetics, the dynamics shows a diffusive exponent with $\alpha = 0.49$. The diffusive nature of the dynamics at an early stage is attributed to the fact that the scalar order $S$ and $T$ reach equilibrium fast in comparison to the director $n$ variable. The defect cores are not well-defined in this period of time.

In the later part of the dynamics, we observe a decrease of the exponent, with exponent values ranging from 0.32 to 0.39, finally regaining the diffusive exponent 0.5. In this intermediate regime of exponents, defect-defect kinetics proceeds via the annihilation of defect-antidefect pair of respective class. At still later stages of the kinetics, a small number of pairs of defects diffuse in the bulk nematic, and a diffusive scaling exponent is obtained.

In Fig. 5.15, we show the data collapse of the structure function as well as the uncollapsed data in the inset. We have, however, been unable to settle the question of the growth exponent conclusively.

### 5.4.3 Visualization of line defects commutation in three dimensions

Fig. 5.13 shows the corresponding uniaxial scalar field $S$ at successive time steps after a biaxial nematic quench from isotropic phase. The inter-commutation of the line disclination is clearly noticeable, as seen in the south corner of the three frames [5.13(b)-5.13(d)]. The pair of lines corresponding to the defect-antidefect pair form a particular class which annihilates by forming a closed loop. Different loops pass through each other to form distinct loops which finally contracts and disappear from the system in the late stage of the kinetics. Superimposed with the scalar field $S$, change of the director field conformation on the stream tube of $S$ is shown in Fig. 5.14 while an inter-commutation of defect line segments takes place.

As proposed from the topological restrictions on biaxial nematic defect classes forming the non-abelian group of quaternions, the inter-commutation of some classes of defect lines is forbidden because of the non-commutativity of the group elements. In our numerics, we do not observe any entanglement events. A plausible reason for the absence could be a local melting of the scalar order parameters while biaxial defect lines locally interact. Topological reasoning indicates that the merging of two defects depends strongly on the path which may or may not accompany the criterion of entanglement. Energetically a $C_0$ defect lies higher in energy landscape than other $C_i$, $(i = x, y, z)$ class of defects. So a $C_0$ defect dissociates into low energetic stable class of defect at late stages prohibiting two $\pi$ defects entangle through a $2\pi$ “umbilical” cord, as been analytically predicted by Kobdaj and Thomas in two dimensions [39]. (The generalization of these results to three dimensions is natural.) The only possible ways of defect entanglement is found in the experimental and theoretical studies of: i) cholesterics or chiral nematics that exhibits of a defect-locked blue phase [48], ii) chiral nematic colloids [68], iii) nontrivial boundary driven nematogenic systems etc. The absence of chirality in our studied system can also be another plausible reason for the absence of defect entanglement.

In Fig. 5.15, we show the data collapse of the structure function as well as the uncol-
5.4. Phase ordering in biaxial nematics

Figure 5.13: Time evolution of uniaxial degree of alignment [Frames 5.13(a)–5.13(d)] in a coarsening 3D biaxial nematic, plotted at an isosurface value 0.5 and volume rendered in false colours.
Figure 5.14: Time evolution of uniaxial degree of alignment in a coarsening 3D biaxial nematic. Frames [5.14(a)-5.14(c)] show zoom of the intercommutation with the director field conformation around the disclination.

Figure 5.15: Data collapse of the structure function $S(k, t)$ with scaled Fourier modes for different times. The inset shows the unscaled correlator at different times.
lapsed data in the inset. However, accurate estimations of the growth exponent have not been carried out due to lack of sufficient data for the statistical averages to be meaningful.

5.5 Conclusion

In this chapter, we have described point and line defects of different homotopy classes which arise in our numerics. We discussed phase ordering kinetics in uniaxial nematic phases, validating the theory by locating integer and half integer defects corresponding to $\pi_i(R)$.

We demonstrate that the late-stage growth exponent in two-dimensional uniaxial nematics is 0.5, confirming scaling expectations. For uniaxial and biaxial nematics in three dimensions, we show the existence of an asymptotic 0.5 growth exponent. This asymptotic behaviour, however, is obtained only after a long crossover regime in which the data can be fit to numbers between 0.32 - 0.39, suggesting that the data of Zapotocky et al. and of other previous workers may have been confined to this crossover regime. We numerically observe defects in biaxial phase ordering but find no evidence for entanglement of defects, as posited by the topological theory of defects. However, we see clear indication for intercommutation of string defects in three dimensions and our novel visualization techniques enable us to track the detailed variation of the order parameter structure through such intercommutation events. These observation suggest that similar methodologies may find powerful application in the study of defect kinetics in these and similar systems with complex defects.