

Spectral Alignment of Mesogens for Three-Dimensional Disclination Localization in Liquid Crystals

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Abstract

Topological defects govern the material properties and dynamics of liquid crystals. Efficiently identifying three-dimensional disclination centerlines from mesogen-resolved datasets remains a fundamental challenge. Traditional diagnostics rely on thresholding local scalar order parameters, which struggle to differentiate between one-dimensional topological defect lines and the three-dimensional volumes within which disorder is present. Herein, we present Spectral Alignment of Mesogens (SPAM) and Discrete Layer Analysis (DLA), a deterministic framework that extracts disclination centerlines directly from unoriented mesogen-scale director fields. This approach casts sign assignment as a continuous spectral relaxation of an Ising-like spin optimization on a distance-weighted interaction graph. We validate this approach on a wide range of molecular-dynamics simulations of calamitic liquid-crystalline assemblies, showing a range of benefits as compared to existing techniques. Together, SPAM and DLA provide a robust framework for three-dimensional topological defect extraction relevant to

a wide range of liquid-crystalline media, including passive nematics, active fluids, and nematic elastomers.

Introduction

In nematic liquid crystals, macroscopic response is heavily influenced by mesoscale orientational order. This coupling between orientational structure and material response underlies applications ranging from liquid-crystal microtechnology and active fluids to nematic elastomers and flow-driven liquid-crystalline materials.^{1–4} Continuum theories represent this order through fields such as the Q -tensor,^{5–7} whose eigenstructure encodes both the magnitude and symmetry of local alignment. Classical elastic theories describe smooth distortions of the director (or Q -tensor) field.^{8,9} Many of the most important structures in nematic materials arise from topological incompatibilities of the order-parameter space.^{10–12} These topological defects include both point and line defects; the present work focuses on disclinations, the line-like defects of three-dimensional nematic assemblies.

The director field is a line field rather than an ordinary vector field. At each point, the orientations $\hat{n}$ and $-\hat{n}$ are physically equivalent (Figure 1i); this head–tail symmetry is central to the topology of nematic defects. A disclination is therefore not identified solely by a local reduction in orientational order. It is characterized by the obstruction to assigning a globally continuous vector representative of the director field throughout a domain enclosing the defect. Equivalently, transporting a chosen director orientation continuously around a closed circuit encircling a half-integer disclination returns the vector representative with reversed sign at the end of the operation (Figure 1ii). Classical loop-based constructions and homotopy arguments make this obstruction precise.^{13,14} The operational challenge in molecular data is to detect this *orientability obstruction* from a finite, noisy, and irregularly sampled set of mesogens.

Local disorder diagnostics provide a common and physically interpretable route for iden-

tifying defect-associated regions in molecular and mesoscopic data. Scalar-order-parameter fields, Q -tensor eigenvalue measures, and related disclination-density constructions identify regions where local orientational alignment is degraded.^{15–19} These methods are valuable near defect cores, where local order is typically reduced. However, the measured object is a finite-width region of reduced alignment, not the one-dimensional centerline of the topological defect. Its apparent location, connectivity, and thickness depend on the coarse-graining length scale, neighborhood definition, and threshold used to define the defect region. In assemblies containing multiple defects, broadened low-order regions can overlap or merge, obscuring the line geometry that one ultimately wants to measure.

This manuscript develops a complementary viewpoint. Rather than beginning with a local disorder threshold, we begin with the global sign-assignment problem created by nematic line-field symmetry. The objective is to assign a sign $s_i \in \{-1, +1\}$ to every mesogen of a given director field with an arbitrary assignment of vector orientations $\hat{n}_i$ so that neighboring oriented vectors $s_i\hat{n}_i$ and $s_j\hat{n}_j$ are mutually consistent, with

$$s_i s_j (\hat{n}_i \cdot \hat{n}_j) \geq 0 \tag{1}$$

whenever possible. In a defect-free simply connected domain, such an assignment can be made without introducing a discontinuity. In the presence of half-integer disclinations, global consistency is topologically obstructed and the aligned vector field must contain discontinuities. In two-dimensional systems, the previously developed Topology-Accommodating Direction-Assignment (TADA) method constructed such discontinuity sets by radial propagation, with endpoints identifying defects or domain boundaries.²⁰ In three dimensions, the analogous discontinuities are no longer curves: they are quasi-two-dimensional surfaces whose boundaries trace disclination lines, disclination loops, or curves on the physical boundary of the sample (Figure 1iii, 1iv).

The shift from two to three dimensions renders this problem substantially more difficult.

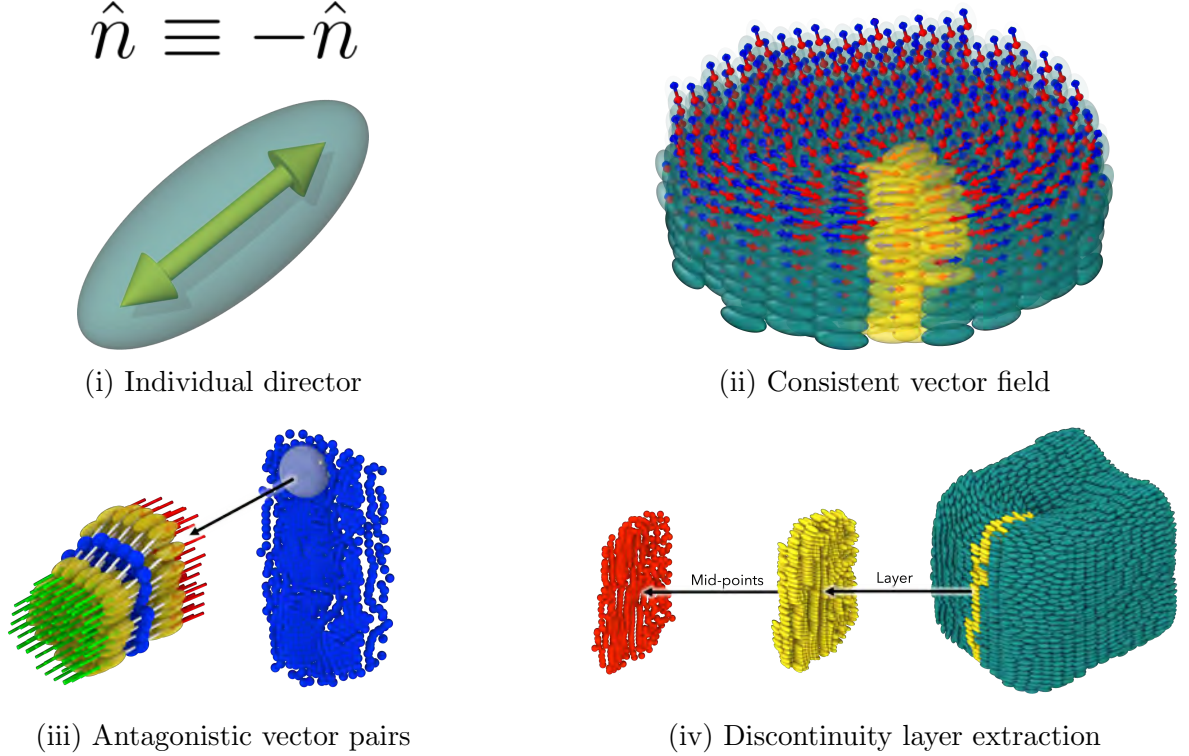


Figure 1: **Layer extraction from sign-aligned nematic data.** (i) Each mesogen contributes an unoriented director, represented as a double-sided axis with $\hat{n} \equiv -\hat{n}$. (ii) A global sign assignment converts the sampled line field into an oriented vector field wherever such an assignment is compatible with the local director structure. (iii) Neighboring mesogens with antagonistic assigned vectors identify discrete samples of the sign-discontinuity set. (iv) The midpoints of antagonistic mesogen pairs form a point-set representation of a quasi-two-dimensional discontinuity layer whose termination traces the associated disclination geometry.

For a single isolated defect, propagation-based assignment can produce a usable discontinuity surface. In more-complex geometries, however, the relevant computational issue is not only the existence of an admissible sign assignment, but the geometry of the discontinuity surface it produces. Propagation-based constructions can encode the same orientability obstruction while generating folded, concave, or closely spaced sheets that do not readily permit subsequent boundary extraction. Robust three-dimensional defect analysis therefore requires two ingredients: (1) a global sign-assignment method that produces geometrically coherent discontinuity surfaces and (2) a layer-analysis procedure that converts those surfaces into disclination centerlines.

Spectral Alignment of Mesogens (SPAM) addresses the first requirement by recasting vector assignment as a global spectral optimization problem. The construction is analogous to orientation problems in computational geometry and surface reconstruction, where locally estimated normals must be oriented consistently to distinguish interior from exterior.^{21–23} It is also naturally analogous to an Ising model: local director compatibility defines weighted couplings, while the unknown signs are binary spin variables.^{24–26} The difference from a lattice Ising system is that the interaction graph is induced by the mesogen point set and by orientation-dependent compatibility between neighboring mesogens.

Discrete Layer Analysis (DLA) addresses the second requirement. After SPAM assigns signs, neighboring mesogens whose assigned vectors are antagonistic define a discrete point-set representation of a discontinuity layer. DLA analyzes this point set as a quasi-two-dimensional object embedded in three-dimensional space. Local volumetric point density identifies regions where the layer becomes sparse, while local plane approximations characterize the nearby sheet geometry. Together, these quantities identify the one-dimensional termination set of the discontinuity layer. Connected termination sets are then reconstructed as disclination centerlines according to the geometry of the extracted layer.

Whereas scalar-order-parameter-based analyses measure finite-width regions of reduced local orientational order surrounding disclination cores, our approach localizes the disclination centerline as the termination of a global sign-discontinuity surface. This distinction enables direct measurement of centerline geometry, connectivity, and arclength. Such measures are relevant for a host of modeling applications, including the calibration of a recent class of continuum models proposed for line defects in liquid crystals.^{27,28}

Molecular systems and motivating examples

We study three-dimensional calamitic nematic assemblies generated by molecular-dynamics simulations and designed to contain both prescribed disclination geometries and defect struc-

tures induced by boundary or exclusion constraints. The first class consists of prescribed single-defect systems. Two assemblies contain straight half-integer disclination lines aligned with the z direction, generated by extruding two-dimensional $+\frac{1}{2}$ and $-\frac{1}{2}$ director patterns into three dimensions. These are referred to as the comet (Figure 2i) and trefoil (Figure 2ii) configurations, respectively. Two additional assemblies contain prescribed disclination loops: a wedge loop (Figure 2iii) and a wedge-twist loop (Figure 2iv). These controlled systems are useful because the expected defect geometry is known from construction.

The second class consists of a cylindrical-exclusion geometry (Figure 5i). A central cylindrical exclusion is introduced into a cuboidal nematic assembly, and mesogens adjacent to the exclusion surface preferentially align parallel to the tangent plane of the local cylindrical wall. This geometry produces a more complex three-dimensional defect landscape in which multiple disclination components occur. It is therefore a more stringent test of whether the vector-assignment method and layer-analysis procedure can separate nearby components and preserve their connectivity.

Methodology

1 Molecular-dynamics simulations

Molecular assemblies are generated using LAMMPS,²⁹ with visualization and post-processing performed in OVITO.³⁰ The systems consist of rod-shaped calamitic mesogens modeled as ellipsoidal particles interacting through the Gay-Berne potential.^{31,32} The Gay-Berne model generalizes the Lennard-Jones interaction³³ by introducing orientation-dependent contact distances and well depths. Following the implementation described by Brown,³⁴ the interaction between two equal-mass ellipsoidal particles with orientations $\hat{u}_1$ and $\hat{u}_2$ and center-

of-mass separation r is written as

$$U(r) = 4\tilde{\epsilon}(\hat{u}_1, \hat{u}_2, r) \epsilon_0 (\tilde{r}^{-12} - \tilde{r}^{-6}),$$

$$\tilde{r} \equiv \frac{r - \tilde{\sigma}(\hat{u}_1, \hat{u}_2, r) + \sigma_0}{\sigma_0}. \quad (2)$$

Here σ_0 and ϵ_0 define characteristic length and energy scales, while $\tilde{\sigma}$ and $\tilde{\epsilon}$ encode the orientation dependence of the effective contact distance and interaction strength (where, following the notation in Brown,³⁴ $\mu = \gamma = \nu = 1$). All quantities are expressed in reduced units defined by σ_0 , ϵ_0 , particle mass m , the time scale $\sqrt{m\sigma_0^2/\epsilon_0}$, density scale m/σ_0^3 , pressure scale ϵ_0/σ_0^3 , and temperature scale k_B/ϵ_0 . The mesogen aspect ratio is fixed at 2.5, and the equations of motion are integrated using a dimensionless time step of 10^{-3} .

The prescribed single-defect systems contain between 24,000 and 34,000 mesogens and are initialized with known positions and orientations. The straight-line cases are generated by extruding two-dimensional half-integer point-defect director patterns along the z direction. The loop cases contain either wedge character, in which the near-field director rotation is tangent to the loop,^{35,36} or mixed wedge–twist character, in which the rotation vector is oriented along the $-y$ direction.¹⁹

For the multiple-defect geometry, a cylindrical exclusion of radius $R = 20$ is introduced parallel to the z axis at the center of a cuboidal domain. Mesogens near the exclusion surface preferentially align parallel to the tangent plane of the local cylindrical wall, consistent with the central role of surface-induced orientation in liquid-crystal ordering.^{37,38} Related geometries occur in studies of nematics around inclusions and nanoporous nematic membranes.^{39,40} These simulations are initialized from a dilute vapor phase at temperature $T = 50$ and number density $\rho = 0.01$, then quenched to $T = 0.01$ and $\rho = 0.5$ using a Nosé–Hoover thermostat and barostat.^{41,42} Defect analysis is performed on configurations equilibrated for a minimum of 300 reduced time units.

2 Local scalar-order-parameter comparison

Scalar-order-parameter analysis provides a local-disorder reference against which SPAM–DLA centerline localization can be compared.^{5,6,15–17,43} For each mesogen i , a neighborhood of nearby mesogens is selected and a local Q -tensor, Q_i , is constructed from the directors in that neighborhood. The scalar order parameter S_i is obtained from the appropriately normalized leading eigenvalue of Q_i . Near a disclination core, neighboring directors sample rapidly varying orientations, so the local orientational coherence decreases and the corresponding scalar order parameter is reduced. The scalar-order field therefore provides a useful indicator of the spatial region associated with a defect core.

The scalar-order field measures a finite-width region of reduced local alignment. The detected low-order region depends on the averaging neighborhood and on the threshold used to classify mesogens by scalar order. For this reason, scalar-order analysis is treated here as a core-region diagnostic rather than as the primary definition of the topological centerline. A broadened set of low- S_i mesogens is therefore interpreted as a core-associated region surrounding the defect, not as a direct line-length measurement. The full calculation of the scalar order parameter can be found in Supplementary Information Sec. 1.

3 Spectral Alignment of Mesogens

The molecular data define a discrete nematic line field on mesogen centers

$$\mathcal{P} = \{\mathbf{r}_i\}_{i=1}^N, \quad \hat{\mathbf{n}}_i \in \mathbb{S}^2, \quad \hat{\mathbf{n}}_i \equiv -\hat{\mathbf{n}}_i.$$

SPAM constructs an oriented representative of this line field by assigning a binary sign, following the same line-field orientability problem⁴⁴ addressed by TADA in two dimensions²⁰ and in a similar spirit to graph-based orientation problems for point-cloud normals.^{21–23}

$$s_i \in \{-1, +1\}, \quad \mathbf{m}_i = s_i \hat{\mathbf{n}}_i.$$

Let

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|, \quad E = \{(i, j) : 0 < r_{ij} \leq d_{\max}\}.$$

For $(i, j) \in E$, we define

$$w_{ij} = \exp\left(-\frac{r_{ij}^2}{2d_{\max}^2}\right),$$

and set $w_{ij} = 0$ otherwise. The weighted director-compatibility matrix is

$$A_{ij} = w_{ij} (\hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j), \quad A_{ij} = A_{ji}, \quad A_{ii} = 0. \quad (3)$$

For a sign assignment $s = (s_1, \dots, s_N)^T$, the weighted alignment is

$$\sum_{i,j=1}^N A_{ij} s_i s_j = s^T A s.$$

Thus, the exact SPAM sign-assignment problem is an Ising/QUBO-type binary optimization over molecularly defined couplings:²⁴⁻²⁶

$$\begin{aligned} & \text{maximize} && s^T A s, \\ & \text{subject to} && s_i^2 = 1, \quad i = 1, \dots, N. \end{aligned} \quad (4)$$

Equivalently, one may minimize the Ising-like energy

$$\theta(A, s) = -s^T A s. \quad (5)$$

Here the binary variables s_i play the role of spins, while the couplings $A_{ij} = w_{ij}(\hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j)$ are determined by molecular proximity and local director compatibility. To obtain a deterministic global approximation, SPAM relaxes the binary constraints to a continuous spectral problem. The binary vector $s \in \{-1, +1\}^N$ is replaced by

$$x \in \mathbb{R}^N, \quad x^T x = N,$$

giving

$$\begin{aligned} & \text{maximize} && x^T A x, \\ & \text{subject to} && x^T x = N. \end{aligned} \tag{6}$$

This is equivalent to maximizing the Rayleigh quotient

$$R(A, x) = \frac{x^T A x}{x^T x}, \quad x \neq 0. \tag{7}$$

Since A is real and symmetric, the maximum is attained by the leading eigenvector,^{45–48}

$$A u_{\max} = \lambda_{\max} u_{\max}, \quad \lambda_{\max} = \max_{x \neq 0} R(A, x).$$

A binary assignment is then recovered by

$$v_i = \text{sign}((u_{\max})_i), \tag{8}$$

and the final oriented field is

$$\mathbf{m}_i = v_i \hat{\mathbf{n}}_i.$$

The assignment is unique up to the global reversal $v \mapsto -v$, which leaves $\theta(A, v)$, all pairwise products $v_i v_j$, and the discontinuity set unchanged. For comparisons across assemblies, we report

$$\bar{E} = \frac{\theta(A, v)}{N} = -\frac{v^T A v}{N}. \tag{9}$$

For TADA, which depends on the initial propagation seed, $\bar{E}$ is reported as a distribution obtained by sweeping the seed over the assembly.

4 Discontinuity layers

After sign assignment, discontinuity layers are constructed from neighboring mesogen pairs whose assigned vectors are antagonistic, extending the discontinuity-layer viewpoint used

in TADA from curve-like cuts in two dimensions to surface-like cuts in three dimensions (Figure 1iii, 1iv).^{13,14,20} A pair (i, j) contributes to the layer when $v_i \hat{n}_i \cdot v_j \hat{n}_j < 0$, under the local neighbor definition used for the interaction graph and layer extraction. The representative layer point can be taken as the midpoint between the two mesogen centers or as an equivalent local marker associated with the pair. The resulting point set samples a quasi-two-dimensional surface across which the assigned vector field changes sign. Full implementation of layer construction can be found in Supplementary Information Sec. 2.

In two dimensions, such discontinuities are curve-like and terminate at point defects or at the domain boundary. In three dimensions, they are surface-like and terminate along line defects, closed loops, or the domain boundary. The physically relevant geometric object is therefore not the entire discontinuity surface but its boundary. SPAM improves this step because global spectral assignment tends to reduce folded and highly concave layers that complicate boundary extraction.

5 Discrete Layer Analysis

DLA converts the point-set representation of each SPAM discontinuity layer into disclination centerline geometry. Each layer is treated as a sampled surface embedded in three dimensions. For every layer point, a local neighborhood is used to estimate surface support through covariance/PCA structure.^{21,49} Points in the smooth interior of a layer have locally planar, two-dimensional support, whereas points near layer terminations exhibit asymmetric support and reduced local volumetric point density. DLA uses these geometric signatures to identify candidate termination points, which are connected through a spatial neighbor graph to reconstruct disclination components. Defect identifiers are assigned to the reconstructed centerlines rather than to the finite-thickness layer itself. Further implementation details for DLA are provided in the Supplementary Information Sec. 3.

6 Defect length as a line observable

Once DLA extracts a connected disclination component, its arclength can be computed from the ordered centerline or from a graph approximation of the boundary component. For an ordered open component with centerline points $c_1, \dots, c_M$, the length is

$$L_{\text{open}} = \sum_{m=1}^{M-1} \|c_{m+1} - c_m\|. \quad (10)$$

For a closed loop, the terminal segment is included,

$$L_{\text{loop}} = \sum_{m=1}^{M-1} \|c_{m+1} - c_m\| + \|c_1 - c_M\|. \quad (11)$$

This arclength is a line observable defined on the reconstructed centerline and should not be confused with the volume or thickness of a finite-width scalar-order core region.

Results and Discussion

1 Prescribed solitary disclinations

The prescribed solitary-disclination geometries (Figure 2) provide controlled cases in which the target defect structure is known by construction. We consider both straight disclination lines and closed disclination loops, allowing the SPAM–DLA workflow to be evaluated on centerline extraction, component connectivity, and arclength measurement.

1.1 Straight half-integer disclination lines

The comet and trefoil assemblies contain prescribed two-dimensional half-integer director patterns extruded along the z direction, producing straight disclination lines at the center of the three-dimensional assemblies. SPAM assigns a globally optimized vector representative to the sampled line field and produces a quasi-two-dimensional discontinuity layer. The

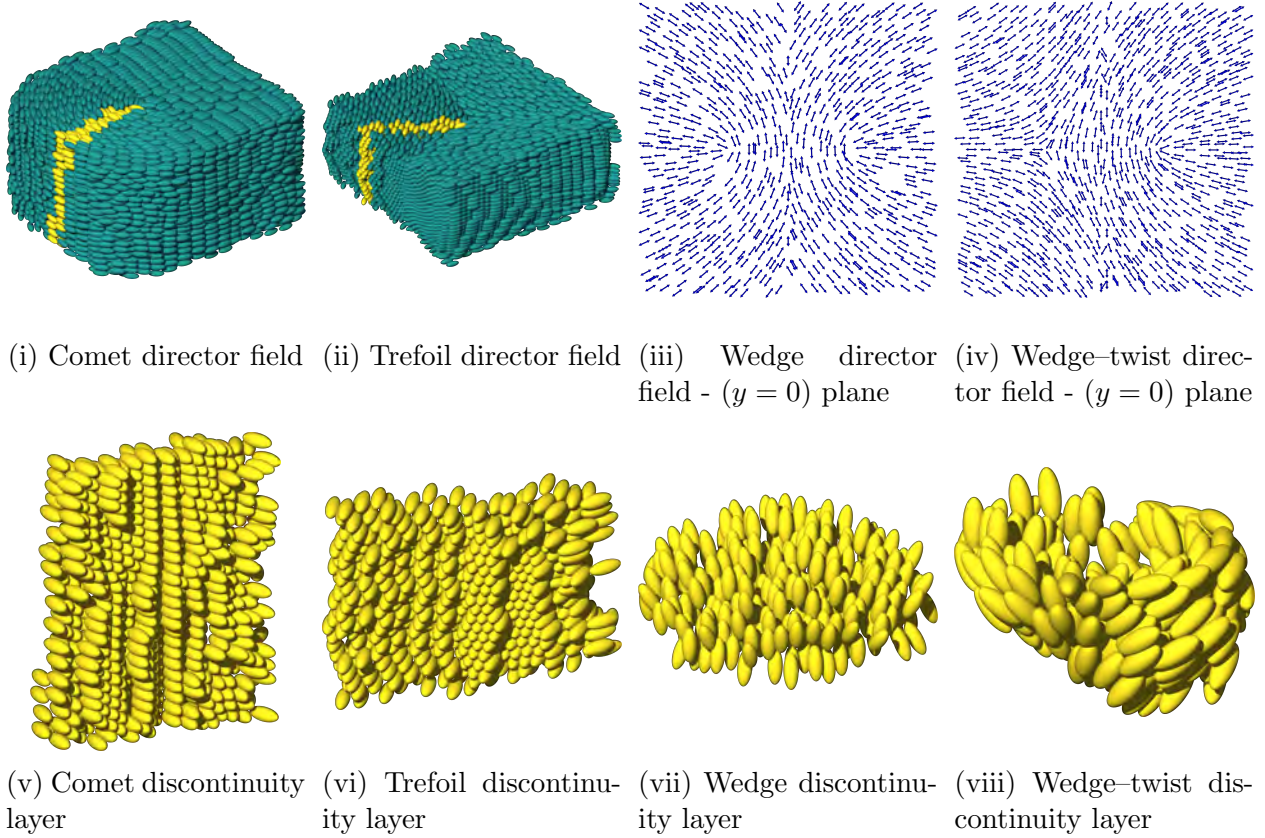


Figure 2: **Prescribed solitary disclinations in nematic assemblies.** The top row shows prescribed director-field configurations for (i-ii) straight half-integer disclination lines and (iii-iv) $y = 0$ plane for disclination loops. The bottom row shows the corresponding SPAM discontinuity layers. For straight-line geometries, the layer terminates along the prescribed disclination line; for loop geometries, the disclination is identified through the closed termination structure of the layer.

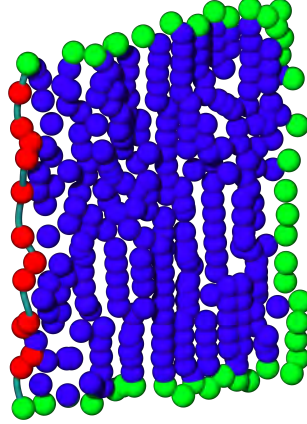
extracted layer geometry is consistent with the imposed topology: the layer terminates along the central disclination line, while its remaining structure is set by the sample boundary and by the global orientation cut. DLA then converts this termination set into a reconstructed centerline whose length can be measured directly (Figure 3i, 3ii).

1.2 Half-integer disclination loops

The wedge and wedge-twist assemblies test the same orientability-based construction for prescribed closed disclination geometries. In both cases, the imposed director field contains a loop-like topological obstruction. SPAM produces discontinuity layers whose terminal boundary follows the prescribed loop geometry, and DLA reconstructs the corresponding closed centerline (Figure 3iii, 3iv). These examples demonstrate that the same layer-boundary representation applies to both straight disclination lines and disclination loops without changing the underlying sign-assignment framework.

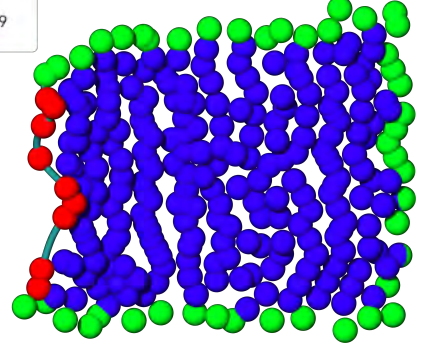
The measured arclengths are reported on the reconstructed DLA centerlines. These measurements therefore evaluate the extracted line geometry rather than the thickness of the discontinuity layer or the extent of a reduced-order core region. The scalar-order fields for the same prescribed geometries are shown as local-disorder references in Figure 4.

Disclinations
Line: $L = 20.553$



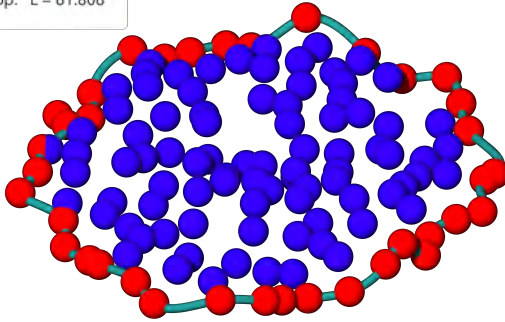
(i) Comet director field

Disclinations
Line: $L = 13.459$



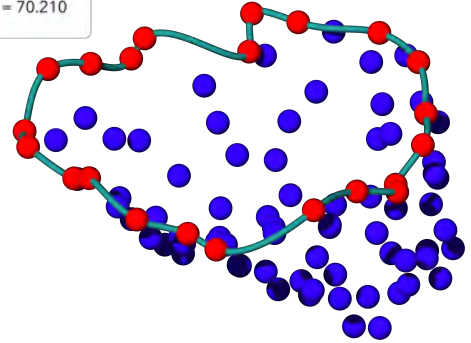
(ii) Trefoil director field

Disclinations
Loop: $L = 61.806$



(iii) Wedge loop director field

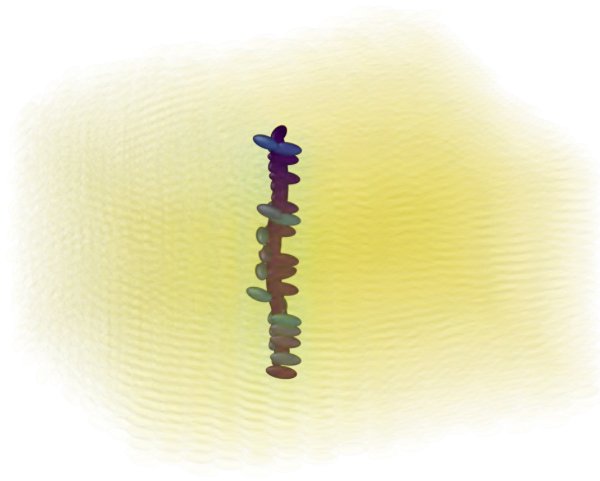
Disclinations
Loop: $L = 70.210$



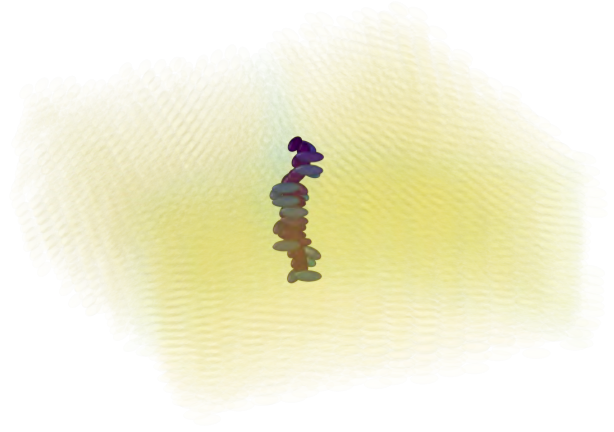
(iv) Wedge-twist loop director field



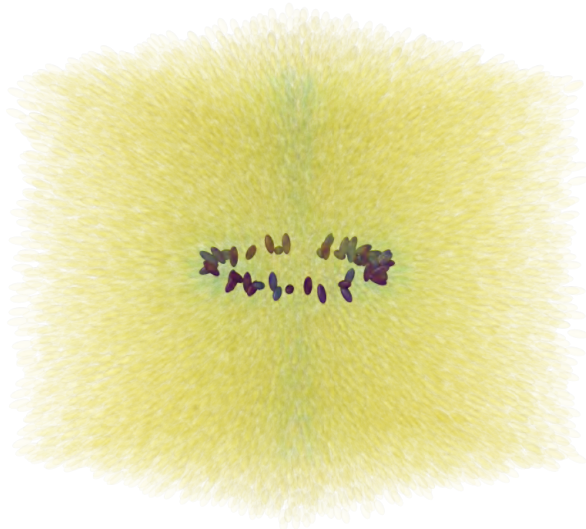
Figure 3: **Disclination length for prescribed solitary geometries.** Straight disclination lines are generated from extruded comet and trefoil director fields, while closed disclination loops are generated from wedge and wedge-twist director fields. SPAM-DLA reconstructs the corresponding centerline geometry and enables direct arclength measurement for each prescribed defect.



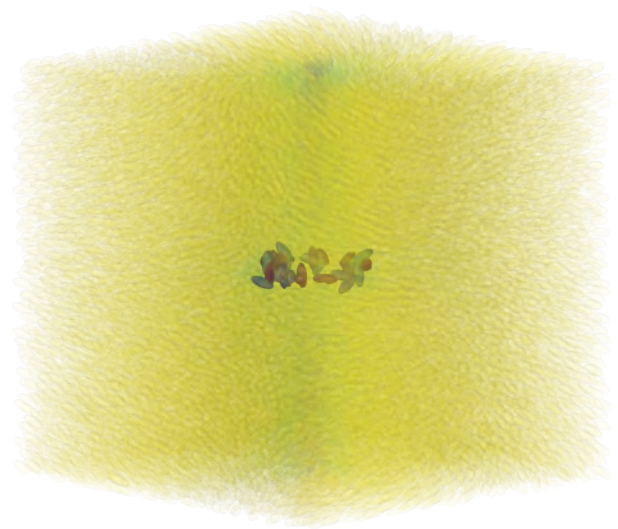
(i) Comet director field



(ii) Trefoil director field



(iii) Wedge director field



(iv) Wedge-twist director field



Figure 4: **Scalar-order-parameter localization of prescribed defects.** Scalar-order visualization identifies finite-width regions of reduced local alignment for the prescribed straight-line and loop geometries. Mesogens away from the core are made more transparent to reveal the reduced-order region.

2 Multiple-defect cylindrical-exclusion geometry

The cylindrical-exclusion geometry provides the strongest test of the framework because multiple disclination components arise in the same assembly. The local anchoring imposed by the central exclusion induces a complex three-dimensional director configuration. In this setting, visual inspection of the director field or scalar-order field alone is insufficient to determine the full component structure. The discontinuity layer must therefore be geometrically clean enough for DLA to resolve the extracted disclination components.

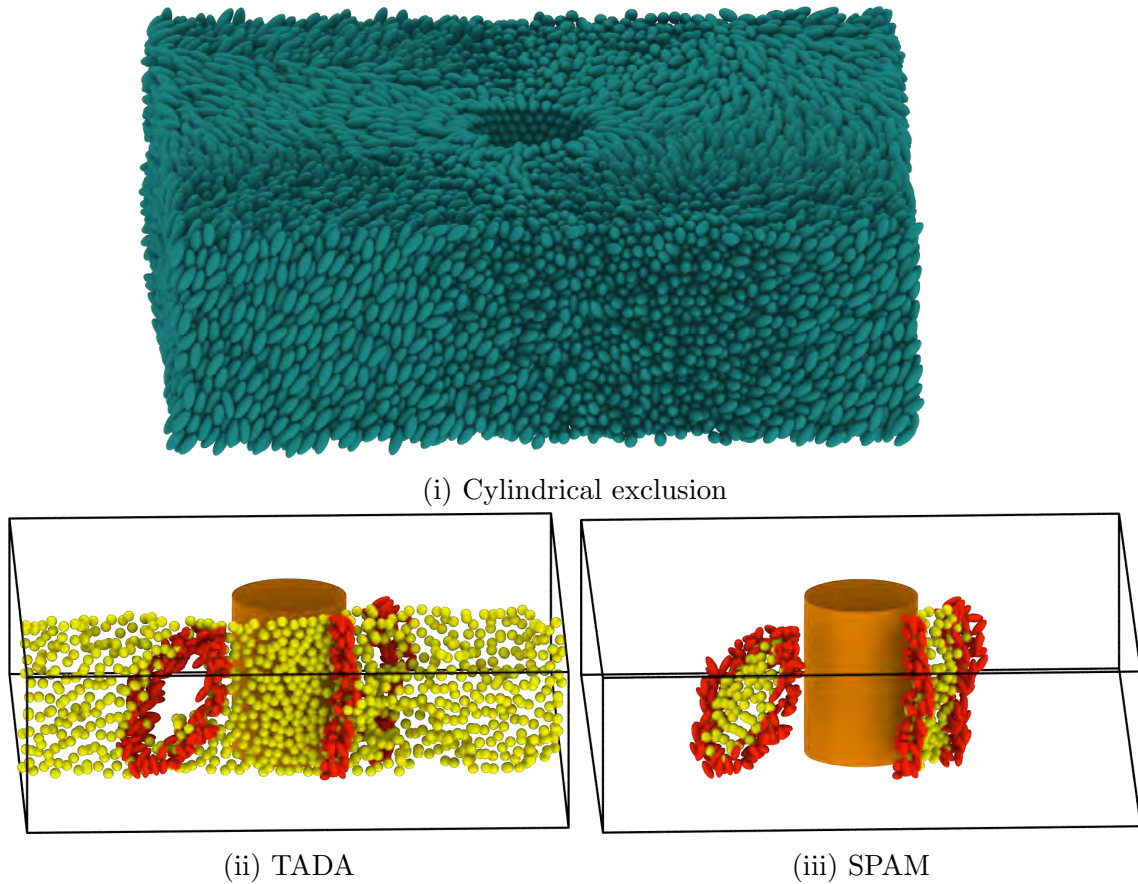


Figure 5: **Vector assignment in the cylindrical-exclusion geometry.** The cylindrical exclusion induces a complex defect configuration. A propagation-based assignment produces one admissible discontinuity layer, while SPAM produces a deterministic layer with reduced geometric complexity. Red mesogens indicate defects identified through local-order calculations. The SPAM layer encodes the same orientability obstruction while providing a cleaner object for DLA boundary extraction.

Figure 5iii shows that SPAM reduces folded and closely spaced sheet geometry relative to

the representative TADA layer. This geometric regularization is important for DLA because folded, concave, or closely spaced sheets make the terminal boundary harder to extract reliably. SPAM therefore improves the conditioning of layer-boundary extraction without changing the underlying topological information encoded by the sign field.

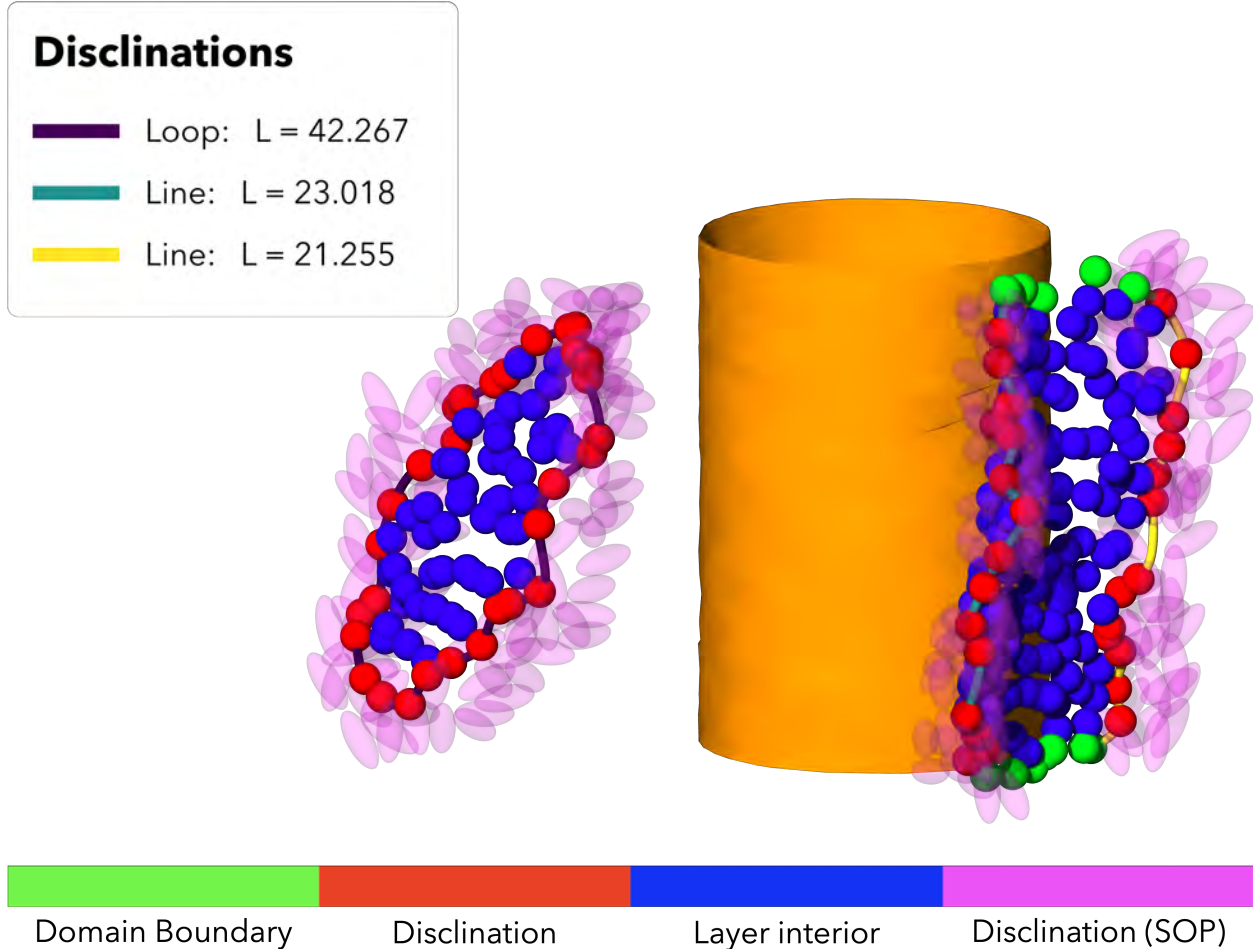


Figure 6: DLA-based disclination detection in the cylindrical-exclusion geometry. For the assembly shown in Figure 5i, the boundaries of the SPAM discontinuity layer are extracted using DLA. The detected line set provides the centerline representation used for component connectivity and arclength measurements; scalar-order-selected mesogens are overlaid as a local-disorder reference.

The scalar-order field marks a wider core-associated zone around the same defect structure, while SPAM–DLA returns the extracted line set used for component connectivity and length measurements (Figure 6). The comparison illustrates why line metrics are computed from DLA centerlines rather than from thresholded core volumes.

3 Energy comparison with propagation-based assignment

The key distinction between TADA and SPAM is the assignment principle. TADA constructs a topology-accommodating orientation field by propagating signs from a selected molecular seed; different seeds can produce different sign assignments and discontinuity layers. SPAM instead treats all signs as globally coupled binary variables on a molecular interaction graph and obtains a direct spectral approximation to the globally optimal assignment. Importantly, the spectral construction is *invariant* to the arbitrary initial signs used to represent the un-oriented mesogen axes. Reversing any subset of the input vectors induces the corresponding sign transformation of the interaction matrix and its leading spectral mode, hence the reconstructed oriented field is unchanged, apart from a physically irrelevant global reversal. The resulting spectral cut, and hence the discontinuity layer, is therefore determined by the interaction graph rather than by either the initial vector-sign distribution or a propagation seed. The numerical robustness of this assignment and its proximity to the discrete energy minimum are examined in Sec. 5 of the Supplementary Information. To compare the two methods quantitatively, the normalized alignment energy in Eq. (9) is evaluated for SPAM and for a family of TADA assignments generated by systematically varying the propagation seed (Figure 7).

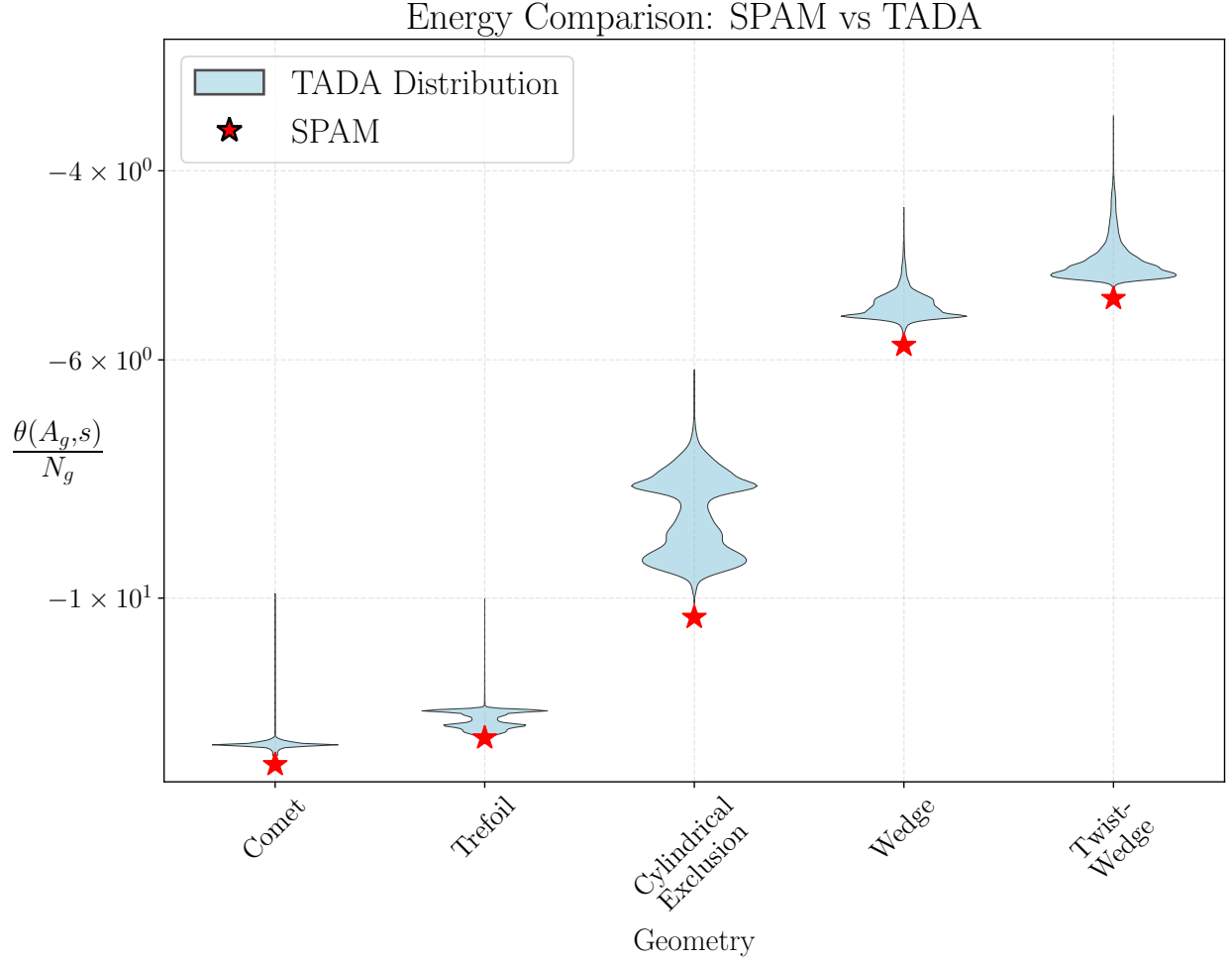


Figure 7: **Normalized alignment energy for TADA and SPAM.** For each geometry g , the normalized energy $\theta(A_g, s)/N_g$ compares the vector assignment produced by SPAM with the distribution of propagation-based TADA assignments. For solitary-defect geometries, TADA and SPAM produce similar energies, with SPAM slightly lower. For the multiple-defect geometry, the difference becomes more pronounced because the geometry of the discontinuity layer is more strongly affected by the propagation construction.

The resulting energies are shown in Figure 7. For solitary straight-line and loop defects, the difference between TADA and SPAM is modest because the topology and discontinuity-surface geometry are relatively simple. The distinction is larger in the multiple-defect assembly, where propagation can produce folded or concave layers and a broader range of energies. By reducing antagonistic neighbor alignments over the complete interaction graph, SPAM produces a lower-energy and generally more regular discontinuity layer for subsequent DLA boundary extraction.

4 Limited near-core director information

We next test whether SPAM can retain defect signatures when director information near the prescribed core is removed (Figure 8). This behavior was observed in the two-dimensional TADA setting and persists in the three-dimensional SPAM formulation. The underlying reason is topological: removing the immediate core does not remove the orientability obstruction carried by loops or surfaces enclosing the defect. Scalar-order-parameter detection relies directly on near-core disorder; if near-core data is absent, the low-order signal can be lost. A global sign-assignment method can still detect that the remaining director data cannot be oriented consistently without introducing a discontinuity.

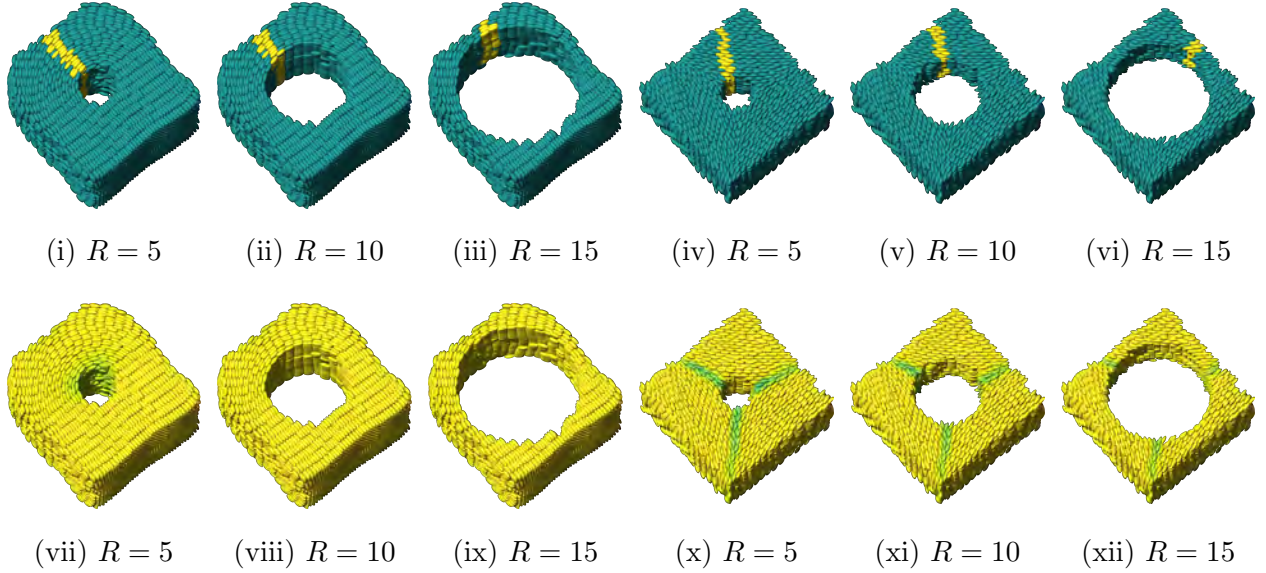


Figure 8: **Defect detection with missing near-core director data.** SPAM and scalar-order-parameter detection are compared on six prescribed-defect configurations with cylindrical regions of missing near-core data: three comet configurations (i–iii, vii–ix) and three trefoil configurations (iv–vi, x–xii), with increasing exclusion radius. The upper row shows SPAM-based discontinuity detection, while the lower row shows the corresponding SOP-based low-order regions. SPAM records the orientability obstruction in the remaining director field, whereas SOP relies on the near-core information of local orientational disorder.

This comparison emphasizes the conceptual distinction between local and global diagnostics. SOP measures local loss of order; SPAM measures the obstruction to global orientation. In experimental or simulation settings where the core is unresolved, occluded, or excluded from the data, global orientability can therefore supply information that is inaccessible to a purely local disorder criterion.

Conclusions

We have introduced SPAM, a deterministic spectral framework for assigning globally consistent vector representatives to three-dimensional nematic director fields sampled from molecular data. The method formulates the head–tail sign choice as an Ising-like alignment problem on a distance-weighted mesogen interaction graph, solves a leading-eigenvector relaxation, and binarizes the result to obtain an oriented vector field. In orientable regions, this produces a smooth vector representative of the sampled line field. In regions containing half-integer disclinations, the obstruction to global orientability appears as quasi-two-dimensional discontinuity layers.

The central geometric observation is that disclination centerlines are encoded by the terminations of these discontinuity layers. Pairing SPAM with DLA converts the point-set representation of each layer into reconstructed disclination components, providing the geometric objects needed for component identity, connectivity, spatial localization, and arclength measurement. This shifts molecular disclination localization from thresholding a local disorder field to extracting the boundary of a global sign-discontinuity surface.

Across prescribed straight disclination lines, prescribed disclination loops, and cylindrical-exclusion assemblies with multiple defects, SPAM produces deterministic vector assignments with alignment energies comparable to or lower than propagation-based assignments. The distinction is most important in complex three-dimensional geometries, where propagation-based constructions can generate folded or closely spaced discontinuity layers. SPAM pro-

duces more regular, better-separated layers, improving the conditioning of the subsequent DLA extraction.

The results support a two-level interpretation of disclination structure. SPAM–DLA identifies the topology and geometry of the disclination centerline, while scalar-order-parameter analysis identifies finite-width regions of reduced local orientational order around defect cores. Treating these as separate observables avoids conflating the thickness of a reduced-order region with the arclength of the underlying topological defect. It also clarifies sensitivity analysis: SPAM depends on the molecular neighbor graph and distance weighting, DLA depends on local geometric neighborhoods used to identify layer terminations, and scalar-order-parameter detection depends on the averaging radius and threshold used to select reduced-order mesogens.

More broadly, the framework places disclination detection at the intersection of topology, geometry, and spectral optimization. The binary sign-assignment formulation could also be treated using stochastic Ising optimizers such as simulated annealing, but the spectral relaxation used here provides a deterministic assignment without an annealing schedule.⁵⁰ The DLA step is naturally related to point-set surface reconstruction and moving-least-squares geometry processing,^{21,51} although the present implementation uses only local neighborhood geometry, point density, and covariance structure. These connections suggest future extensions for regularizing discontinuity layers, estimating uncertainty in centerline extraction, and characterizing defect-core structure around the reconstructed line. Together, SPAM and DLA provide a deterministic geometric route for localizing and quantifying three-dimensional disclination lines and loops directly from molecular nematic assemblies.

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Supplementary Information

1 Scalar Order Parameter and Defect Identification

In this section, we outline the computation of the scalar order parameter and its use as a diagnostic for identifying regions associated with disclination cores. The procedure follows Callan-Jones *et al.*;¹⁶ related formulations and tensor-based diagnostics are discussed in Refs.^{6,15,17,43} The central idea is to construct a locally averaged second-order tensor whose leading eigenstructure quantifies the degree of orientational alignment in a neighborhood.

For mesogen i , the unsigned director aligned with the major axis of the particle is denoted by

$$\hat{\mathbf{n}}_i = (n_x, n_y, n_z), \quad \hat{\mathbf{n}}_i \equiv -\hat{\mathbf{n}}_i.$$

From this director, we construct the symmetric traceless tensor

$$Q_i = \begin{bmatrix} n_x^2 & n_x n_y & n_x n_z \\ n_y n_x & n_y^2 & n_y n_z \\ n_z n_x & n_z n_y & n_z^2 \end{bmatrix} - \frac{1}{3} I_{3 \times 3}, \quad (12)$$

which is invariant under the nematic symmetry $\hat{\mathbf{n}}_i \rightarrow -\hat{\mathbf{n}}_i$.

To incorporate spatial averaging, we define a nondimensional radial coordinate

$$x_{ij} = \frac{2\|\mathbf{r}_i - \mathbf{r}_j\|}{d_{\max}}, \quad (13)$$

where $\mathbf{r}_i$ and $\mathbf{r}_j$ are the mesogen center positions and $d_{\max}$ is the averaging cutoff. The locally averaged tensor at mesogen i is

$$Q_{i,\text{avg}} = \frac{\sum_{j \in N(i)} w(x_{ij}) Q_j}{\sum_{j \in N(i)} w(x_{ij})}, \quad N(i) = \{j : \|\mathbf{r}_i - \mathbf{r}_j\| \leq d_{\max}\}. \quad (14)$$

The radial weight is chosen to be smooth and compactly supported:

$$w(x) = \begin{cases} \frac{1}{6} (3x^3 - 6x^2 + 4), & 0 \leq x < 1, \\ \frac{1}{6} (2 - x)^3, & 1 \leq x \leq 2, \\ 0, & x > 2. \end{cases} \quad (15)$$

The scalar order parameter associated with mesogen i is then computed as

$$S_i = \frac{3}{2} \lambda_i, \quad (16)$$

where λ_i denotes the largest eigenvalue of $Q_{i,\text{avg}}$. With this convention, $S_i = 0$ corresponds to locally isotropic orientational disorder, while $S_i = 1$ corresponds to perfect local alignment.

2 Layer Identification

For particle-based representations of nematic assemblies, discontinuities in the assigned vector field are discretized by pairs of nearby mesogens whose assigned vectors are antagonistic. After SPAM assigns signs, each mesogen has an oriented representative

$$\mathbf{m}_i = v_i \hat{\mathbf{n}}_i, \quad v_i \in \{-1, +1\}.$$

A neighboring pair (i, j) is antagonistic when

$$\mathbf{m}_i \cdot \mathbf{m}_j < 0. \quad (17)$$

The corresponding layer point is taken as the midpoint of the two mesogen centers,

$$\mathbf{p}_{ij} = \frac{1}{2} (\mathbf{r}_i + \mathbf{r}_j). \quad (18)$$

The collection of such midpoint samples defines a discrete point-set representation of the discontinuity layer. For disclination lines and loops, this layer is a quasi-two-dimensional surface whose terminations coincide with the underlying disclination geometry.

The selection of antagonistic mesogen pairs follows a recursive nearest-neighbor procedure. The procedure is designed to identify mutually antagonistic mesogen pairs while avoiding duplicate pair assignments.

1. For each mesogen k , construct a neighbor list $N(k)$ containing mesogens within a maximum radial distance $d_{\max}$.
2. If there exists at least one mesogen $j \in N(k)$ satisfying

$$\mathbf{m}_j \cdot \mathbf{m}_k < 0,$$

then a discontinuity in the assigned vector field is present within the local neighborhood. Among such neighbors, designate one antagonistically aligned mesogen as MAV_i .

3. Construct a new neighbor list centered at MAV_i , again using the cutoff $d_{\max}$. From this list, select the closest mesogen whose assigned vector is antagonistic to that of MAV_i , and denote it by CM_i .
4. Relabel CM_i as MAV_{i+1} and repeat Step 3. If the subsequently identified CM_{i+1} coincides with the original MAV_i , then the pair $(\text{MAV}_i, \text{MAV}_{i+1})$ is accepted as an antagonistic mesogen pair and removed from the search space. If this condition is not satisfied, the procedure is iterated with $i \rightarrow i + 1$ until convergence.

The accepted antagonistic pairs define the layer samples used in the subsequent DLA procedure.

3 Discrete Layer Analysis

DLA identifies terminations of the discontinuity-layer point set using two local geometric diagnostics: normalized volumetric point density and angular coverage in a locally fitted tangent plane. The discontinuity layer is treated as a sampled surface embedded in three dimensions. The present implementation uses local neighborhood geometry, point density, and covariance-based plane estimation; this viewpoint is related to point-cloud surface reconstruction and moving-least-squares surface descriptions,^{21,51} but does not require an explicit reconstructed surface. Unless stated otherwise, the results presented here use a neighborhood radius of

$$d_{\max} = 3.5\sigma_0.$$

3.1 Radial Distribution

Points near a layer termination are surrounded by fewer neighboring layer samples within a fixed radial distance than points in the smooth interior of the layer. This local-density contrast persists for quasi-two-dimensional surfaces represented by discrete point sets and is illustrated in Figure 9; related local-neighborhood arguments are standard in point-cloud geometry processing.^{21,22}

For a layer point i , let $N(i)$ denote the set of layer points within distance $d_{\max}$. We define the local volumetric point density

$$\rho_N(i) = \frac{|N(i)|}{\frac{4}{3}\pi d_{\max}^3}, \quad (19)$$

and the normalized density

$$\rho_N^*(i) = \frac{\rho_N(i)}{\max_i \rho_N(i)}. \quad (20)$$

For sufficiently uniform sampling, points near layer terminations have lower ρ_N^* than points in the layer interior. To accommodate concave regions, nonuniform point spacing, and surface

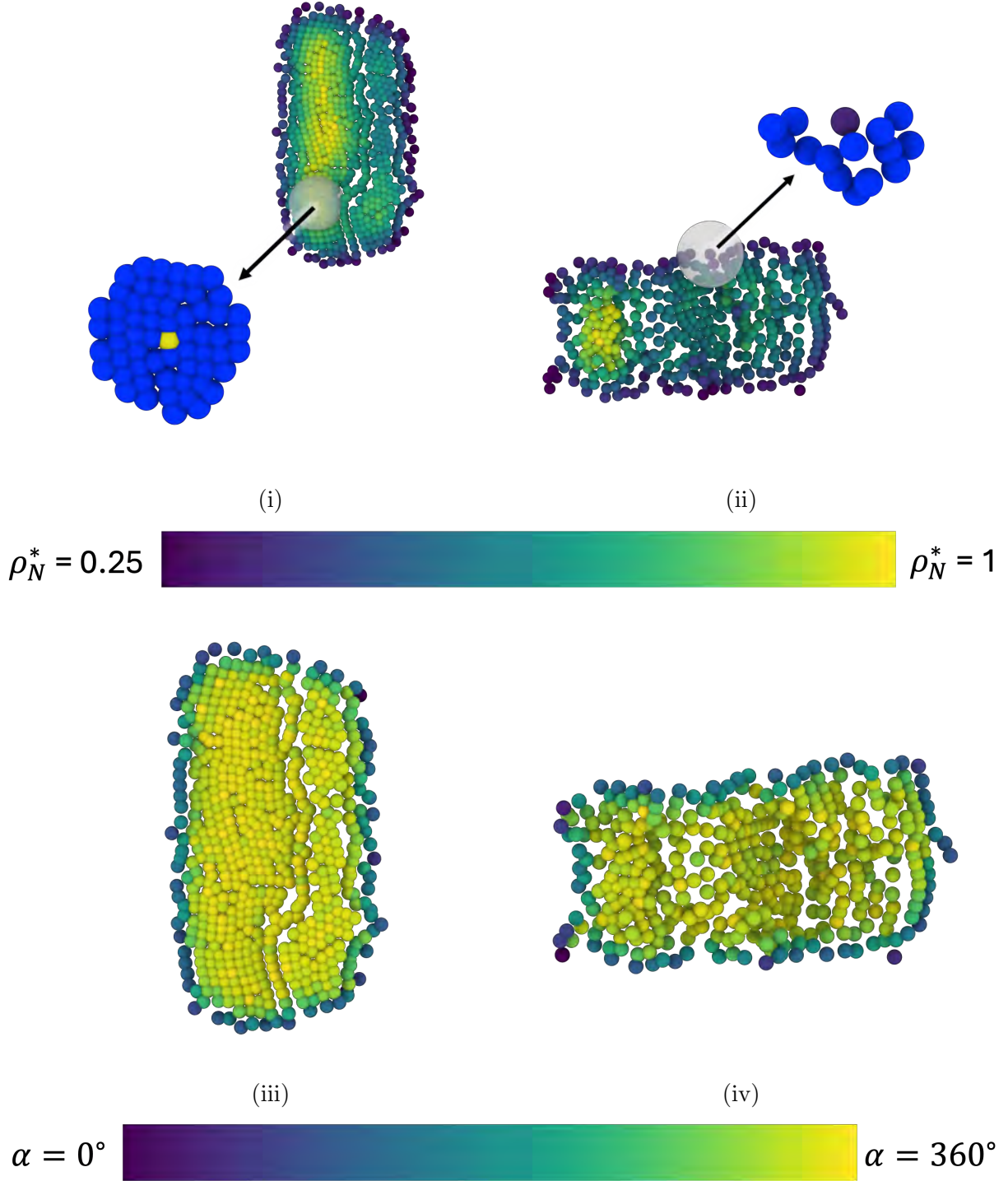


Figure 9: **Local neighborhood analysis of representative layer geometries.** (i–ii) Normalized local volumetric point density identifies sparse layer-termination candidates. (iii–iv) Angular coverage after local plane projection further distinguishes layer terminations from concave or under-sampled interior regions.

undulations, we adopt the conservative threshold

$$\rho_N^*(i) \leq 0.65 \quad (21)$$

to identify candidate layer-termination points. This density criterion alone is not sufficient, since interior points in strongly curved or under-sampled regions may also have reduced neighborhood cardinality.

3.2 Coverage

To distinguish true layer terminations from sparse interior regions, DLA also evaluates local angular coverage. Points in the smooth interior of a layer are expected to be surrounded by neighboring layer samples in all directions within a locally fitted tangent plane. Their projected neighbors therefore subtend an angle close to $\alpha = 360^\circ$. Points near a layer termination exhibit incomplete angular coverage.

For each layer point, a local best-fit plane is constructed using principal component analysis, as described in Supplementary Information 4. Neighboring points are projected onto this plane and the total angular coverage α is computed around the central point. To account for finite sampling and surface undulations, a point is classified as a layer-termination point when

$$\alpha \leq 240^\circ. \quad (22)$$

A representative comparison between layer terminations identified by DLA and scalar-order-selected mesogens is shown in Figure 10.

4 PCA-Based Local Plane Construction and Coverage

For each layer point, DLA estimates the local sheet geometry from neighboring layer samples and measures how completely those samples surround the point within the local tangent

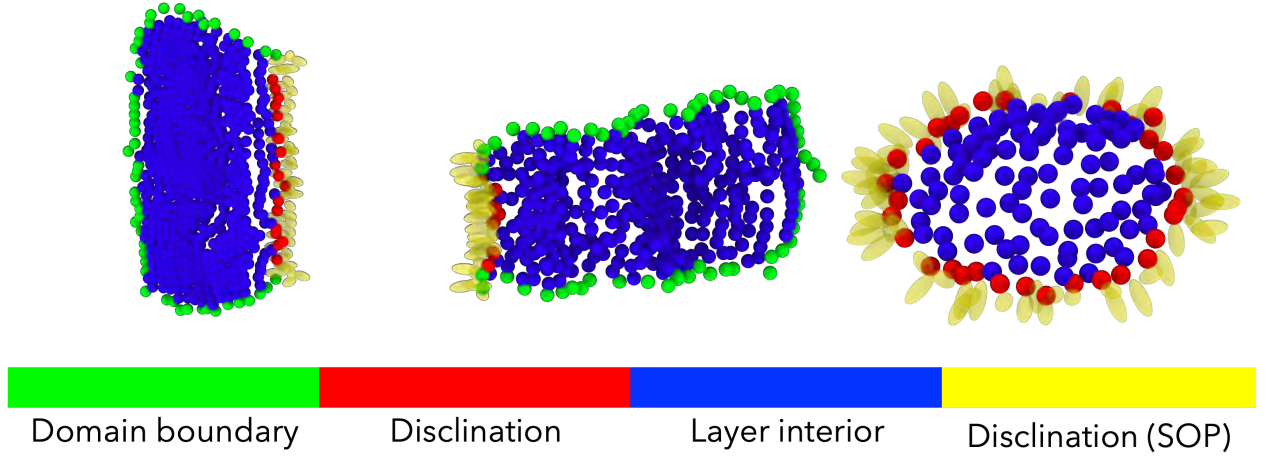


Figure 10: **Local neighborhood analysis.** Points on the discontinuity layer identified as belonging to the disclination line are shown in red, while points classified as terminating at the sample boundary are shown in green. Scalar-order-selected mesogens are overlaid in yellow as a local-disorder reference.

plane. Let $\mathbf{p}_c$ denote a layer point and let

$$N(\mathbf{p}_c) = \{\mathbf{p}_j : \|\mathbf{p}_j - \mathbf{p}_c\| \leq d_{\max}\}$$

be its neighboring layer points. A local principal-component frame is computed from $N(\mathbf{p}_c)$. The two dominant principal directions define the local tangent plane, while the third direction defines the local normal $\mathbf{n}_c$. For each neighbor, the relative vector

$$\mathbf{r}_j = \mathbf{p}_j - \mathbf{p}_c$$

is projected onto the local tangent plane by removing its normal component,

$$\mathbf{q}_j = \mathbf{r}_j - (\mathbf{r}_j \cdot \mathbf{n}_c)\mathbf{n}_c. \tag{23}$$

The projected neighbor vectors $\{\mathbf{q}_j\}$ are then used to define an in-plane reference direction,

$$\hat{\mathbf{a}}_c = \frac{\sum_{j \in N(\mathbf{p}_c)} \mathbf{q}_j}{\left\| \sum_{j \in N(\mathbf{p}_c)} \mathbf{q}_j \right\|}, \quad (24)$$

provided the denominator is nonzero. If the projected neighborhood is degenerate, or if fewer than two projected neighbors remain after removing the center point, the coverage is set to 360° . Each projected neighbor is assigned a signed angle relative to $\hat{\mathbf{a}}_c$,

$$\theta_j = \text{sgn}[\mathbf{n}_c \cdot (\hat{\mathbf{a}}_c \times \mathbf{q}_j)] \cos^{-1} \left(\frac{\mathbf{q}_j \cdot \hat{\mathbf{a}}_c}{\|\mathbf{q}_j\|} \right), \quad (25)$$

with zero-length projections assigned $\theta_j = 0$. The local angular coverage is defined as the span of these signed angles,

$$\alpha_c = \left| \max_j \theta_j - \min_j \theta_j \right| \frac{180^\circ}{\pi}. \quad (26)$$

Interior layer points have broad angular support in the local plane, whereas points near layer terminations have incomplete angular support and therefore smaller α_c . To account for concave boundaries, a layer point is marked as a candidate boundary when

$$\alpha_c < 240^\circ. \quad (27)$$

This coverage criterion is then combined with the precomputed boundary indicator to distinguish terminations associated with the sample boundary from those associated with the disclination centerline.

5 Sign-Gauge Invariance of $\theta(A, v^m)$

The SPAM interaction matrix is defined on an unoriented director field. Therefore, changing the arbitrary sign convention of the input directors should not change the physical alignment

energy, provided the sign transformation is applied consistently.

Let

$$A_{ij} = w_{ij} (\hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j)$$

be the interaction matrix associated with one arbitrary choice of vector representatives for the input line field. Let

$$\boldsymbol{\phi} = (\phi_1, \dots, \phi_N)^T, \quad \phi_i \in \{-1, +1\},$$

be an arbitrary sign gauge, and define the diagonal sign matrix

$$D_\phi = \text{diag}(\phi_1, \dots, \phi_N).$$

Applying this sign convention to the input directors,

$$\hat{\mathbf{n}}_i \rightarrow \phi_i \hat{\mathbf{n}}_i,$$

transforms the interaction matrix to

$$A_\phi = D_\phi A D_\phi. \tag{28}$$

Since $D_\phi^T = D_\phi$ and $D_\phi^2 = I$, the matrices A and A_ϕ are orthogonally similar and therefore have the same spectrum. If

$$A u^m = \lambda_m u^m, \tag{29}$$

then

$$A_\phi (D_\phi u^m) = D_\phi A D_\phi D_\phi u^m = D_\phi A u^m = \lambda_m D_\phi u^m. \tag{30}$$

Thus, $D_\phi u^m$ is the corresponding eigenvector of A_ϕ . The binarized SPAM assignments

transform in the same way:

$$v^m = \text{sign}(u^m), \quad v_\phi^m = \text{sign}(D_\phi u^m) = D_\phi v^m, \quad (31)$$

assuming no zero eigenvector entries. If zero entries occur, their signs may be chosen consistently without affecting the gauge argument. Using the SPAM energy convention

$$\theta(A, v) = -v^T A v, \quad (32)$$

we obtain

$$\begin{aligned} \theta(A_\phi, v_\phi^m) &= -(v_\phi^m)^T A_\phi v_\phi^m \\ &= -(D_\phi v^m)^T (D_\phi A D_\phi) (D_\phi v^m) \\ &= -(v^m)^T D_\phi D_\phi A D_\phi D_\phi v^m \\ &= -(v^m)^T A v^m \\ &= \theta(A, v^m). \end{aligned} \quad (33)$$

Therefore, the SPAM alignment energy is invariant under arbitrary sign-gauge choices of the input nematic directors:

$$\theta(A_\phi, v_\phi^m) = \theta(A, v^m). \quad (34)$$

This invariance reflects the fact that SPAM acts on the underlying line field rather than on a particular arbitrary vector representation of that line field.