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Estimation of unordered core size using a robustness measure for topological defects in discretized orientation and vector fields

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We show how the finite sizes of unordered defect cores in discretized orientation and vector fields can reliably be estimated using a robustness measure for topological defects. Topological defects, or singular points, in vector and orientation fields are considered in applications from material science to life sciences to fingerprint recognition. Their identification from discretized two-dimensional fields must deal with discontinuities, since the estimated topological charge jumps in (half-)integer steps upon orientation changes above a certain threshold. We use a recently proposed robustness measure [Hoffmann & Sbalzarini, Phys. Rev. E 103(1), 012602 (2021)] that exploits this effect to quantify the influence of noise in a vector field, and of the path chosen for defect estimation, on the detection reliability in two-dimensional discrete domains. Here, we show how this robustness measure can be used to quantify the sizes of unordered regions surrounding a defect, which are known as *unordered cores*. We suggest that the size of an unordered core can be identified as the smallest path radius of sufficient robustness. The resulting robust core-size estimation complements singular point and index estimation and may serve as uncertainty quantification of defect localization, or as an additional feature for defect characterization.

1 Introduction: singular points and their robustness

A *topological (point) defect* is a singular point in an otherwise continuous vector field over a domain X. In two-dimensional orientation fields, where orientations or nematic vectors are defined by identifying antipodal polar vectors or by a $\mathbf{Q}$-tensor, topological defects are classified by their half-integer *index* or *charge*. In orientation fields over discrete domains, defect charge is identified from the total orientation change accumulated along a closed path around the query point [1,2]. Due to the discrete nature of a defect, its existence cannot depend continuously on a discretized orientation field, rendering defect identification challenging in applications with noisy or otherwise imperfect orientation measurements. Based on this observation, we have previously introduced a robustness measure for topological defects, which quantifies the largest admissible change in any single orientation value along the path that does not alter the defect estimator [3]. It therefore measures the sensitivity of a defect estimate to noise or temporal dynamics of the orientation field in a discrete domain. This enabled quantifying the tradeoff between defect robustness and localization precision and comparing different closed path shapes [4].

Closed paths of different shapes can therefore be used to measure the *total* topological charge in the enclosed area. This generalizes to the case when singular points are surrounded by an unordered region known as *defect core*. In contrast to singular points, defect cores are extended objects, and one can ask what their size is.

2 Defect cores and their size

Identifying an unordered defect core, or defining its size, can be done using closed paths of different sizes: Paths of the smallest possible length, around a single spatial discretization element (pixel or triangle), identify individual point defects, which we refer to as *microscopic* defects. Larger paths identify clusters of defects with their sum of charges. Paths larger than the size of an unordered core add no further charge to the estimate, but lead to increasing estimation robustness approaching the theoretical limit of robustness [3]. Making the paths too large might start fusing nearby unordered cores, leading to fluctuating charge and robustness estimates.

To construct a robust estimator of defect core size, we investigate how the estimated total charge and its robustness, as well as the total number of enclosed microscopic defects, change as a function of the radius of a circular closed path used for detection. For these numerical experiments, we generate synthetic defect cores in an otherwise smooth orientation field by varying the magnitude of the orientation radially around predefined defect center and adding Gaussian noise to the orientations. We fix two radii R_1, R_2 between which the orientation magnitude is linearly attenuated (see Fig. 1**b,c**, bottom panels). The ground truth radius of the core is somewhere between R_1 and R_2, and the uncertainty with which it can be estimated is proportional to the core interface thickness $R_2 - R_1$.

In this synthetic data, we first detect microscopic defects from all single-pixel paths (Fig. 1**a**). We then use a watershed algorithm to cluster these microscopic defects. For each detected cluster, we determine the center of mass $(x_{\text{clust}}, y_{\text{clust}})$ of all

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a b c

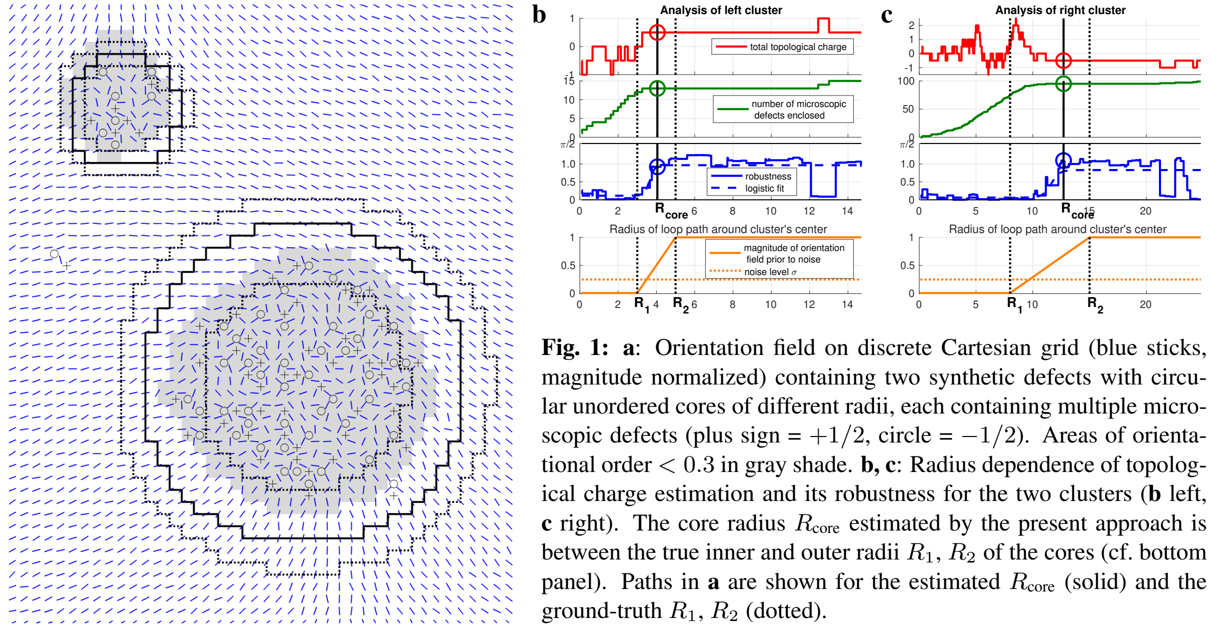

Fig. 1: **a**: Orientation field on discrete Cartesian grid (blue sticks, magnitude normalized) containing two synthetic defects with circular unordered cores of different radii, each containing multiple microscopic defects (plus sign = $+1/2$, circle = $-1/2$). Areas of orientational order < 0.3 in gray shade. **b, c**: Radius dependence of topological charge estimation and its robustness for the two clusters (**b** left, **c** right). The core radius R_{core} estimated by the present approach is between the true inner and outer radii R_1, R_2 of the cores (cf. bottom panel). Paths in **a** are shown for the estimated R_{core} (solid) and the ground-truth R_1, R_2 (dotted).

defect locations (unit weights) in that cluster. We use discretized circular paths around the center point to compute the total topological charge, robustness [3,4], and the total number of microscopic defects enclosed by increasing path radii $r \in (0, \infty)$.

We find that paths smaller than the inner core radius R_1 lead to erratically fluctuating index estimates of low robustness (Fig. 1**b,c**). Paths larger than the outer core radius R_2 yield a constant total charge (red line) with high robustness (blue line). When paths grow too large and start to include portions of other cores, the robustness decreases significantly and the charge changes again. Therefore, the radius of a defect core can be estimated as the radius from a cluster's center at which the robustness saturates at high level for constant total charge. We identify such points by fitting a logistic function to the observed robustnesses for radii up to 1.1 times the distance to the nearest neighboring cluster center (Fig. 1**b,c**, dashed blue line). Deliberately including radii that contain parts of at least one neighboring cluster compensates for potential over-segmentation in the initial clustering of microscopic defects. The defect core radius is then estimated as the 95% quantile of the logistic fit. The thus estimated core radii R_{core} are consistent with ground truth in Fig. 1, i.e., $R_1 < R_{\text{core}} < R_2$. The estimated cores defined by radius R_{core} are comparable to or slightly larger than the unordered area (gray shade in Fig. 1**a**), which is defined by orientational order on 7×7 pixel patches below threshold 0.3. Differently from the radial core-size estimation, the unordered region approach cannot guarantee robustness nor connectedness of the identified cores, may miss some microscopic defects, and requires to set an absolute threshold (for this synthetic data chosen as the known noise level $\sigma = 0.3$).

While we find the core radius estimator to work reliably in our benchmarks, other heuristics are possible as well. For example, one could alternatively fit a piecewise constant function to identify the onset of the robustness plateau at the core size radius, or employ a magnitude-aware version of the robustness measure [3]. One could also include information about the total *number* of enclosed microscopic defects, which also plateaus beyond the core radius (Fig. 1**b,c**, green line). This being a monotonic function may simplify detection, but the increase when reaching the neighboring cluster would need to be considered. Finally, one can generalize to path shapes other than circles, e.g. by "expansion over the critical edge" [3], and use the same heuristics to quantify core size in terms of area rather than radius.

The present approach bears similarities with defect identification methods that define defects as locations where orientational order falls below some threshold [1]. Indeed, regions of low orientational order are characterized by large orientation differences between nearby discretization points, resulting in low robustness according to our definition. The observed plateau of high robustness for path radii above R_{core} also explains why estimating topological charge using paths that are maximally distant from any defect performs well in practice [5], although this cannot determine core size. Overall, the presented core-size estimation by saturating robustness complements singular point detection, exemplifies the usefulness of robustness information in topological charge estimation, and may be applied to data validation or as an additional feature for defect tracking.

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