Liquid Crystal Droplet Simulations for Materials Exploration

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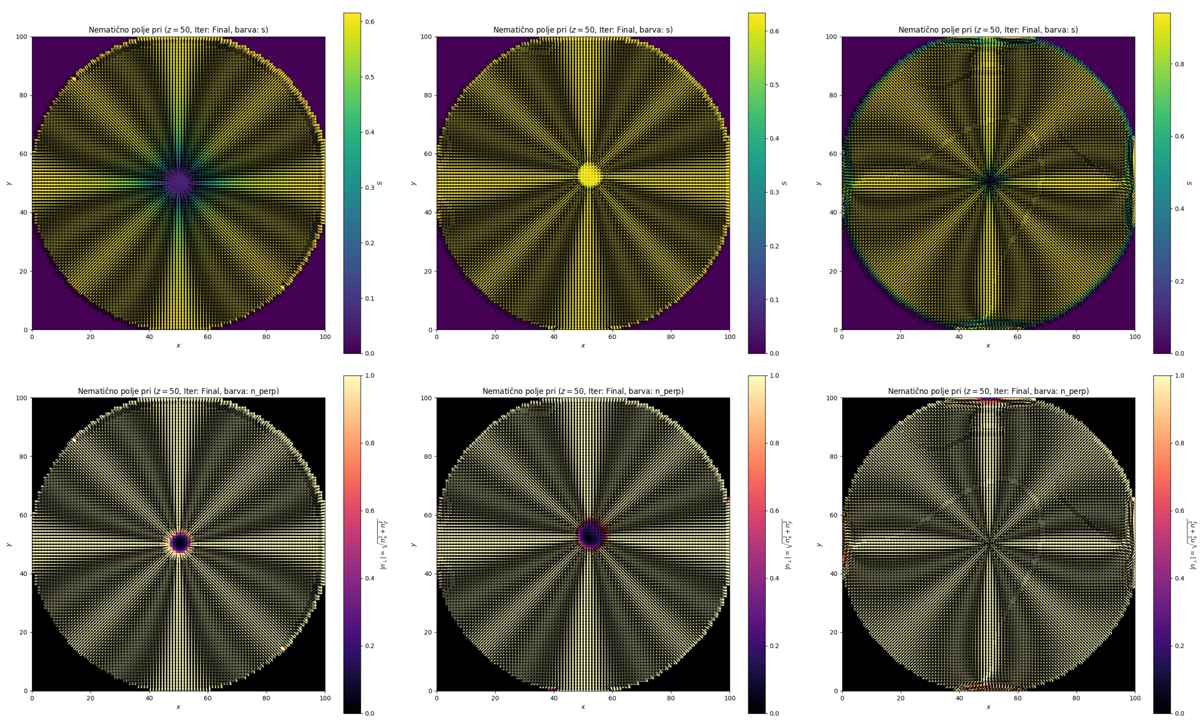


Introduction

Phase transitions in soft matter, such as the isotropic-nematic transition in liquid crystals (LCs), are governed by universal symmetry-breaking principles. According to the Kibble-Żurek mechanism (KZM), the rapid transition through a critical point "freezes" local fluctuations into a mosaic of topological defects. While KZM is well-established for infinite systems, its validity in confined geometries—where surface anchoring and finite-size effects dominate—remains a subject of intense research. This study explores the emergence of complexity in LC droplets, bridging the gap between cosmological scaling laws and soft matter biophysics.

Aim of the Study

The primary objective is to investigate the scaling laws of defect formation in nematic droplets following a thermal quench. We hypothesize that despite the strong topological constraints imposed by radial anchoring and finite droplet size, the system preserves a "topological memory" of the quench velocity, manifesting in universal power-law scaling of the defect density.

Methodology

We used a 3D LdG phenomenological theory in a spherical droplet with strict radial anchoring (homeotropic) at the surface. We then used a linear quench protocol, cooling from the isotropic phase to the shallow and deep nematic phase at varying rates τ_Q. To achieve this, we also used a finite-difference discretization on a high-resolution mesh to capture both the escaped-radial core and standard LdG singular structure. We also automated the detection of defect density ρ_D and correlation length ξ as a function of quench speed.

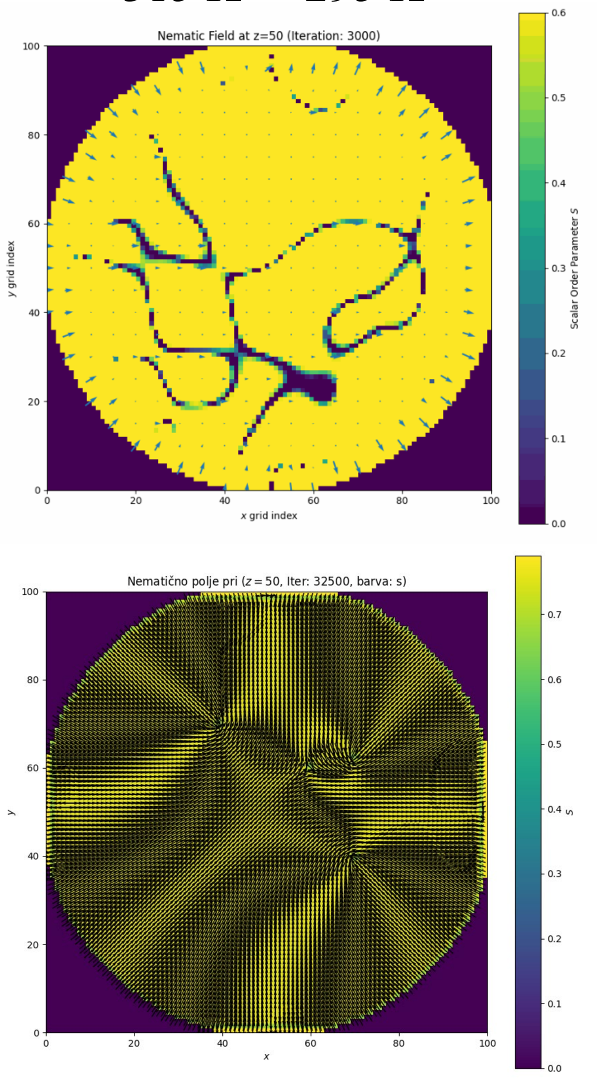
Results

Observation of a transition from high-density defect networks ("string-like" disclinations) to a single stable radial hedgehog core during relaxation. Correlation length ξ_p supposedly exhibits saturation (≈ 0.04) due to finite-size constraints of the droplet. Observed defect density follows an apparent power-law $\rho_D \propto \tau_Q^{-1/4}$, which may or may not be physically accurate for our system, but the quantitative trends align with theoretical expectations. We also successfully Identified defect structures and escaped-radial behavior depending on the spatial resolution and quench depth ΔT.

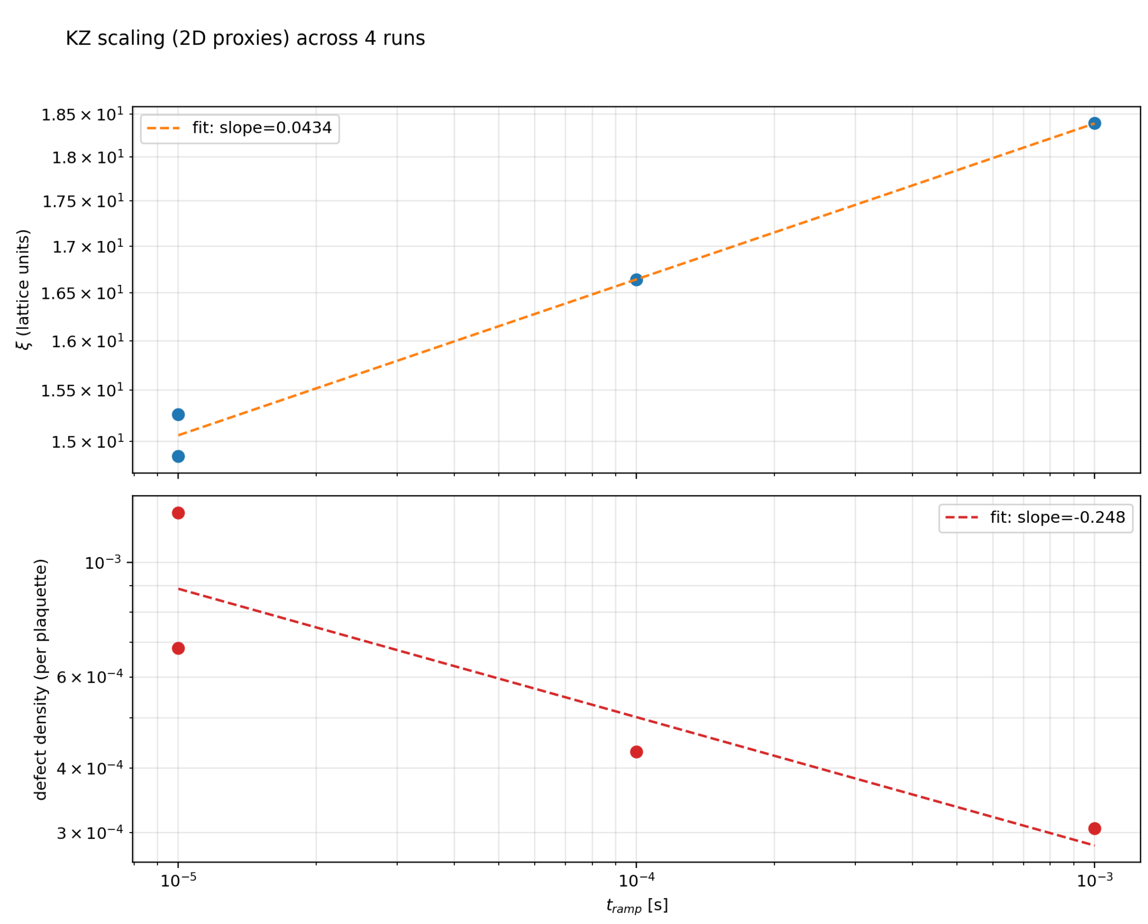
Discussion

The recovered exponents exhibit values that differ from those predicted by the infinite-system KZM, yet the overall trends align perfectly with theoretical expectations for $\rho_D(\xi_p)$. In infinite systems, mean-field KZM predicts an exponent of ¼ for the correlation length ξ_p. In our confined 3D system, strong geometric constraints and the nature of disclination lines seemingly lead to a reduction in effective dimensionality as the disclination lines are forced to align with the preferred radial director field, effectively suppressing fluctuations in other dimensions and leading to 1D-like scaling behavior. The observed $\rho_D \sim \tau_Q^{-1/4}$ scaling indicates that the topological defect count scales linearly with the inverse of the KZ correlation length, rather than the volumetric ξ_p^{-3}. This implies that the topological memory of the quench is preserved despite the saturation of the correlation length, which is limited by the droplet's radius. Our results suggest that KZM in extremely confined spaces offers a unique window into topological stabilization, and our findings provide a robust numerical foundation for further exploration of LC-based adaptive materials.

315 K → 295 K



312 K → 305 K



Conclusions

The KZM remains a valid framework for predicting defect formation in confined nematics. NDs retain information about transition speed through density of trapped disclinations. We observe that topological confinement seemingly decouples the theoretically predicted scaling of ξ_p from ρ_D, yet the universal signatures of the mean-field universality remain detectable in the defect statistics. These results may be crucial for the development of LC-based thermal sensors, where the sensitivity and accuracy are dictated by the precise control of phase transition dynamics.

References

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