Numerical Experiments in Domain Decomposition for Simulating Liquid Crystal Defects

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Abstract

In this project we explore a domain decomposition method to improve the overall runtime of a finite element method approximation to the solution of a liquid crystal model. Both the Ericksen model and the Landau-deGennes model will be considered. The numerical experiments intend to show the effect of the domain decomposition method on the runtime. Specifically we vary two parameter: (1) the size of the subdomain and (2) the number of iterations within the subdomain.

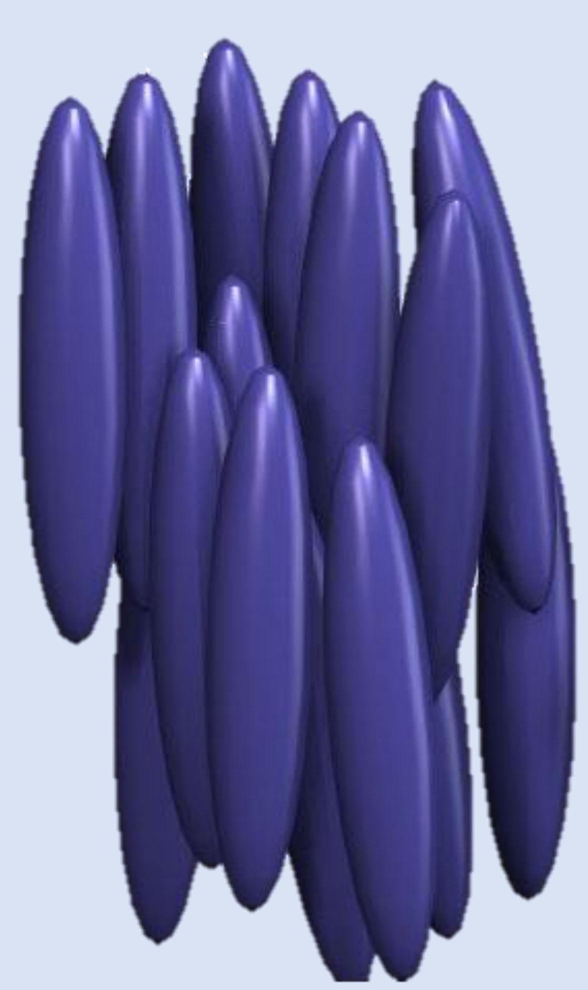
Introduction

The liquid crystalline phase is an intermediate state of matter of certain materials consisting of rod-like molecules with properties characteristic of both liquids and crystals.

LCs tend to orientations that minimize local differences in alignment.

LCs have a variety of applications:

- Assembly of microstructures
- LCD screens
- Material design



Ericksen Model

Energy model with respect to director vector $\mathbf{n}$ and scalar order parameter s:

$$E[s,\mathbf{n}] = \frac{1}{2}\int_\Omega (b_0|\nabla s|^2 + s^2|\nabla \mathbf{n}|^2)\mathrm{d}\mathbf{x} + \frac{1}{\epsilon_{\mathrm{dw}}^2}\int_\Omega \psi(s)\mathrm{d}\mathbf{x}$$

Effective at modeling integer order defects, e.g. ± 1 defects.

Director describes orientation; scalar order parameter describes degree of alignment.

Landau-deGennes Model

Energy model with respect to an order tensor $\mathbf{Q}$:

$$E[\mathbf{Q}] = \frac{1}{2}\int_\Omega |\nabla \mathbf{Q}|^2 \mathrm{d}\mathbf{x} + \frac{1}{\eta_B^2}\int_\Omega \psi(\mathbf{Q})\mathrm{d}\mathbf{x}$$

Effective at modeling half integer defects, e.g. $\pm\frac{1}{2}$ and ± 1 defects.

Order tensor models a line field, i.e. a vector field without orientation.

Defects in Liquid Crystals

Boundary conditions lead to defects in the liquid crystals represented by rapid changes (and discontinuities) in the solution.

Defects are of interest in physical applications.

More difficult to simulate than LCs without defects.

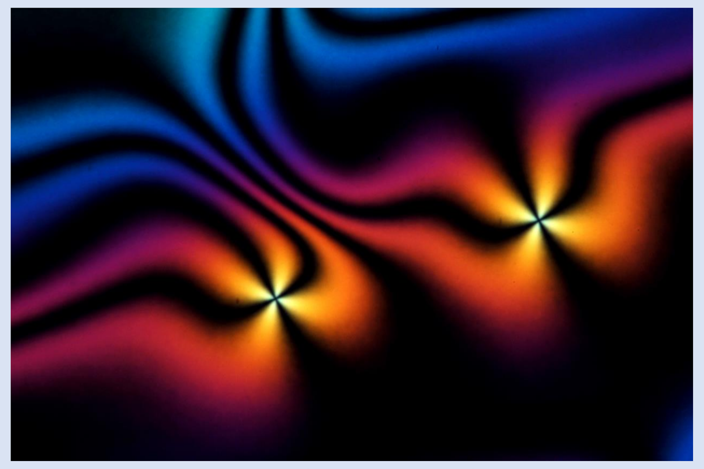


image of a point defect

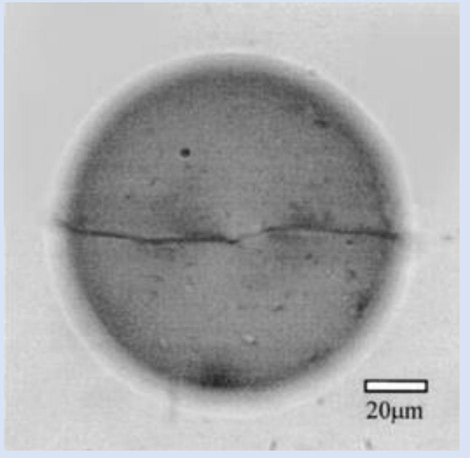


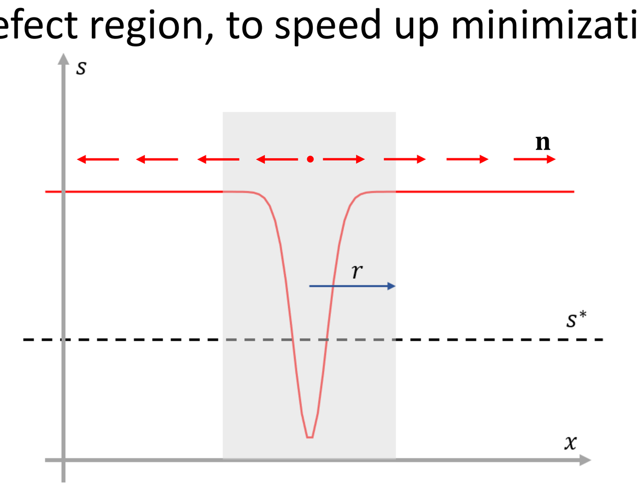
image of a "Saturn Ring" defect

Domain Decomposition and Subdomain Iterations

Regions near the defect are extremely stiff with respect to gradient flow iterations.

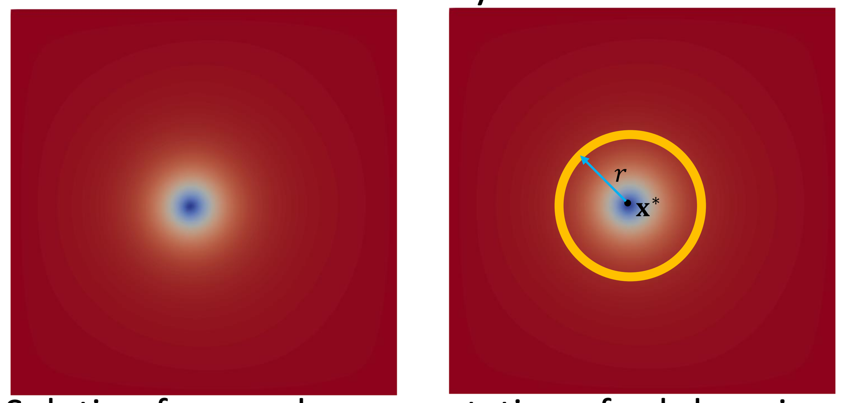
The model parameters $\mathbf{n}$ and s are tightly coupled near the defects.

Use alternating Schwarz method, with extra steps in the defect region, to speed up minimization.



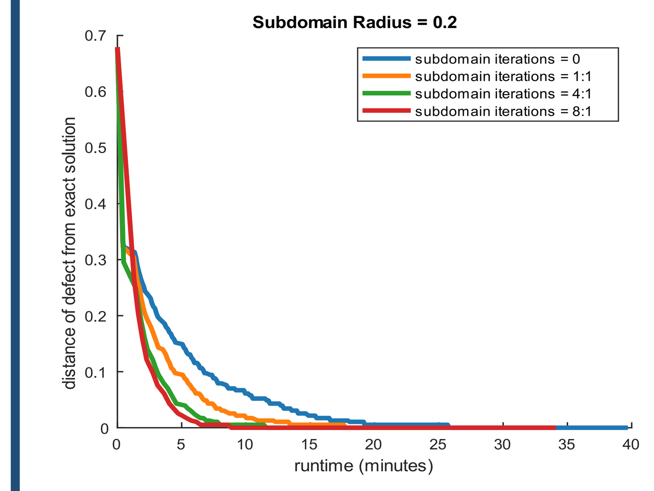
Proposed algorithm:

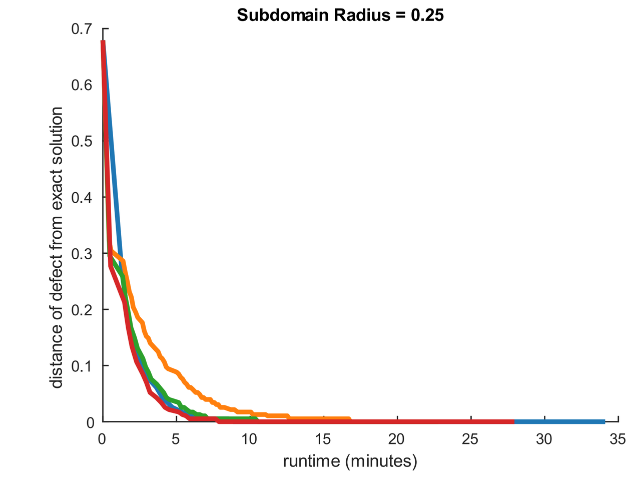
1. For $i = 1 \ldots n$
   1. Perform a gradient flow step for the whole domain.
   2. Determine subdomain
      let $\mathbf{x}^* = \min_{\mathbf{x}} s(\mathbf{x})$
      $S^* = \{\mathbf{x} \in \Omega : |\mathbf{x} - \mathbf{x}^*| < r\}$
   3. Perform k gradient descent steps inside S^* using exterior of S^* as boundary conditions.

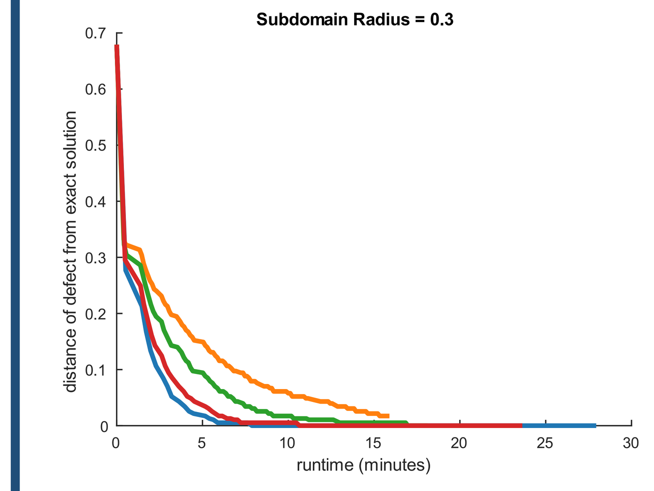


Solution for s and representation of subdomain

2D Results



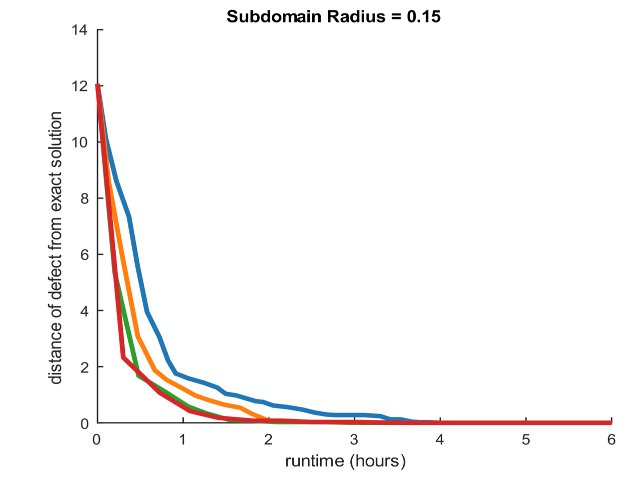


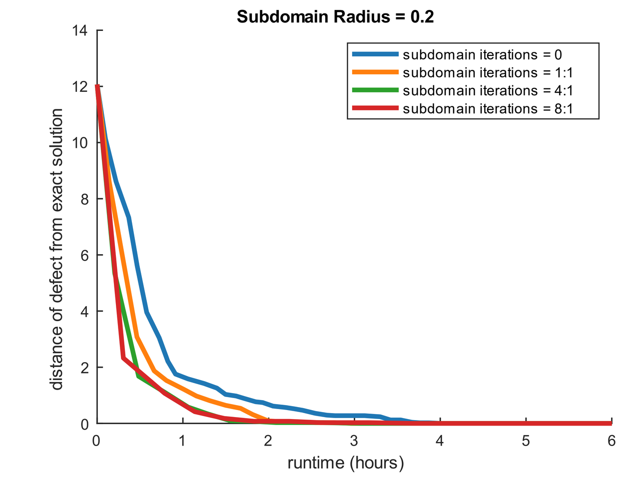


Increasing the number of iterations in the subdomain improves runtime.

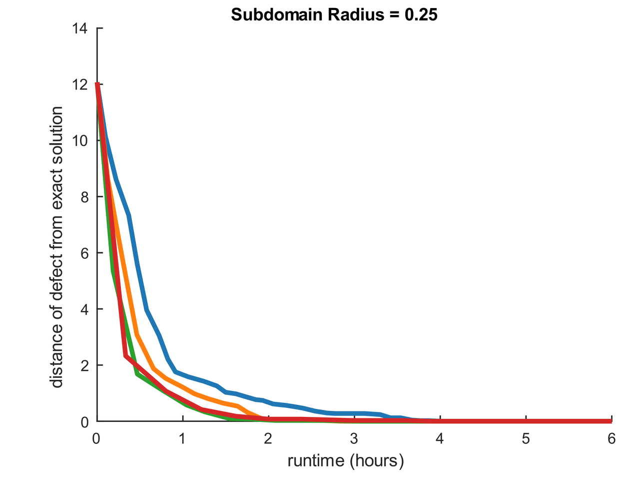
Small subdomains are more successful than large subdomains.

3D Results

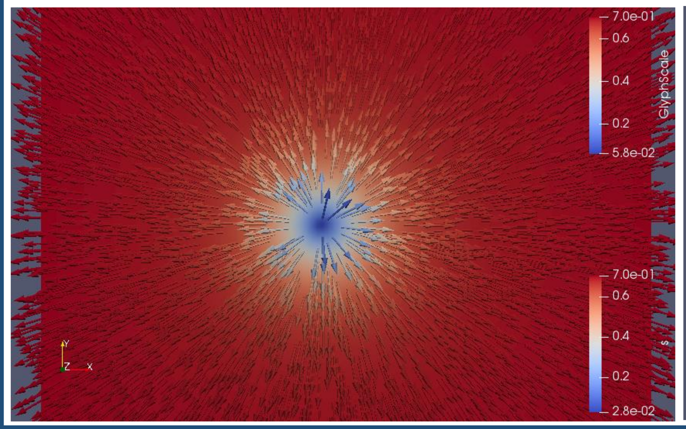




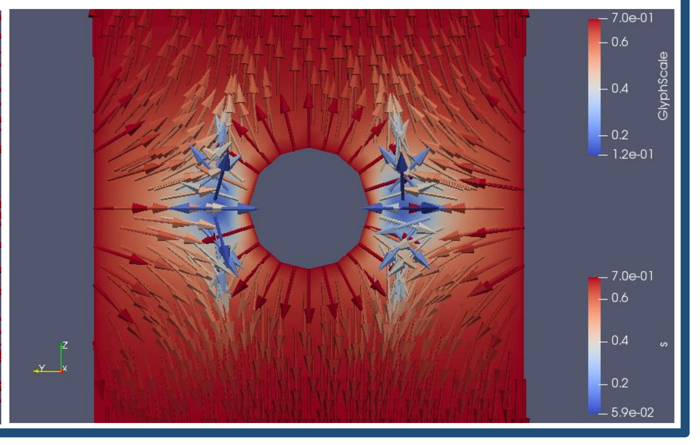
The difference for 3D simulations is on the order of hours.



2D Point Defect



Cross-section of Saturn Ring Defect



Literature cited

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Acknowledgments

The author acknowledges financial support by the NSF via DMS-1555222 (CAREER) with additional support from the Center for Computation & Technology at Louisiana State University and computer support is provided by HPC@LSU computing.