# Instabilities of 3D dry active nematics: particle-based simulation and perturbation analysis


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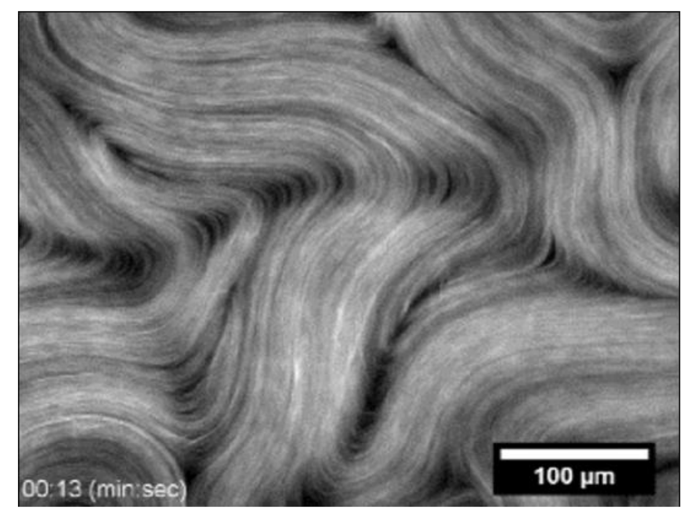
## Background

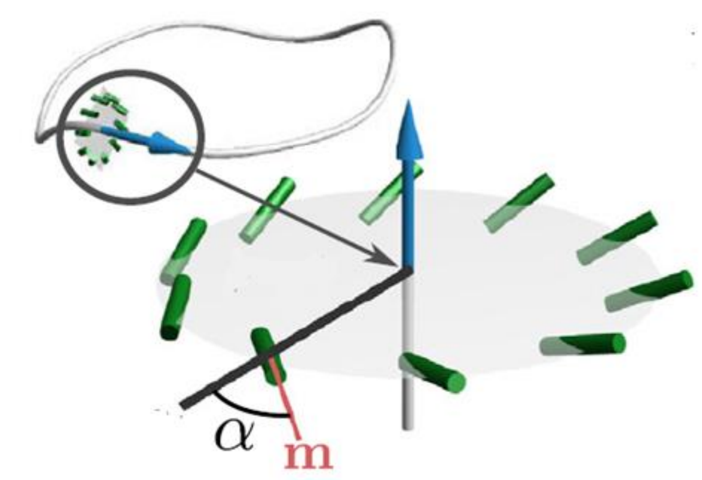
With self-propelled velocity, nematics may deviate from aligned ordered state to form pairs of topological defects. In 3D, such defects will be line-like and the simplest model is disclination loop. To analyze the location and density of defects can strongly help us understand the configuration and dynamics of active nematics.

### 2D active nematics



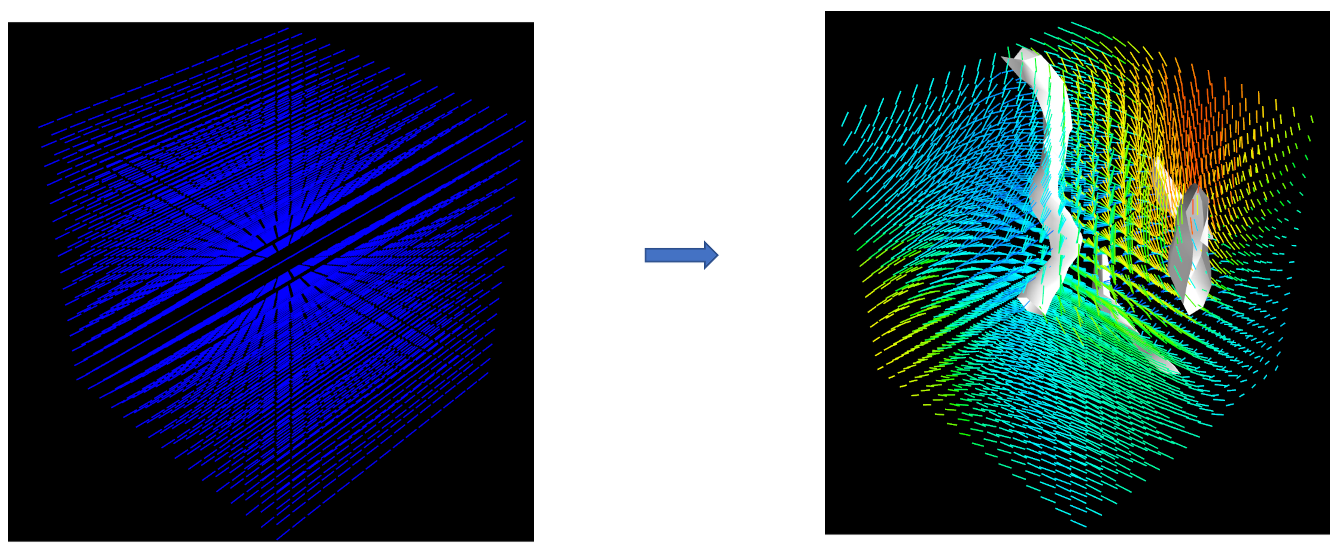

DeCamp, *et al*, **Nature**, 2015

### 3D disclination loop




J. Binysh, *et al*, **Phys. Rev. Lett.**, 2020

## Instability



**Colored dash:** director and its orientation

**White region:** disordered lines

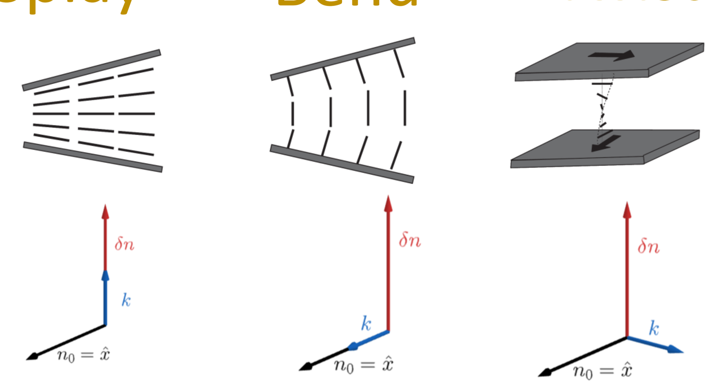
## Introduction

Unlike the previous research, in this project we focused on the **DRY** system, namely there is no hydrodynamics interaction or no solvent. This can help us understand how only active force and filaments' alignment influence the emergent dynamics.

We aimed to investigate the **instability** of 3D active nematics: how the filaments reorient from initial aligned state and form disclination loops.

## Question 1: What deformation appears first? By perturbation analysis on continuum description

There are 3 different kinds of deformation modes in nematics. With $\delta n$ (linear perturbation) and Fourier transform, we can depict each mode by orientation of wave vector $k$.




Also by such perturbation analysis, we investigate the equation in the right, to find which orientation of $k$ is the most unstable.

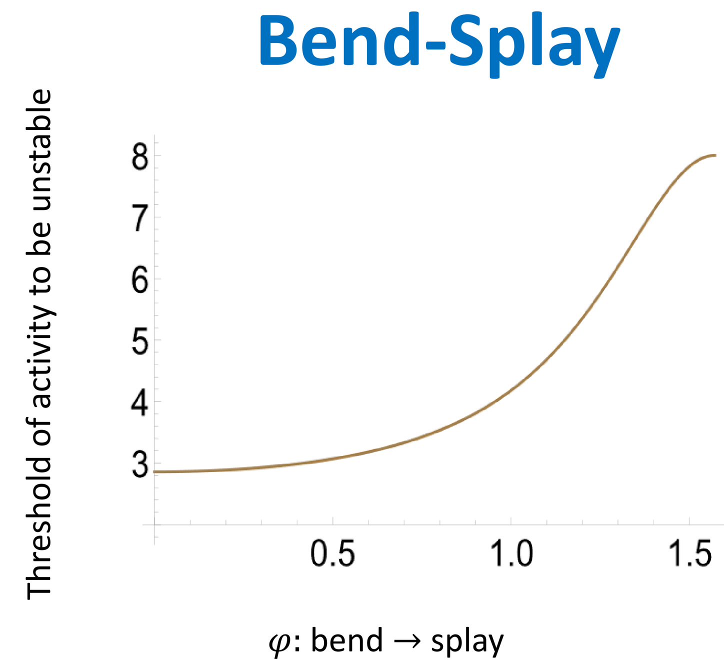
Material derivative — Free energy — Rotation — Activity induced flow alignment

$$\partial_t \mathbb{Q} + \mathbf{u}\cdot(\nabla\mathbb{Q}) = -\frac{1}{\gamma}\frac{\delta\mathcal{F}}{\delta\mathbb{Q}} + (\mathbb{Q}\Omega - \Omega\mathbb{Q}) + \lambda\left[\mathbb{Q}\mathrm{E} + \mathrm{E}\mathbb{Q} - \frac{2}{3}\mathrm{Tr}(\mathrm{E}\mathbb{Q})\mathbb{I}\right] + \lambda\rho\left[\mathrm{E} - \frac{1}{3}\mathrm{Tr}(\mathrm{E})\mathbb{I}\right]$$

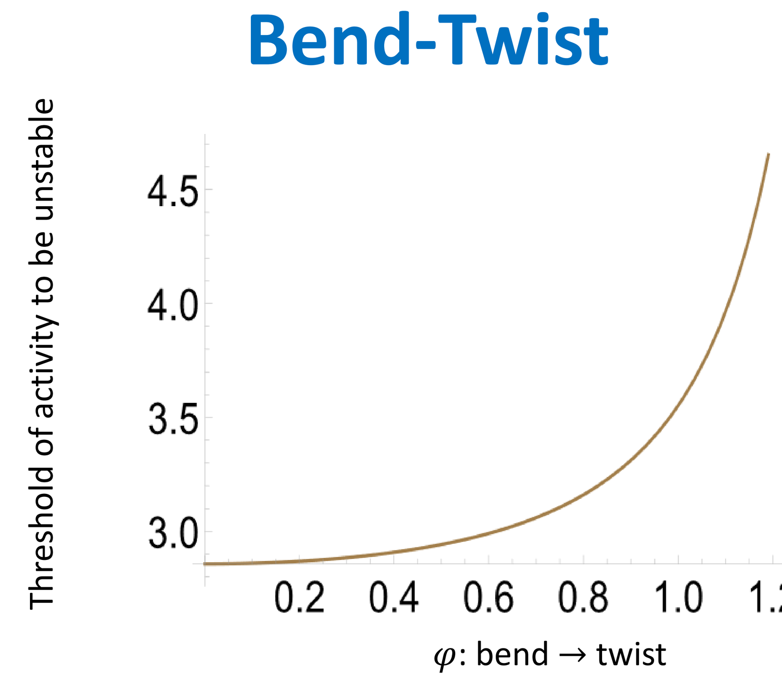
$-\zeta\mathbf{u} = \alpha\nabla\cdot\mathbb{Q}$ **DRY** system: velocity only comes from activity

Considered the system of two coupled deformations for simplicity:

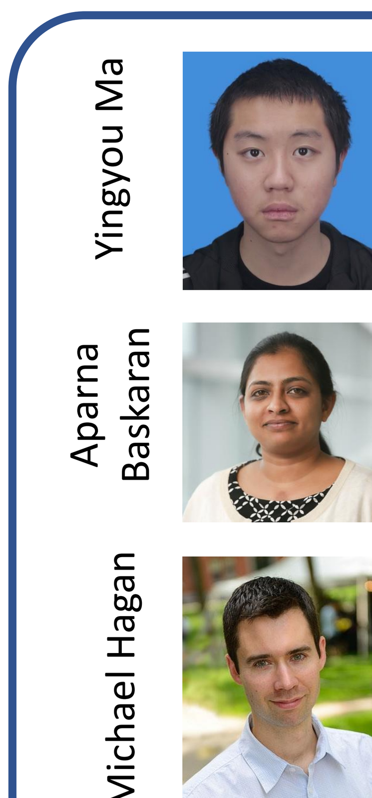
### Bend-Splay



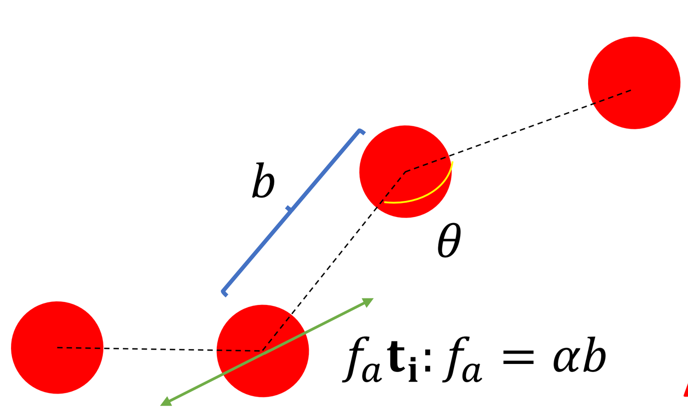

### Bend-Twist




**Conclusion: Bend** will firstly go unstable

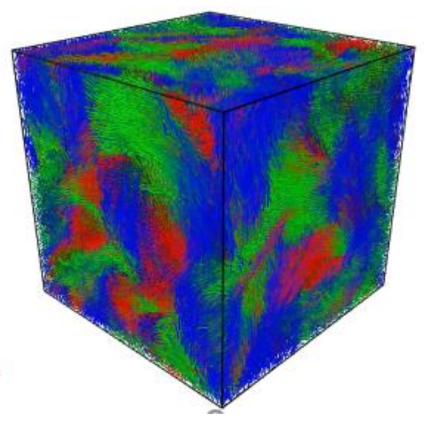



## Question 2: How disclination loops emerge? By particle-based simulation (semi-flexible filaments)

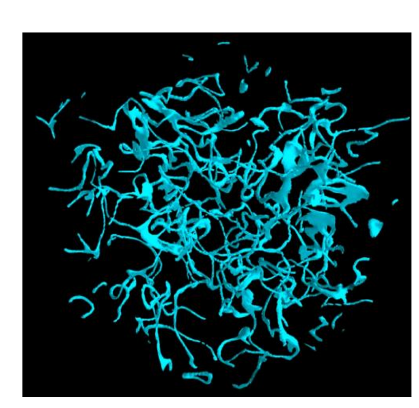



$$m_i\ddot{r}_i = f_i^a - \gamma\dot{r}_i - \nabla_{r_i}U(r_{ij}) + R_i(t)$$

Activity — Friction — Potential — Thermal Noise

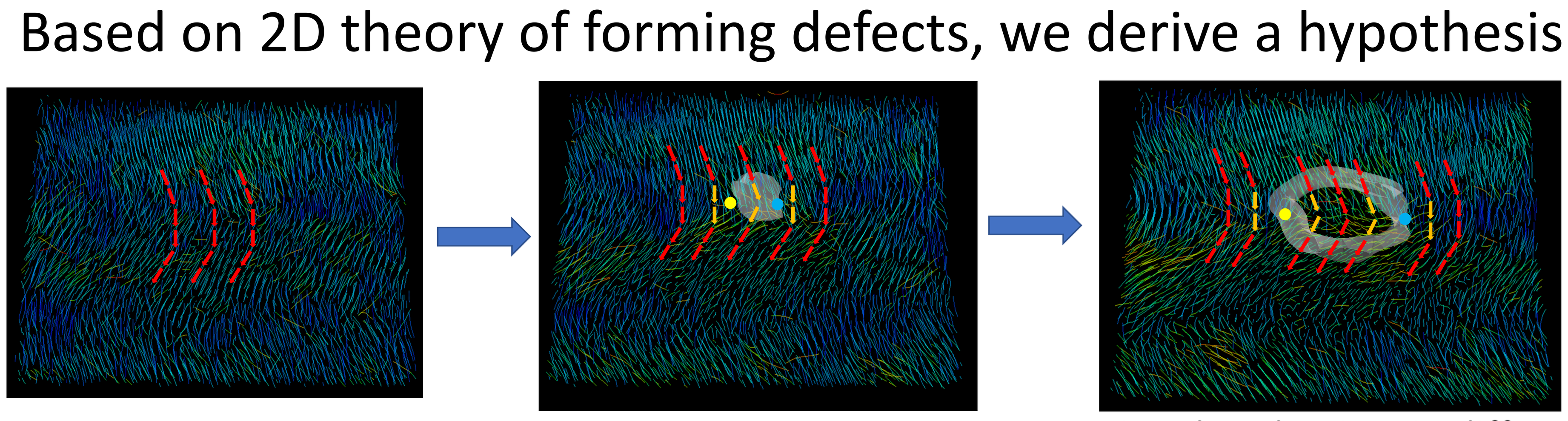


**DRY** system: Only particles of nematics



The network of disordered regions

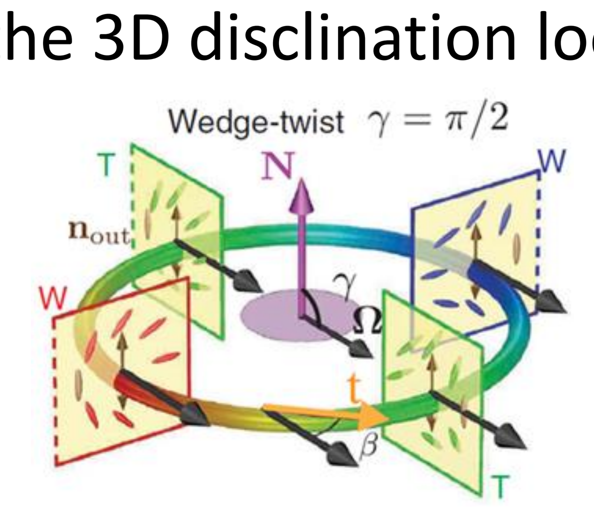
Based on 2D theory of forming defects, we derive a hypothesis of the 3D disclination loops' appearing (white: disordered):



Start with bend instability (supported by question 1)

Net active force form defects (analog to 2D theory)

Disordered points in different slices form a loop




This hypothesis will always form wedge-twist loops. In the shown trial, every loop is wedge-twist.

G. Duclos, *et al*, **Science**, 2020

**Conclusion: 2D-analog** hypothesis

## Summary

We investigated the initial instability period of active dry nematic.
The perturbation analysis shows bend is always firstly unstable.
A mechanism of forming a disclination loop was proposed.

## Future work

Check if there is another way of forming a loop.
Investigate the evolving and interaction of loops.
Check the results by continuum simulation.