An Open Problem in Pattern Forming Systems

Edward McDugald

University of Arizona

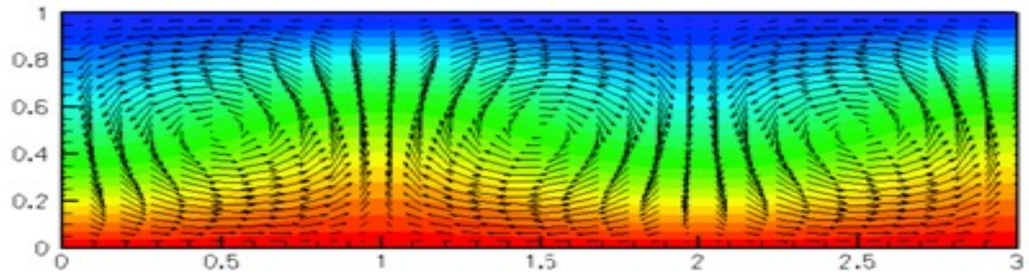
Advised by Shankar Venkataramani and Alan Newell

Overview

- This work concerns pattern forming systems, that arise as microscopic gradient flows that are translationally and rotationally invariant.
  - Informally, any PDE admitting straight parallel roll solutions on an infinite domain satisfies this description.
- We will find that there is a universal macroscopic model that governs such microscopic systems.
- We will pose an open problem- a behavior observed in the microscopic model not deduced by the macroscopic model.
- We will discuss ML-based approaches to analyze the problem.

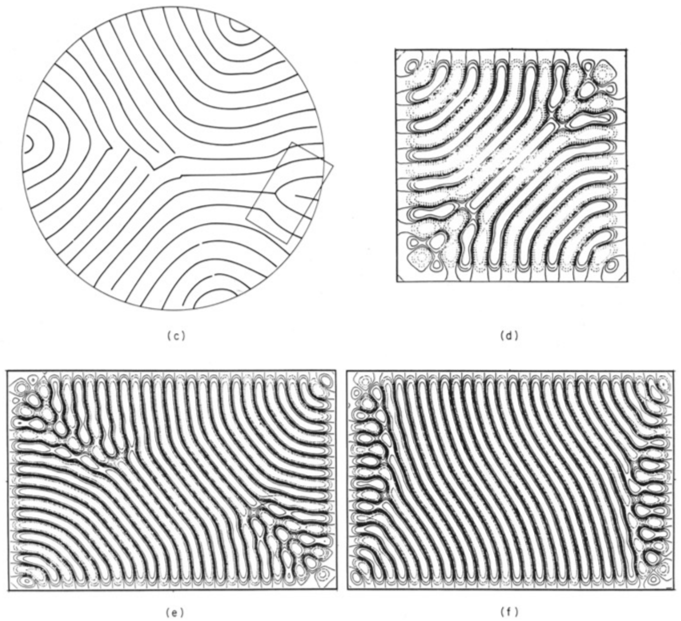
The Microscopic Model (Convection)

- The canonical example of such patterns in nature is given by Rayleigh-Benard convection.



- We take as our example microscopic model the Swift-Hohenberg PDE:

$$w_t = -(1+\nabla^2)^2 w + Rw - w^3.$$



Derivation of Macroscopic Model- Procedure

1. Introduce a small parameter and modulational ansatz
2. Average the energy functional
3. Compute variations of the averaged energy with respect to amplitude and phase, up to desired order
4. Obtain macroscopic equations

$$w = \sum A_n(k^2)\cos(n\theta) \quad \text{(for real fields)}$$
$$w = A(k^2, \boldsymbol{X}, T)e^{i\theta(\boldsymbol{x},t)} \quad \text{(for complex fields).}$$

$$\begin{aligned} \boldsymbol{X} &= \epsilon \boldsymbol{x} \\ T &= \epsilon^2 t \\ \Theta(\boldsymbol{X}, T) &= \epsilon\theta(\boldsymbol{x}, t) \\ k &= \|\boldsymbol{k}\| \\ \epsilon &= \frac{l}{L} \quad \text{The inverse aspect ratio.} \end{aligned}$$

$$\nabla_{\boldsymbol{x}} w = e^{i\theta}(i\boldsymbol{k} + \epsilon\nabla_{\boldsymbol{X}})A$$

$$\overline{E} = \frac{1}{2\pi}\int E\,d\theta$$

The Unregularized Macroscopic Model

- For complexified Swift-Hohenberg, we have:

$$E = \int \left((\nabla^2 + 1)w(\nabla^2 + 1)w^* - Rww^* + \frac{1}{2}w^2 w^{*^2} \right) dx.$$

- After applying the modulational ansatz, this becomes:

$$E = \int \left((k^2 - 1)^2 A^2 - RA^2 + \frac{1}{4}A^4 + K \right) d\boldsymbol{x}$$
$$+ \epsilon^2 \int \left((2\boldsymbol{k} \cdot \nabla A + \nabla \cdot \boldsymbol{k}A)^2 + 2(1 - k^2)A\nabla^2 A \right) d\boldsymbol{x}.$$

$$\delta E = \frac{\delta E}{\delta w}\delta w + \frac{\delta E}{\delta w^*}\delta w^* = -2A_t \delta A - 2A^2 \Theta_t \delta\theta.$$

- Analyzing the leading order terms, one obtains:
  - The Eikonal Solution: $A^2 = R - (K^2 - 1)^2.$
  - The Unregularized CN: $A^2 \Theta_T + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{k} B(k^2) = 0$
  - Where: $B(k^2) = A^2(k^2) \frac{dA^2(k^2)}{dk^2}$

The Regularized Macroscopic Model

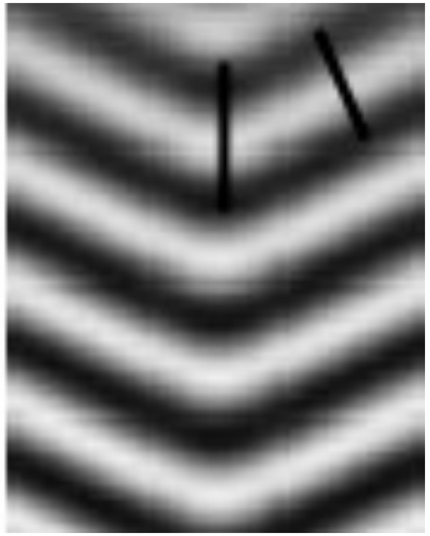
- For the unregularized Cross-Newell Equation to be well posed, we require that:

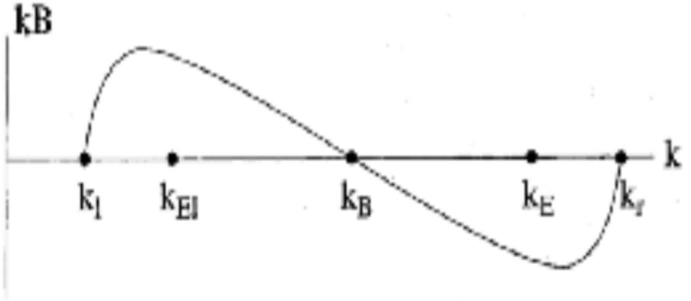
$$\frac{d}{dk}(kB(k^2)) < 0$$
$$B(k^2) < 0.$$

$$A^2\Theta_T + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{k}B(k^2) = 0$$

- But, this can be easily violated, as along line defects, the wavenumber is outside the Busse balloon.
- Bringing in the $O(\epsilon^2)$ terms yields the RCN:

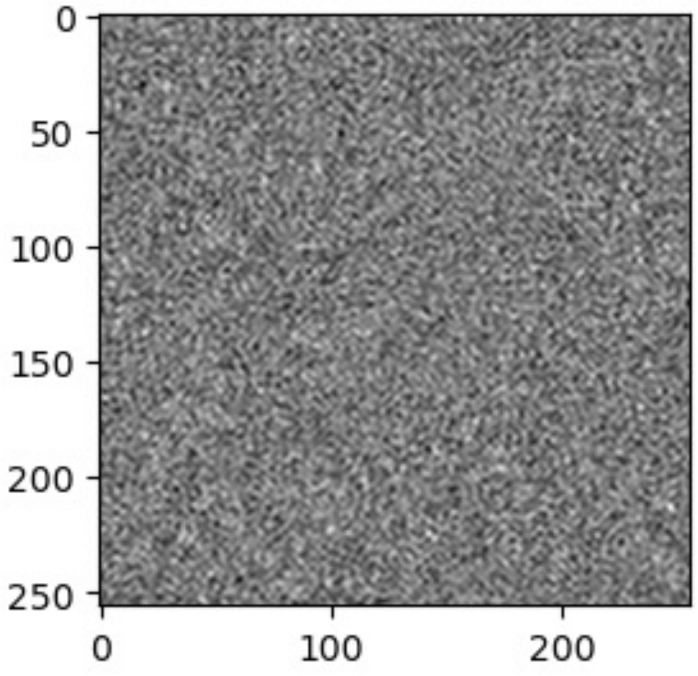
$$A^2(k_B^2)\Theta_T + \nabla \cdot \boldsymbol{k}B + \epsilon^2 A^2(k_B^2)\nabla^4\Theta = 0.$$

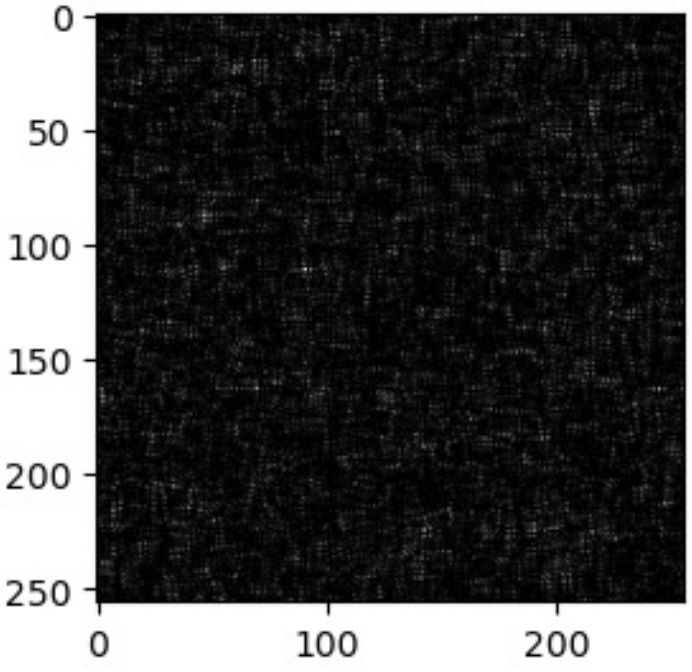




RCN for Real Fields

- The RCN: $\langle w_\theta^2 \rangle \Theta_T + \nabla \cdot \boldsymbol{k} B + \epsilon^2 \langle w_\theta^2 \rangle \nabla^4 \Theta = 0.$





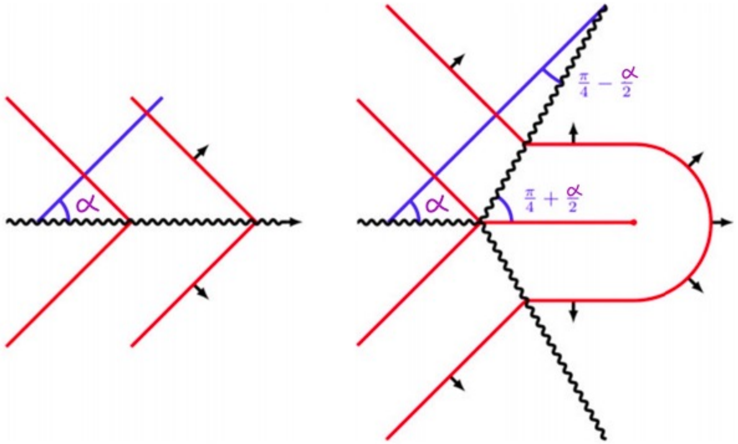
Macroscopic Energy Functional and Self-Dual Solutions

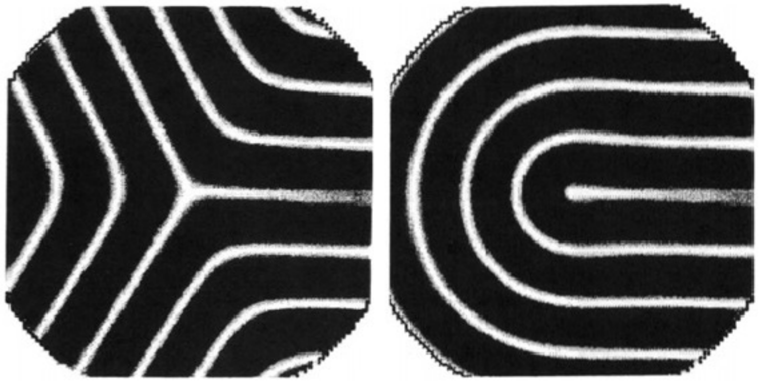
- The macroscopic energy consists of a sum of a “bending” energy and a “stretching energy”.

$$\eta \nabla^4 \theta + \nabla \cdot \boldsymbol{k} B = -\frac{\delta \overline{E}}{\delta \theta}$$

$$\overline{E} = \int \left(\frac{1}{2}\eta |\nabla^2 \theta|^2 + \frac{\alpha}{2} G^2 \right) d\boldsymbol{x}$$

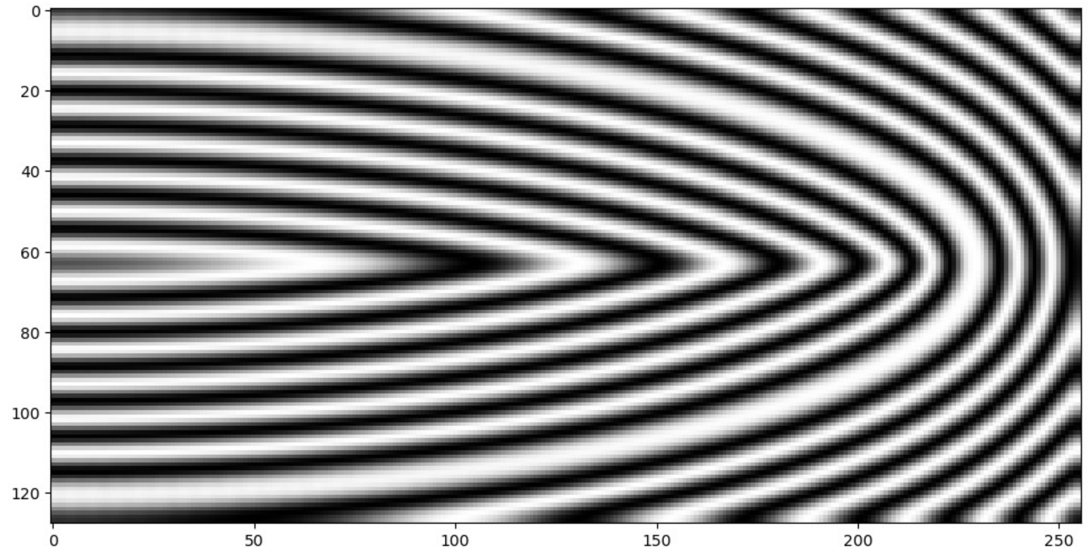
- Stationary solutions can be deduced by balancing the strain and bending energies.

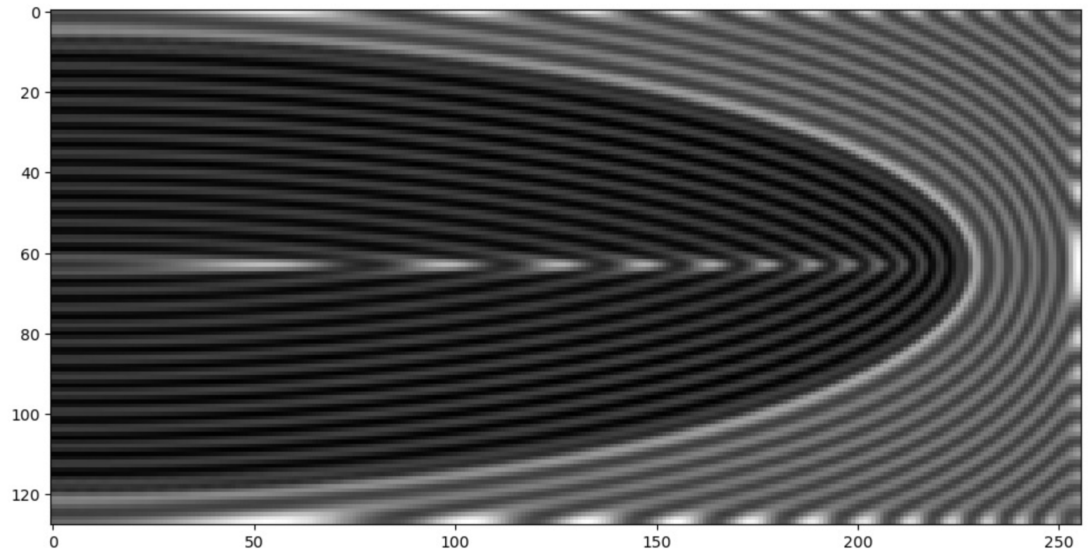




An Open Problem

- There is a behavior observed when solving SH on an ellipse that is not deduced by the macroscopic equations.
- Some possibilities:
  - The behavior is captured by RCN, we just don't know how
  - The RCN should include some higher order terms
  - A new order parameter emerges





ML Motivation and SINDy ("Discovering" SH)

- A basic statement of the problem is that there is a behavior in a microscopic model that the macroscopic model does not predict.
- This raises the possibility that the macroscopic equation is incomplete, and there is an additional term required to capture the microscopic behavior.
- Perhaps an additional term could be obtained through SINDy-like approaches.

$$\mathbf{U}_t = \mathbf{\Theta}(\mathbf{U},\mathbf{Q})\xi$$

$$\begin{bmatrix} u_t(x_0,t_0) \\ u_t(x_1,t_0) \\ u_t(x_2,t_0) \\ \vdots \\ u_t(x_{n-1},t_m) \\ u_t(x_n,t_m) \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & u(x_0,t_0) & u_x(x_0,t_0) & \dots & u^5u_{xxx}(x_0,t_0) \\ 1 & u(x_1,t_0) & u_x(x_1,t_0) & \dots & u^5u_{xxx}(x_1,t_0) \\ 1 & u(x_2,t_0) & u_x(x_2,t_0) & \dots & u^5u_{xxx}(x_2,t_0) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & u(x_{n-1},t_m) & u_x(x_{n-1},t_m) & \dots & u^5u_{xxx}(x_{n-1},t_m) \\ 1 & u(x_n,t_m) & u_x(x_n,t_m) & \dots & u^5u_{xxx}(x_n,t_m) \end{bmatrix}} \begin{bmatrix} \\ \\ \xi \\ \\ \\ \end{bmatrix}$$

$$\xi = \mathrm{argmin}_{\hat{\xi}} \|\Theta(u)\hat{\xi} - u_t\|_2^2 + \lambda\|\hat{\xi}\|_0.$$

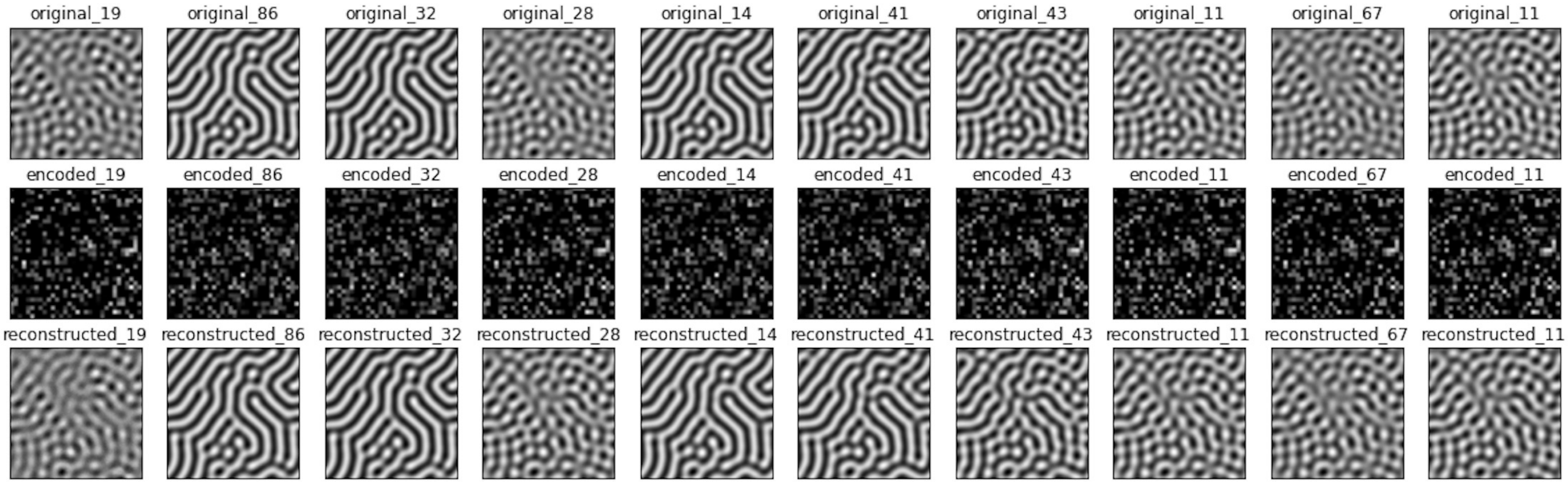
```
c = TrainSTRidge(X,u_t,10**-5,1)
print_pde(c, description)
```

```
u_t = (-0.507735 +0.000000i)u
    + (-1.016235 +0.000000i)u^3
    + (97.489916 +0.000000i)u_{xx}
    + (97.490143 +0.000000i)u_{yy}
    + (-99.522287 +0.000000i)lapu
    + (-1.016119 +0.000000i)biharmu
```

[find_sh.ipynb]

Adding an Autoencoder for macroscopic discovery

- SINDy methods have been combined with an autoencoder to predict governing equations in a different coordinate system. For example, deducing $\ddot{\theta} = \sin(\theta)$ from video of a swinging pendulum. The autoencoder gives a latent space representation, on which the SINDy procedure is applied. [autoencoder_swift_hohenberg.ipynb]



Other applications of ML

- In analyzing the evolution of solutions and energy on the ellipse, we would like to track the wavenumber $k = |\nabla\theta|$ and the Gaussian curvature $\theta_{xx}\theta_{yy} - {\theta_{xy}}^2$ of the pattern.
- The wave vector is difficult to compute, even with Hilbert transforms.
- We can generate patterns with prescribed wave vectors and train a neural net to predict the vector field.
- Once the wave vector is obtained, the gaussian curvature is easy to compute.

Next Steps

- Compute the macroscopic derivation for real fields by hand. This is more delicate than it was for complex fields.
- Understand the relationship between the Jacobian of the map from cartesian coordinates to the wave vector, and its relation to self-dual solutions.
- Tune the autoencoder and add SINDy procedure to loss function.
- Use a neural net to estimate wavenumbers from numerical data.

References

- Rudy, Samuel H, Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. "Data-driven Discovery of Partial Differential Equations." Science Advances 3.4 (2017): E1602614. Web.
- Champion, Kathleen, Bethany Lusch, J Nathan Kutz, and Steven L Brunton. "Data-driven Discovery of Coordinates and Governing Equations." Proceedings of the National Academy of Sciences - PNAS 116.45 (2019): 22445-2451. Web.
- Alan C. Newell and Shankar C. Venkataramani. ”The Universal Behavior of Modulated Stripe Patterns.” (2022)
- Newell, A.C., T. Passot, C. Bowman, N. Ercolani, and R. Indik. "Defects Are Weak and Self-dual Solutions of the Cross-Newell Phase Diffusion Equation for Natural Patterns." Physica. D 97.1 (1996): 185-205. Web.