Predicting Emergent Dynamics

Project 01

Introdution:

kinetic model

$$\Psi(\mathbf{x}, \mathbf{p}, t)$$

Smoluchowski equation,

$$\frac{\partial \Psi}{\partial t} + \nabla_{\mathbf{x}} \cdot (\dot{\mathbf{x}}\Psi) + \nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}}\Psi) = 0,$$

$$\dot{\mathbf{x}} = \mathbf{u} - d_T \nabla_{\mathbf{x}} \log \Psi,$$

$$\dot{\mathbf{p}} = (\mathbf{I} - \mathbf{pp}) \cdot (\nabla \mathbf{u} + 2\zeta \mathbf{D}) \cdot \mathbf{p} - d_R \nabla_{\mathbf{p}} \log \Psi.$$

Stokes flow as

$$-\Delta \mathbf{u} + \nabla P = \nabla \cdot \boldsymbol{\Sigma}, \quad \nabla \cdot \mathbf{u} = 0,$$

$$\boldsymbol{\Sigma} = \alpha \mathbf{D} + \beta \mathbf{S} : \mathbf{E} - 2\zeta\beta (\mathbf{D} \cdot \mathbf{D} - \mathbf{S} : \mathbf{D}).$$

zeroth and second moments c and $\mathbf{D}$.

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = d_T \Delta c,$$

$$\mathbf{D}^{\nabla} + 2\mathbf{S} : \mathbf{E} = 4\zeta (\mathbf{D} \cdot \mathbf{D} - \mathbf{S} : \mathbf{D}) + d_T \Delta \mathbf{D} - 2d d_R \left(\mathbf{D} - \frac{c}{d}\mathbf{I}\right).$$

$$\mathbf{D}^{\nabla} = \partial \mathbf{D}/\partial t + \mathbf{u} \cdot \nabla \mathbf{D} - \left(\nabla \mathbf{u} \cdot \mathbf{D} + \mathbf{D} \cdot \nabla \mathbf{u}^{\top}\right)$$

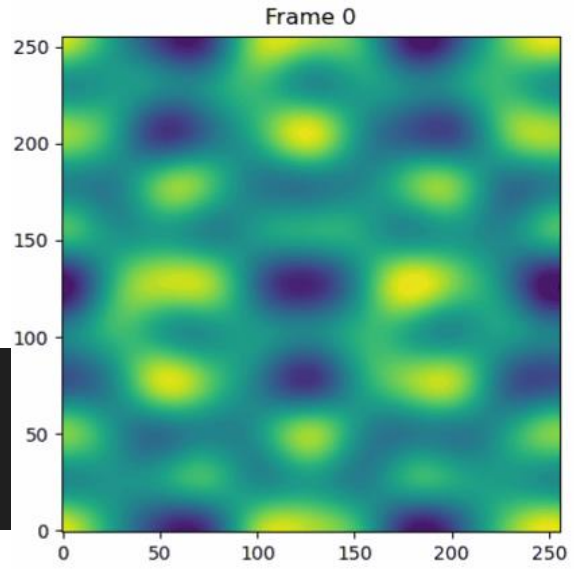
Varied Physical Parameters. $\alpha \in \{-1,-2,-3,-4,-5\}$ $\beta = 0.8$; $\zeta \in \{1,3,5,7,9,11,13,15,17\}$.

Fields present in the data. concentration (scalar field), velocity (vector field), orientation tensor (tensor field), strain-rate tensor (tensor field).

```
Number of simulation repetitions: 24

Size of each repetition: torch.Size([81, 256, 256, 11])

Field names: ['concentration', 'velocity_x', 'velocity_y', 'D_xx', 'D_xy', 'D_yx', 'D_yy', 'E_xx', 'E_xy', 'E_yx', 'E_yy']
```



The goal:

Forecast the time evolution of observables/features extracted from the dataset.

Visualize temporal trends, compute autocorrelation, and assess characteristic timescales.

```
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```

Observable	Formula (in discrete form)	Physical meaning
Mean concentration	$\langle c \rangle$ = mean(`concentration`)	Average density
Kinetic energy	$\langle (vx^2+vy^2)/2 \rangle$	Flow intensity
Enstrophy	$\langle (\partial x\, vy - \partial y\, vx)^2 \rangle$	Vorticity measure
Strain rate magnitude	$\langle \sqrt{(E\_xx^2 + E\_xy^2 + E\_yx^2 + E\_yy^2)} \rangle$	Deformation strength
Nematic order	$\langle \sqrt{(D\_xx^2 + D\_xy^2 + D\_yx^2 + D\_yy^2)} \rangle$	Orientation strength
Cross-correlation	$\langle vx D\_xx + vy D\_yy \rangle$	Flow–orientation coupling

Global Plan:

1. Obtain the time-series trough feature extraction
2. Define the forecasting window
3. Apply base forecasting models: ARIMA, Persistence, linear regression, CNextU-net
4. Compare and report model performance

Next week work:

Review and implement advanced ML forecasting models RNNs, LSTMs, and attention-based models

Dataset	FNO	TFNO	Unet	CNextU-net
active_matter	0.3691	0.3598	0.2489	**0.1034**