Learning phase-transition kinetics from in situ STEM videos

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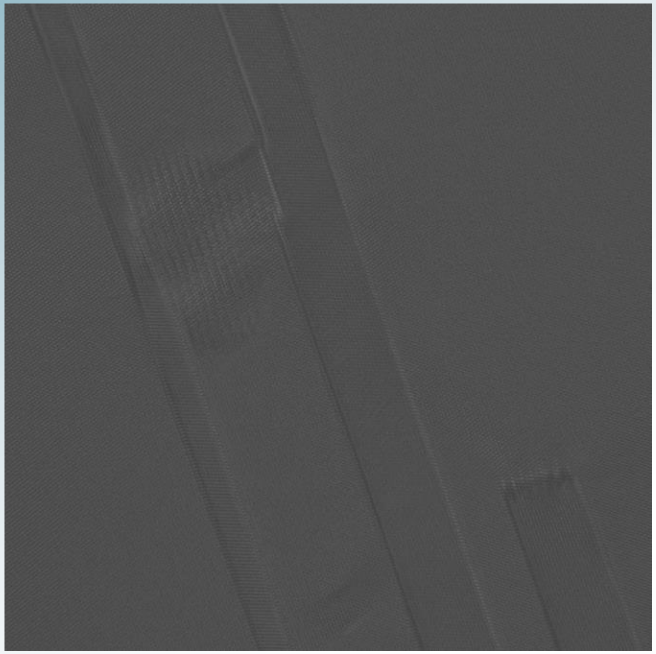
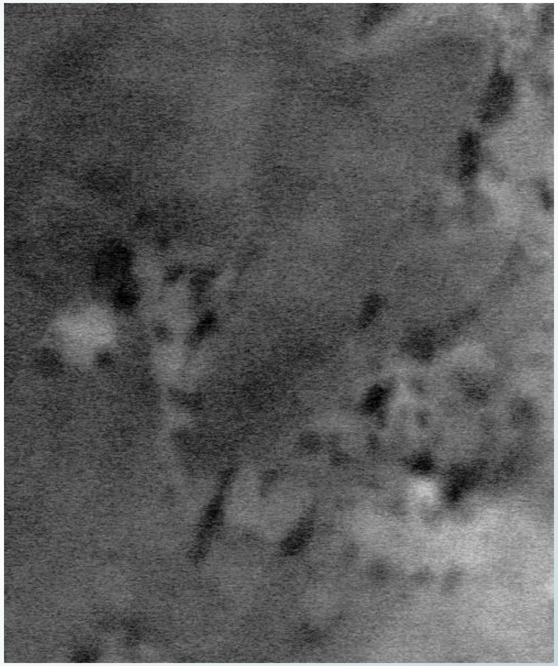
Recording phase-transition kinetics





Question:

Learning phase-transition kinetics from in situ STEM videos

Quantitative description of phase-transition kinetics

Domain knowledge: Phase-field models

Model A: Allen-Cahn equation

$$\frac{1}{M}\frac{\partial \phi}{\partial t} = \kappa \Delta \phi - g(\phi)$$

Model B: Cahn-Hillard equation

$$\frac{1}{M}\frac{\partial c}{\partial t} = \Delta\left(g(c) \; - \gamma \Delta c\right)$$

Bulk free-energy density

$$g(\phi) = \frac{\partial f}{\partial \phi}$$

$$g(c) = \frac{\partial f}{\partial c}$$

$\phi(t, x, y)$: phase field
$c(t, x, y)$: concentration field

Using domain knowledge

Learning phase-transition kinetics from in situ STEM videos

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To parametrize phase-field model based on in situ STEM videos

- For experimentalists:
  - Quantitative description of experiments.
  - Quantitative relationship between processing paras and kinetics.
- For simulation community:
  - Realistic models directly obtained from experiments.

Challenge

Phase field models are **partial differential equations**

Noise accumulation and amplification make it hard to use explicit methods

E.g., Finite difference -> high noise

First smoothing -> highly biased by smoothing parameters

An elegant solution

Data: $I^n(t^n, x^n, y^n), \qquad n = 1 \ldots N$

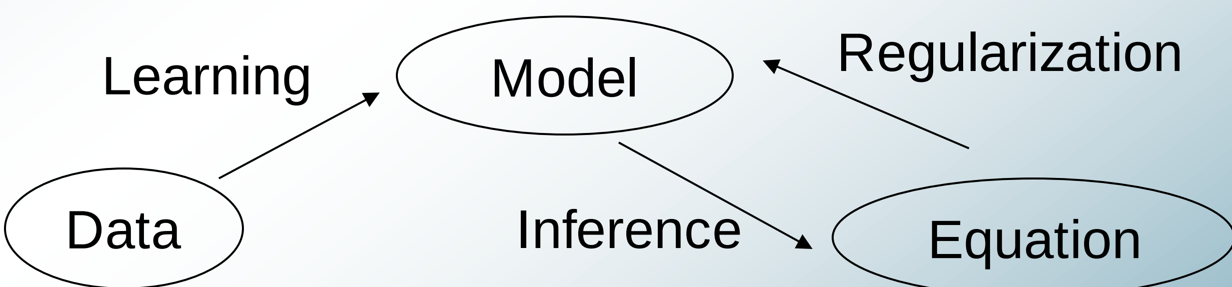
Physics-informed neural networks

$$Loss = \sum_{n=1}^{N} |I(t^n, x^n, y^n) - I^n|^2 + \sum_{n=1}^{N} |\mathrm{Residual}(I(t^n, x^n, y^n))|^2$$

data-fidelity term   Penalizing inequality of equation

Traning parameters: weights in NNs and paras in Eqns.

Raissi et al., Science (2020).
J. Comput. Phys. (2019).



To summarize the pathway

In situ STEM

data

Neural networks

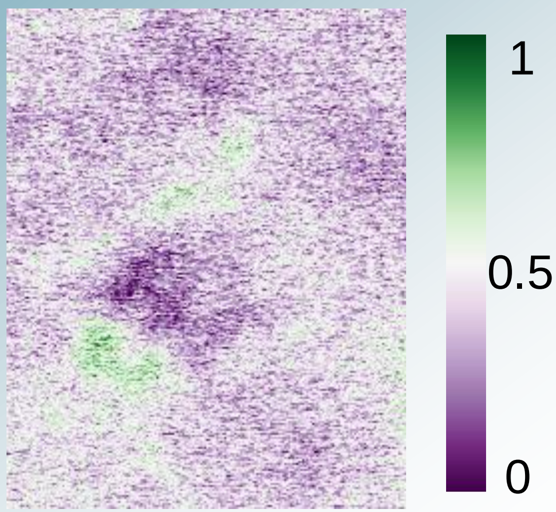
machine learning algorithm

→

Parametrized phase field model

describing phase-transition kinetics quantitatively

How to interpret intensity?



intensity

$I^n(t^n, x^n, y^n)$

Phase field

$\phi^n(t^n, x^n, y^n)$

Allen-Cahn equation

$$\frac{1}{M}\frac{\partial \phi}{\partial t} = \kappa\Delta\phi - g(\phi)$$

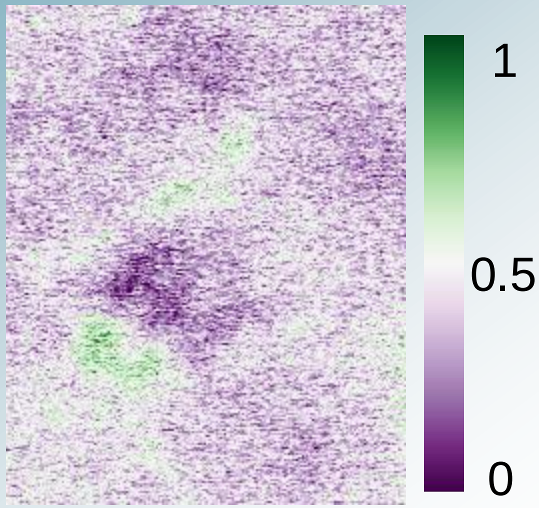
Concentration field

$c^n(t^n, x^n, y^n)$

Cahn-Hillard equation

$$\frac{1}{M}\frac{\partial c}{\partial t} = \Delta\left(g(c) \;- \gamma\Delta c\right)$$

First try



- Interpreting intensity $I(t,x,y)$ as phase field

$I(t,x,y)$: 0 – 255

$\phi(t,x,y)$: 0 – 1

- To parametrize Allen-Cahn equation:

$$\frac{1}{M}\frac{\partial \phi}{\partial t} = \kappa \Delta \phi - g(\phi)$$

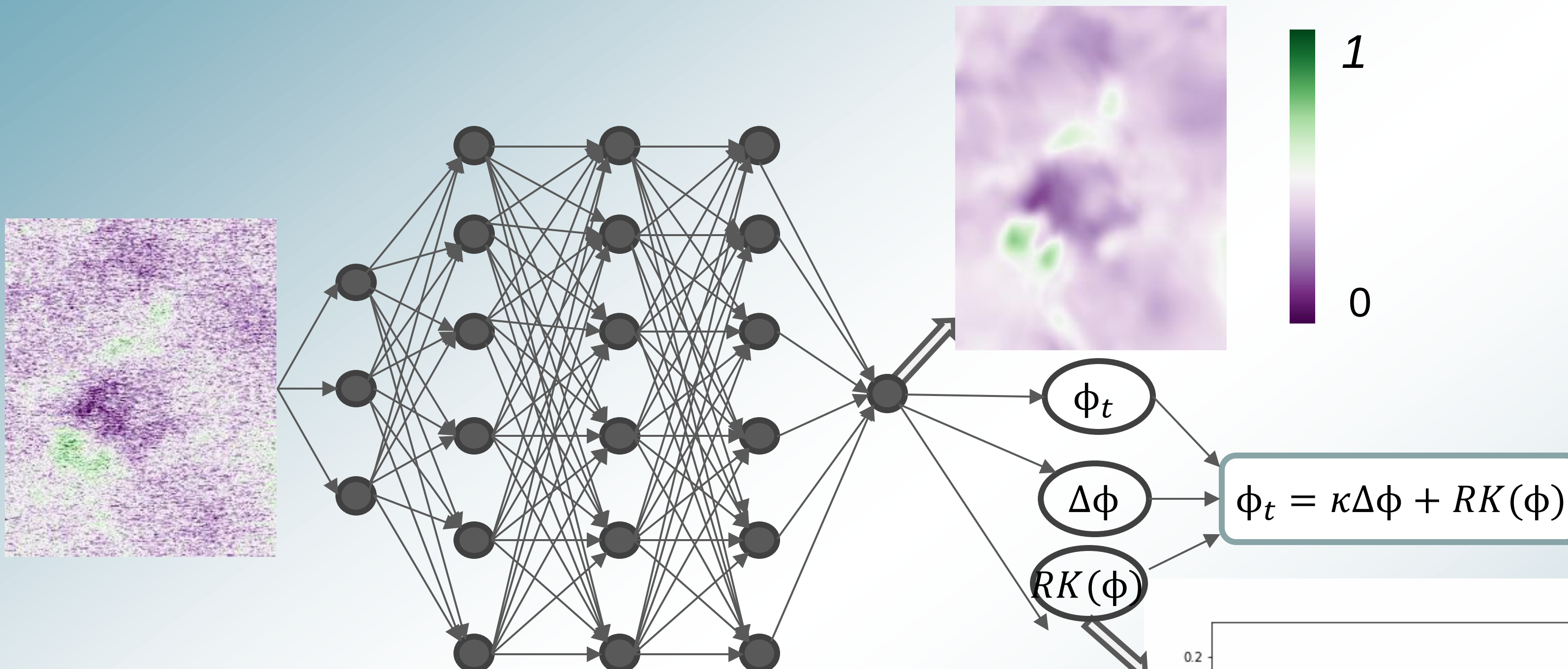
- Use Redlich-Kister polynomial to approximate $g(\phi)$

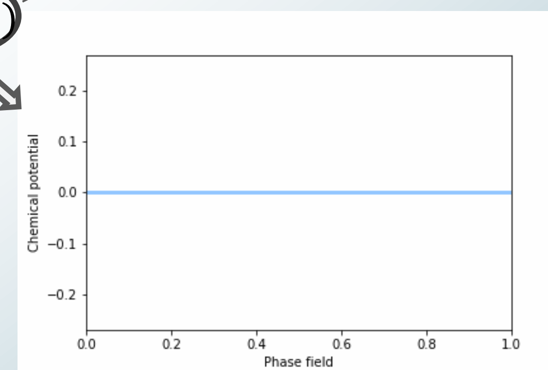
$$g(\phi) = \sum_{n=0}^{N} \alpha_n \cdot \phi(1-\phi)\,(1-2\phi)^n$$

- Training parameters: weights in NNs +

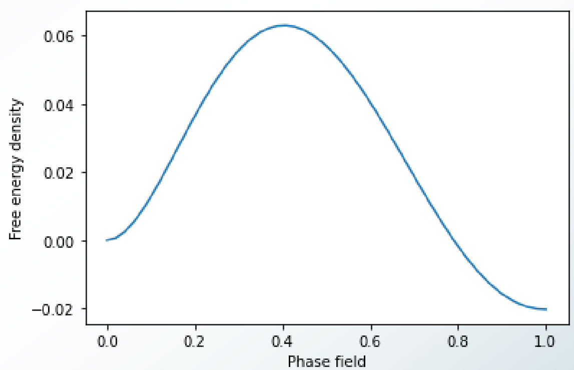
$\kappa,\ \alpha_0, \alpha_1, \alpha_2$

- number of data points: 220,400,000





Free energy:



Nice, but negative κ not physical

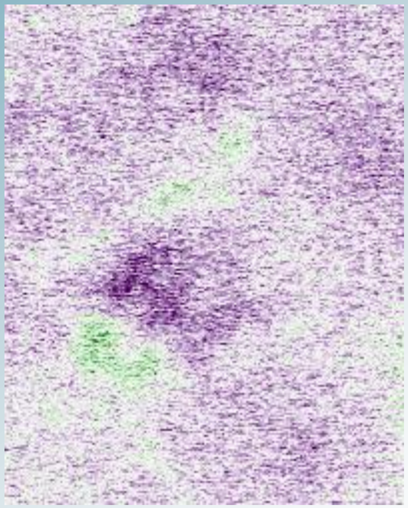
First try

Why negative?

Phase-transition mechanism in Allen-Cahn:
only interface migration but no diffusion

It looks that we have to interpret the intensity as concentration field,
use Cahn-Hillard equation to fit the video.

Second try – toy Cahn-Hillard



- Interpreting intensity $I(t,x,y)$ as concentration field

$I(t,x,y)$: 0 – 255

$c(t,x,y)$: 0 – 1

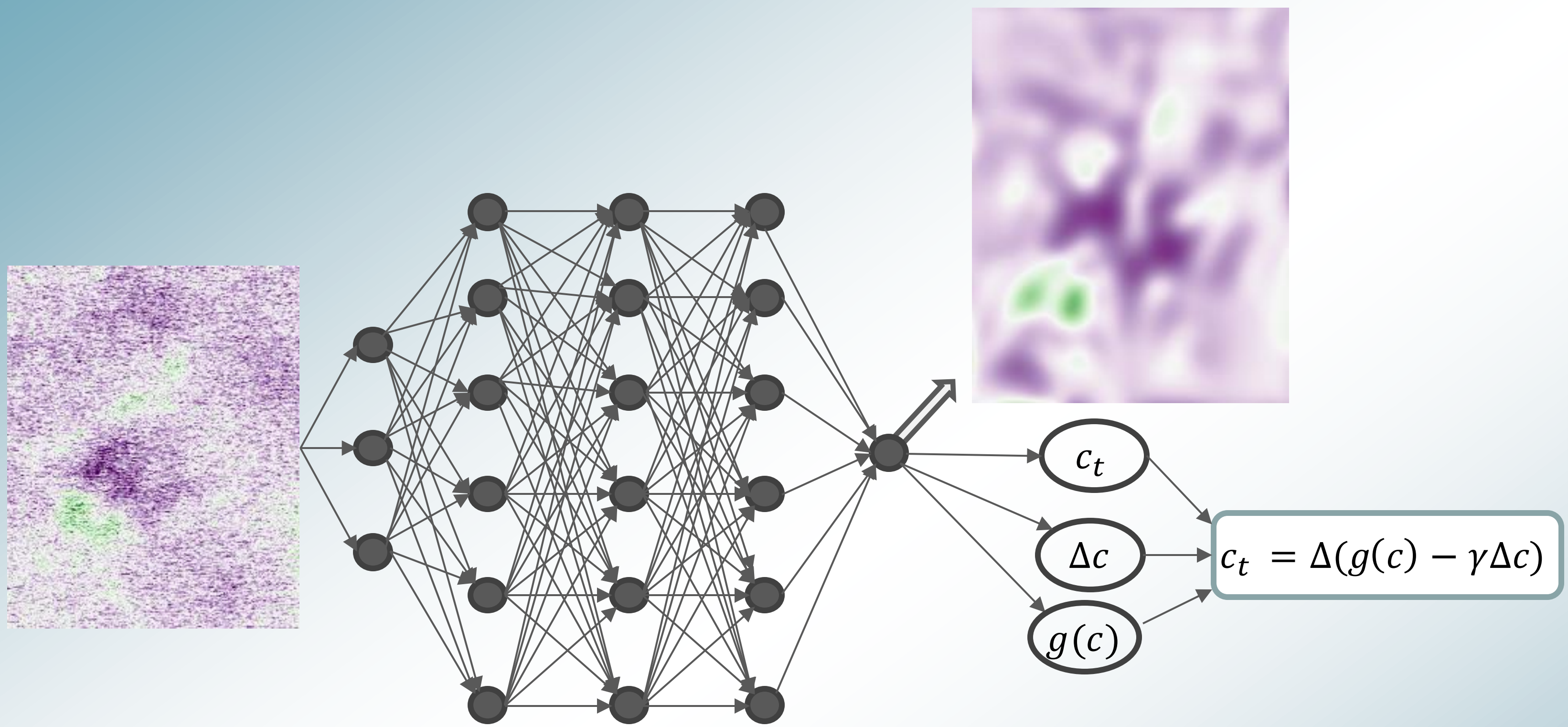
- to parametrize Cahn-Hillard equation:

$$\frac{1}{M}\frac{\partial c}{\partial t} = \Delta(g(c) \ - \gamma\Delta c)$$

- $g(c) = \alpha \cdot c(1-c)(1-2c)$, the derivative of double-well potential

- number of data points: 220,400,000

Second try – toy Cahn-Hillard



γ converges to ~10 pixel,
which looks a reasonable value

Summary

- Developing machine-learning method to learn phase-transition kinetics from in situ STEM
- Got unphysical parameter from Allen-Cahn equation
- Results from Cahn-Hillard equation reasonable

Thanks for your attention!