A Modified Cahn-Hilliard? It's Convoluted

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Acknowledgements

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Binary alloy mixtures separates into their two distinct elements over time.

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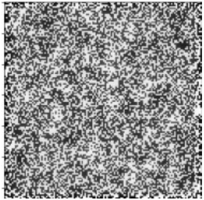

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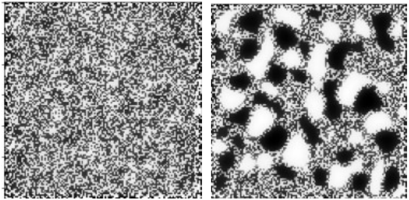

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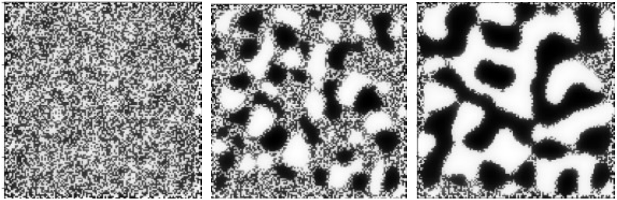

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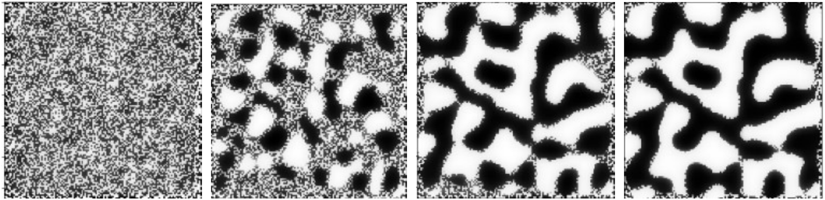

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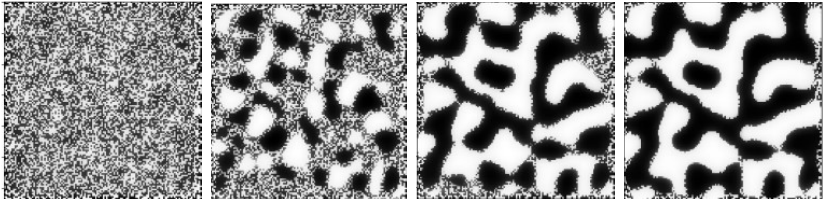
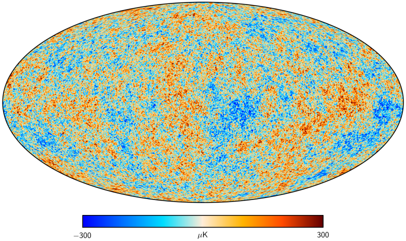


This happens when there is no thermodynamic barrier to phase separation.

Applications

- The classical Cahn-Hilliard modeled spinodal decomposition, especially for binary alloys of metal or polymers
- The introduction of non-local operators came with diblock copolymers
- The big bang theory describes how the universe originates from an initial state of high heat and high density



The Classical Cahn Hilliard Equations

The CHE uses the Laplacian to model changes on the local level.

$$\partial_t \phi = \Delta\mu$$
$$\mu = -\Delta\phi + F'(\phi)$$

- $F(\phi)$ is a double well
- μ is a chemical potential function
- The classical Cahn Hilliard has been well-studied and established

Adjustments to the classical CHE

We studied the doubly non-local Cahn-Hilliard (dnCHE). These operators are taken with respect to probability kernels.

$$\begin{aligned} \partial_t \phi\left(x,t\right) &= \mathscr{L}_J\left(\mu\left(x,t\right)\right) \\ \mu\left(x,t\right) &= -\mathscr{L}_K\left(\phi\left(x,t\right)\right) + F'\left(\phi(x,t)\right) \end{aligned}$$

The inclusion of non-local operators allows for a more robust model.

Non-local Operator

The non-local operator is defined to be:

$$\begin{aligned}
\mathscr{L}_J\mu &= \int_\Omega J(x-y)(\mu(y)-\mu(x))dy \\
&= \int_\Omega J(x-y)(\mu(y))dy - \int_\Omega J(x-y)(\mu(x))dy \\
&= J * \mu - \mu(x)a_J
\end{aligned}$$

Fractional Time Calculus

Fractional Time Calculus

The fractional time derivative accounts for system memory. In order to define it, we must first define fractional time integral.

$$J_t^\alpha = g_\alpha * f(t)$$

where g_α is a piece wise Γ function defined as

$$g_\alpha = \begin{cases} \frac{1}{\Gamma(\alpha)} t^{\alpha-1} & \text{if } t > 0 \\ 0 & \text{if } t \leq 0 \end{cases}$$

and $*$ represents time convolution.

Fractional Time Derivative

Now, using J_t^α, we define the fractional time derivative.

$$cD_t^\alpha = J_t^{1-\alpha}(f'(t))$$

where $D_t^1 = \frac{d}{dt}$, and $\alpha \in (0,1)$.

$$cD_t^{\frac{1}{4}} = J_t^{1-\frac{1}{4}}(f'(t))$$

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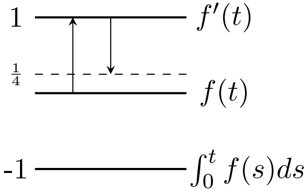

FDE Solution

Consider the standard FDE:

$$\begin{cases} cD_t^\alpha u(t) = u(t) \quad t > 0 \\ u(0) = u_0 \end{cases}$$

We apply the fractional integral to both sides:

$$u(t) = u_0 + J_t^\alpha u(t)$$
$$u(t) = u_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} u(s) ds$$

Modified Doubly Non-Local Cahn-Hilliard

We modify the dnCHE using time convolution.

$$\begin{aligned} k * \partial_t \phi(x,t) &= \mathscr{L}_J(\mu(x,t)) \\ \mu(x,t) &= -\mathscr{L}_K(\phi(x,t)) + F'(\phi(x,t)) \end{aligned}$$

k is a kernel that we can select as we like. Hence we choose $g_{1-\alpha}$ as our kernel k, modeling after the Caputo fractional derivative.

$$\begin{aligned} g_{1-\alpha} * \partial_t \phi(x,t) &= \mathscr{L}_J(\mu(x,t)) \\ \mu(x,t) &= -\mathscr{L}_K(\phi(x,t)) + F'(\phi(x,t)) \end{aligned}$$

Existence Overview

We define our set Y to be functions that are:

- Bounded in space by M
- Continuous in time from $[0, T^*]$
- Where $M = 2\|\phi_0\|_{L^\infty(\Omega)}$ and $T^* \leq \left(\frac{\alpha\Gamma(\alpha)\|\phi_0\|_{L^\infty(\Omega)}}{2\|J\|_{L^1} M\left(2\|K\|_{L^1} + C_M\right)}\right)^{\frac{1}{\alpha}}$

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We also define Picard Iterates:

$$\phi_n(x,t) = \phi_0 + \int_0^t g_\alpha(t-s)(J * \mu_{n-1} - a_J\mu_{n-1})ds$$

$$\mu_{n-1}(t,x) = -(K * \phi_{n-1}) + a_K\phi_{n-1} + F'(\phi_{n-1})$$

Bounded in Space

Assuming the previous iterate is bounded, we can bound the next iterate.

$$
\begin{aligned}
\|\phi_n\|_{L^\infty(\Omega)} &= \left\| \phi_0 + \int_0^t g_\alpha(t-s)(J * \mu_{n-1} - a_J \mu_{n-1})(s) ds \right\|_{L^\infty(\Omega)} \\
&\leq \|\phi_0\|_{L^\infty(\Omega)} + \left(\frac{2}{\alpha \Gamma(\alpha)} \|J\|_{L^1} (2 \|K\|_{L^1} + C_M) M \right) (T^*)^\alpha \\
&\leq \|\phi_0\|_{L^\infty(\Omega)} + \|\phi_0\|_{L^\infty(\Omega)} \\
&\Rightarrow \|\phi_n\|_{L^\infty(\Omega)} \leq M
\end{aligned}
$$

Continuous in Time

We proved for all n:

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- $\|\phi_{n+1} - \phi_n\|_{L^\infty(\Omega)} \leq C(g_{(n+1)\alpha} * 1) = \frac{Ct^{(n+1)\alpha}}{\Gamma((n+1)\alpha)(n+1)\alpha}$

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We then found:

$$\begin{aligned}
\|\phi(t,x)\|_{L^\infty(\Omega)} &\leq \|\phi_0\|_{L^\infty(\Omega)} + \sum_{n=0}^{\infty} \|\phi_{n+1} - \phi_n\|_{L^\infty(\Omega)} \\
&\leq \|\phi_0\|_{L^\infty(\Omega)} + \sum_{n=0}^{\infty} \frac{Ct^{(n+1)\alpha}}{\Gamma((n+1)\alpha)(n+1)\alpha} \\
&= \|\phi_0\|_{L^\infty(\Omega)} + E_{\alpha,1}(t^\alpha)
\end{aligned}$$

By M-Test and ULT, ϕ is continuous in time.

Uniqueness

Theorem (Gronwall's Fractional Inequality)

Let a, g be non-decreasing and $g(t) \leq C$ for all $t \in [0, T]$ and $0 < \beta < 1$. If $x \in L^{\infty}_{+}$ and

$$x(t) \leq a(t) + g(t) \int_0^t (t-s)^{\beta-1} x(s) ds$$

then,

$$x(t) \leq a(t) E_{\beta}(g(t)\Gamma(\beta)(t^{\beta})).$$

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then, $$x(t) \leq a(t) E_\beta(g(t)\Gamma(\beta)(t^\beta)).$$

Assume ϕ and ψ are both solutions,

$$\|\phi - \psi\|_{L^\infty(\Omega)} = \left\| \phi_0 + \int_0^t g_\alpha (J * \mu_\phi - a_J \mu_\phi) - \left(\phi_0 + \int_0^t g_\alpha (J * \mu_\psi - a_J \mu_\psi) \right) \right\|_{L^\infty(\Omega)}$$

$$\leq 0 \cdot E_{\alpha,1}(C\Gamma(\alpha) t^\alpha) = 0 \implies \phi = \psi$$

Approximating $g_{1-\alpha} * \partial_t \phi = \mathscr{L}_J \mu$

For the RHS we use:

- Riemann Sums

$$\mathscr{L}_J \mu(t_n, x_m) = \int_\Omega J(x_m - y)\,(\mu(y) - \mu(x_m))\,dy$$

$$\approx \Delta x \sum_{i=1}^{M} J(x_m - x_i)\,(\mu(x_i) - \mu(x_m))$$

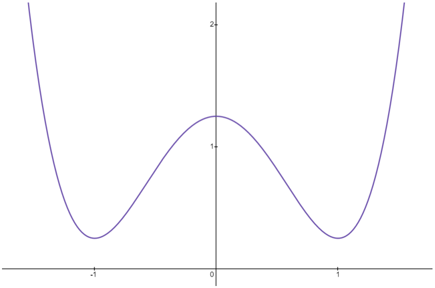
  - Recall $\mu = -\mathscr{L}_K \phi + F'(\phi)$

Approximating $F'(\phi)$

Recall $F(\phi)$ is a double-well potential function:

- Two minima at -1 and 1
- Can be approximated using a fourth degree polynomial
- Take $F(\phi) = \frac{1}{4}\phi^4 - \frac{1}{2}\phi^2$

$$\implies F'(\phi) = \phi^3 - \phi$$



Approximating $g_{1-\alpha} * \partial_t \phi = \mathscr{L}_J \mu$

For the LHS we use:

- Forward Differencing

$$g_{1-\alpha} * \partial_t \phi(t_{n+1}, x_m) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \, \partial_s \phi(t_{n+1}, x_m) \, ds$$

Approximating $g_{1-\alpha} * \partial_t \phi = \mathscr{L}_J \mu$

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$$\approx \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n} \frac{\phi(x,t_{n+1}) - \phi(x,t_n)}{\Delta t} \int_{t_j}^{t_{j+1}} (t_{j+1} - s)^{-\alpha} ds$$

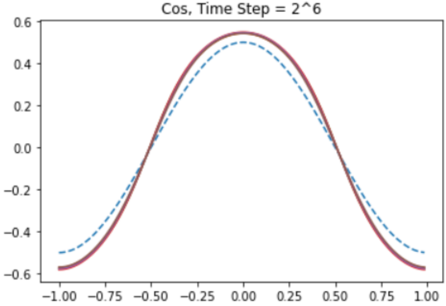
Then we equate the two approximations and solve for $\phi(t_{n+1}, x_m)$

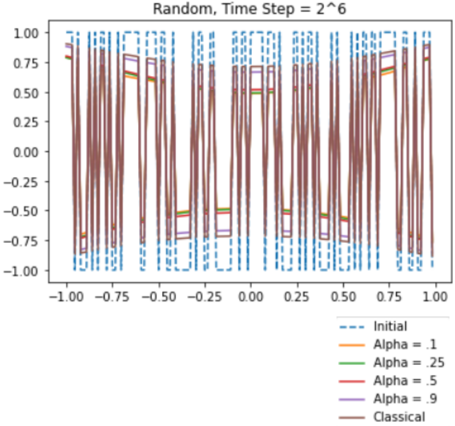
Numerics Results

Simulations details:

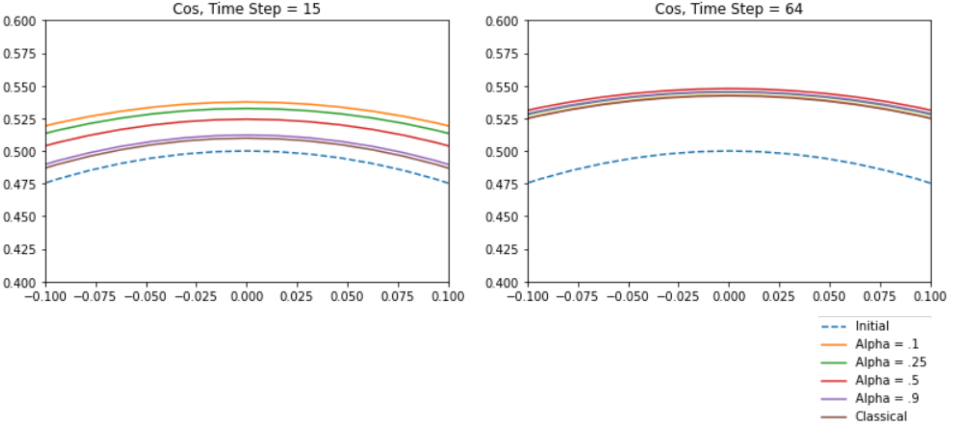
- $x \in (-1, 1)$ - taking 2^7 steps
- $t \in [0, 1]$ - taking 2^6 steps
- Values of $\alpha = .1, .25, .5, .9$
- One dimension
- Initial Conditions $\in Y$:
  - $\phi_0 = .5\cos(\pi x)$
  - $\phi_0 =$ random values of -1 and 1

Numerics Results (Everything)

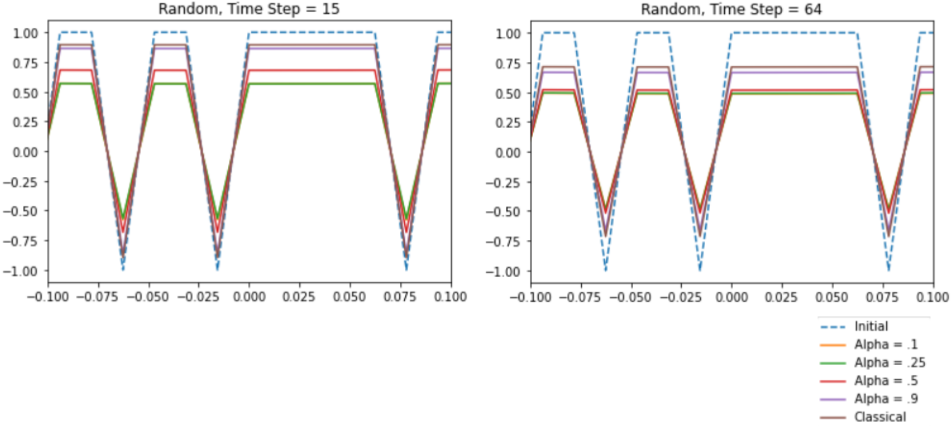




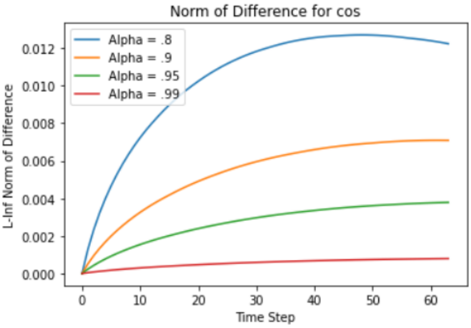
Numerics Results (Cos)

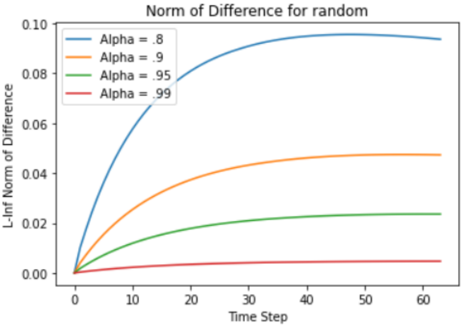


Numerics Results (Random)



Numerics Results Convergence





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- We proved existence and uniqueness of solution for the dnCHE with a fractional time derivative
- We provided basic numerics to show convergence of our fractional derivative approximation to the classical derivative approximation.
- Using a different numerical scheme, we might have better results or have less computation time heavy simulations.
- We can explore what other kernels k can be applied to our modified dnCHE and find what applications such models would have.

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