The Meta-Stability of the Allen Cahn Fractional Differential Equation

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Abstract

The Allen-Cahn equation is a partial differential equation that models the phase changes of certain chemical elements. To determine the areas where a phase change occurs, the stability and metastability of the equation needs to be investigated. Using MATLAB, initial plots of the bifurcation diagrams for the Allen-Cahn equation were created, which gave a basic notion of the approximate locations of the equilibrium points. Furthermore, AUTO, a computer software designed to investigate bifurcations, helps determine the exact bifurcation points in both 1D and 2D. Extending the model to 3D is the next step. From here, we are able to gain a deeper insight into the Allen-Cahn equation and its stability.

Introduction

Allen-Cahn Equation

The Allen-Cahn equation is a reaction-diffusion equation that is used to model phase changes in iron and other chemical alloys. A phase change like slush can be modeled, and investigating the graph of the solutions shows the stability of such a phase. Additionally, the fractional version of the Allen-Cahn equation is more accurate in modeling certain processes. To implement the fractional space component in the Allen-Cahn equation, the $K\Delta$ was changed to $-K(-\Delta)^{\alpha/2}$, where K is a positive constant. If $\alpha = 2$, then the equation is back to its normal version without a fractional component

$$\partial_t u = K\Delta u + u - u^3.$$

In this equation, u is a function of x and t, with x being contained in the finite domain in dimension 1, 2, or 3. The Laplacian operator Δ is equal to the divergence of the gradient of u. We note that the function has homogeneous Neumann boundary conditions, which means the derivative is equal to zero on the boundary. To examine the solutions of this equation, many different numerical methods had to be used. Using finite differences approach, a system of linear equations is solved at each time step, where the left hand size of the matrix contains the fractional component. However, many difficulties arise when the spatial dimension is increased. Thus, spectral methods were used.

Spectral Methods

One way to solve partial differential equations is by using the Discrete Cosine Transform (DCT). The DCT is used when the PDE has Neumann boundary conditions, which set the derivative of the function equal to some value at the endpoints. The main idea is to write the solution in terms of a basis function that is nonzero over the whole domain. The interpolating function using the DCT is written as

$$u(x) = a_0 + \sum_{n=1}^{\infty} a_n \cos(\frac{\pi n x}{L})$$

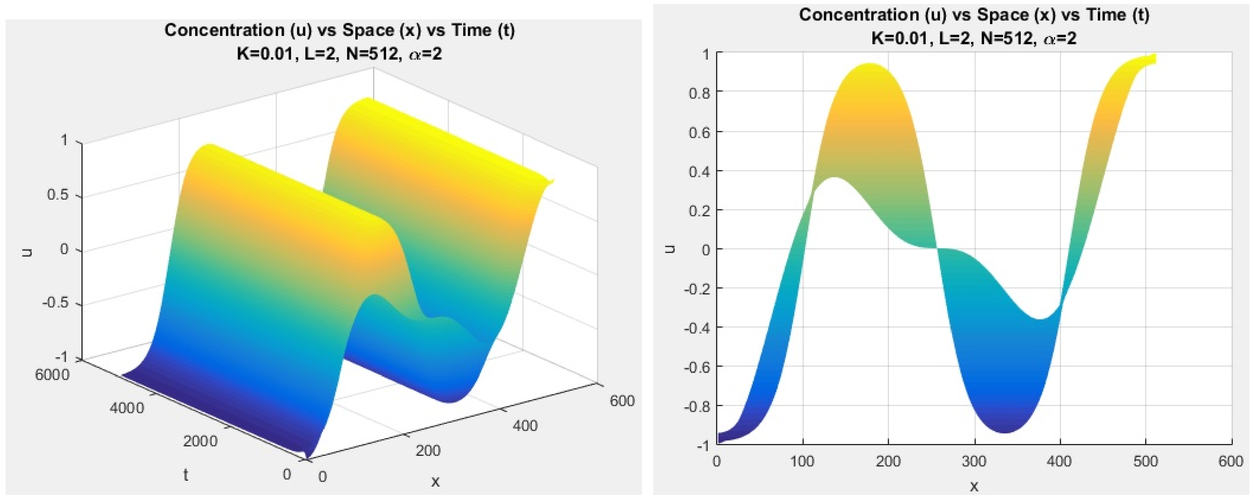
where L is the length of the interval, and a_0 to a_n are the Fourier coefficients. Using the transform and it's inverse allows one to formulate and later solve the problem that is now only based on a series of cosine functions. Due to the global ability of Spectral Methods, they often provide less error than a finite difference approach.

Methods

First consider the one dimensional Allen-Cahn equation

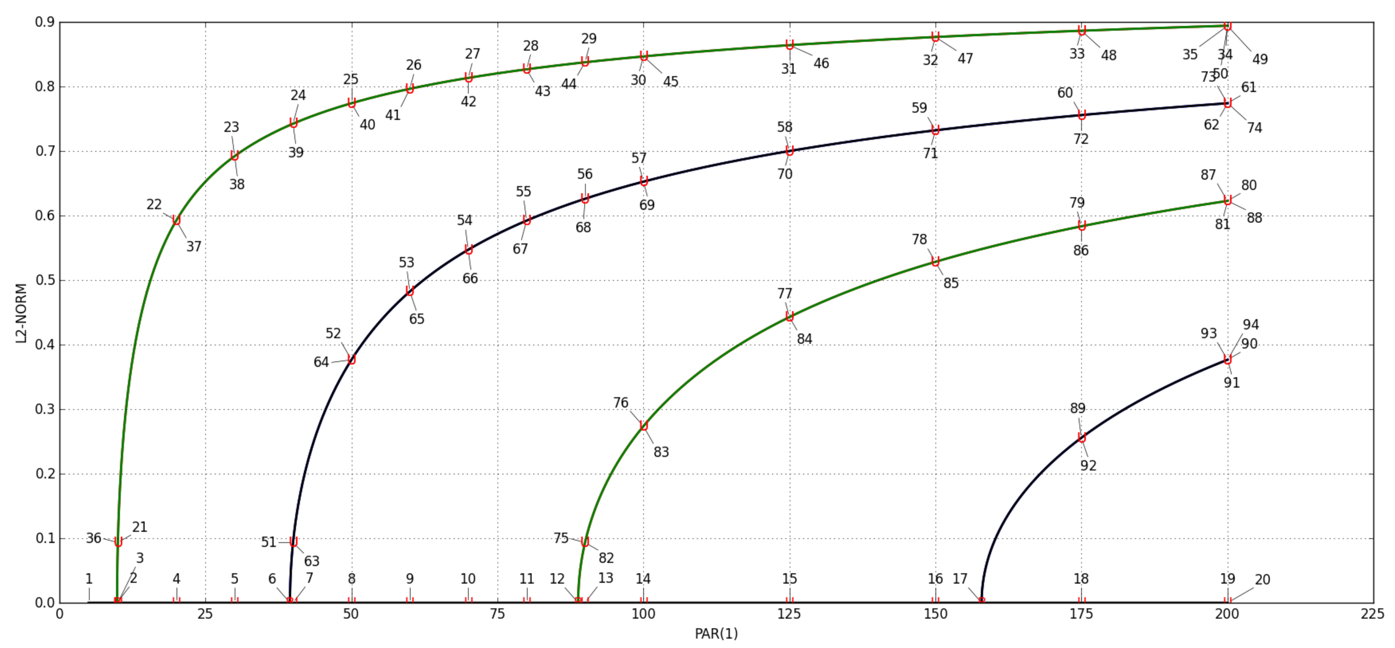
$$\partial_t u = K\Delta u + u - u^3.$$

The solution to this PDE is displayed below (Bueno-Orovio), where N is the size of discretization:



$$L = 2;\ N = 512;\ K = 0.01;\ \alpha = 2;$$

Furthermore, the bifurcation diagram for the $\alpha = 2$ case is seen below:



A portion of this research is devoted to understanding the changes in the bifurcation diagram when the fractional laplacian is implemented. The equation for the fractional Allen Cahn equations is

$$\partial_t u = K(-\Delta)^{\alpha/2} u + u - u^3.$$

After discretizing this space, the "differentiation constant" was investigated as changes were made to the fractional power. Let this differentiation constant be $\kappa = \pi^2 k^2$, where $k = \{1, 2, 3, ...\}$. Changing this requires raising it to a fractional power

$$\kappa^{\alpha/2} = (\pi^2 k^2)^{\alpha/2} = \pi^\alpha k^\alpha = (\pi k)^\alpha.$$

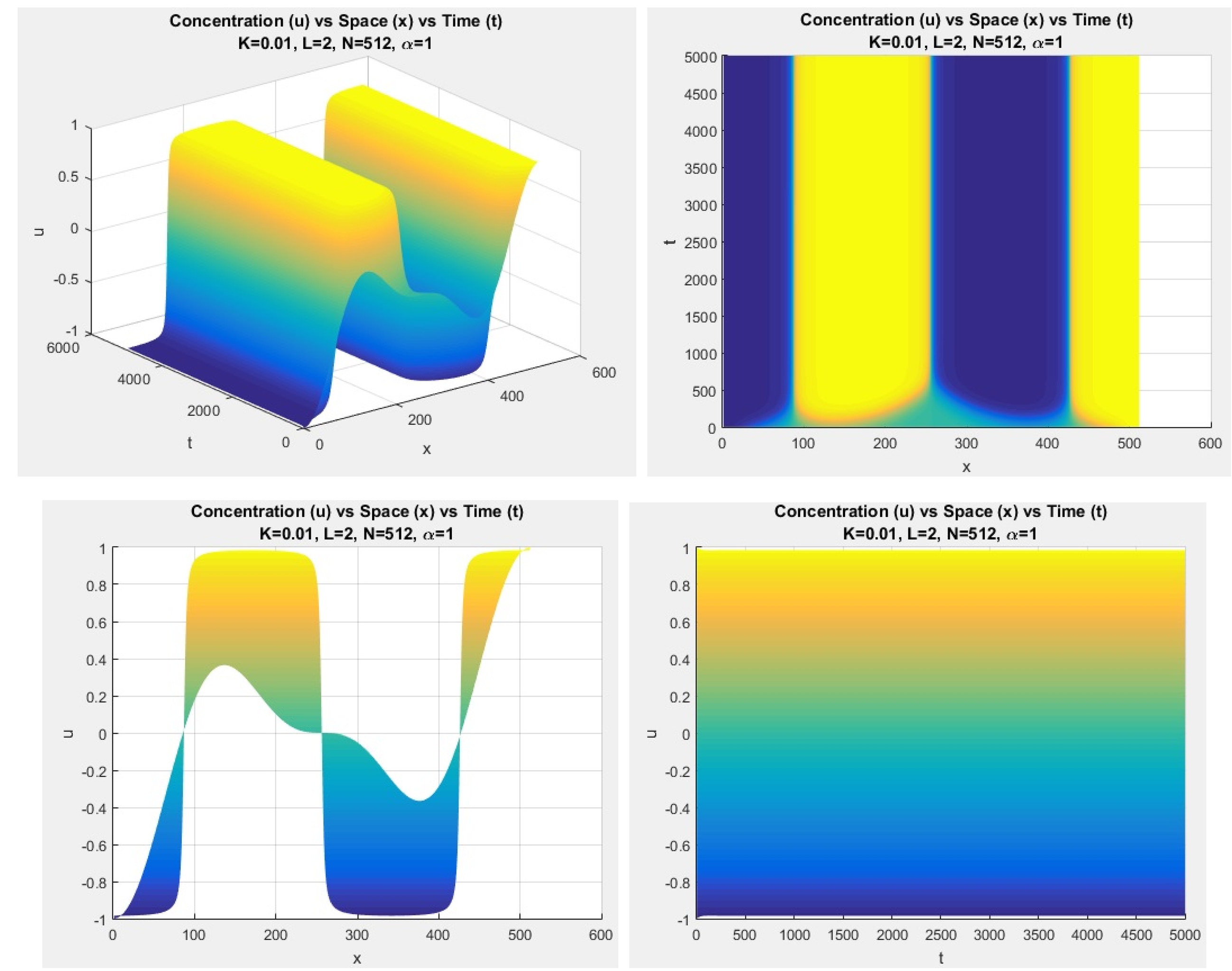
and the corresponding cosine sum is equal to

$$u(x) = a_0 + \sum_{n=1}^{\infty} n^\alpha a_n \cos(\pi n x).$$

In doing so, a more particular adjustment can be looked at of the bifurcation diagram.

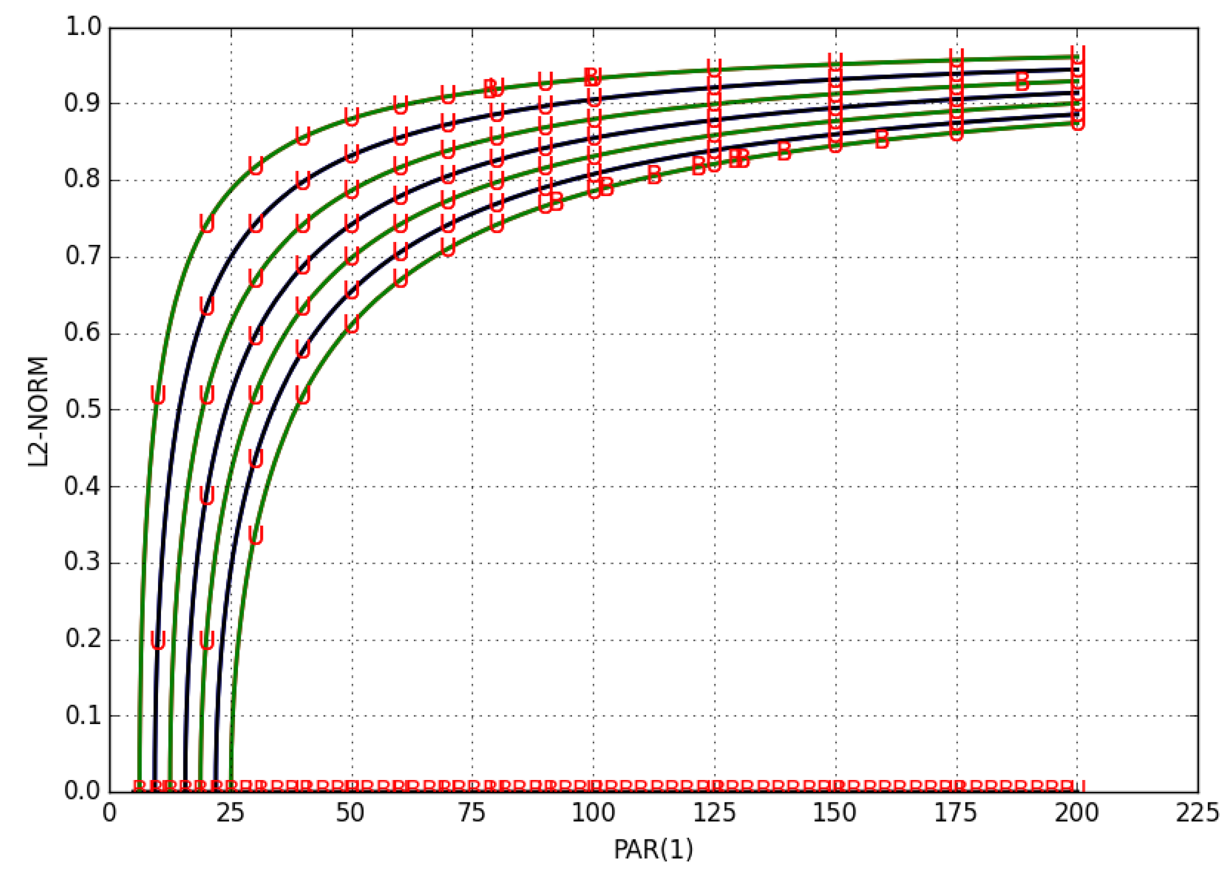
Results and Conclusion

The solution of the Fractional Allen-Cahn equation is displayed here. N refers to the discretization size and L is the length of the interval. The top left image left is the 2 dimensional solution to the equation and the bottom left image is a cross section of the solution.



$$L = 2;\ N = 512;\ K = 0.01;\ \alpha = 1;$$

Below is the bifurcation diagram for the fractional Allen-Cahn equation when $\alpha = 1$.



Acknowledgments

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Bueno-Orovio, Alfonso, David Kay, and Kevin Burrage. "Fourier spectral methods for fractional-in-space reaction-diffusion equations." BIT Numerical Mathematics 54.4 (2014): 937-954.