PHASE SEPARATION DYNAMICS IN MULTICOMPONENT ALLOYS

Undergraduate Research in Computational Mathematics

Hanein Edrees
John Price

George Mason University

April 5, 2008

Abstract

Abstract

Our topic is mathematical models describing pattern formation and phase separation/transition within multicomponent metal alloys. Specifically, we are studying the Cahn-Morral system of partial differential equations, a model for these phenomena. We use numerical bifurcation and continuation to study equilibria for the system in one and two dimensions. This allows us to understand the behavior seen in simulations.

Outline

–Overview

- Phase Separation
  - Spinodal Decomposition
  - Nucleation
- Cahn Morral System
  - Gibbs Simplex
  - Relevant Parameters

–Methods

- Bifurcation Diagrams
- Numerics

–Results

- 1-Dim
- 2-Dim

–Conclusion

Overview

Within homogeneous multicomponent alloys the occurrence of phase separation is an interesting phenomenon. Research of mathematical models providing qualitative descriptions of these separations will be our topic.

Motivation

Simulations of the stochastic Cahn-Morral system exhibit interesting pattern formation behavior. By examining the bifurcations for several of the system's parameters, we can determine if the same behavior is present in the model itself.

PHASE SEPARATION

Transformation of a homogenous system in 2 or more phases

1. Spinodal Decomposition
   "Spontaneous separation"
   A mixture of 2 or more materials separate into regions with different concentrations throughout the material. The homogeneous equilibrium is unstable.
2. Nucleation
   The homogeneous equilibrium is stable, but small noise pushes it out of the stability region. May be visible in the formation of bubbles or droplets formed throughout the alloy. These droplets can have different compositions.

Cahn-Morral Equation

- Cahn Morral System describes the process of phase separation. Specifically, we utilize these equations to describe the mechanism that makes these droplets form.

Cahn Morral System

$$u_t = -\triangle(\epsilon^2 \triangle u + f(u))$$

$$\frac{\partial u}{\partial v} = \frac{\partial \triangle u}{\partial v} = 0 \; on \, \partial\Omega$$

$$u_1 + u_2 + ... + u_N = 1$$

Cahn Morral System

$$u_t = -\triangle(\epsilon^2 \triangle u + f(u))$$
$$\frac{\partial u}{\partial v} = \frac{\partial \triangle u}{\partial v} = 0 \; on \, \partial\Omega$$
$$u_1 + u_2 + ... + u_N = 1$$

- → u : order parameter, u ϵ G $\subset \mathbb{R}$
- → G is the Gibbs simplex
- → $\epsilon > 0$, small parameter – interaction length
- → $\triangle$: Laplacian is a differential operator – divergence of the gradient
- → 1-D Domain: Ω = [0,1]
  2-D Domain: Ω = [0,1] X [0,1]

$$F(u_1, \ldots, u_N) = \prod_{i=1}^{N} \left(u_1^2 + \ldots + u_{i-1}^2 + \sigma \cdot (u_i - 1)^2 + u_{i+1}^2 + \ldots + u_N^2\right)$$

Relevant Parameters

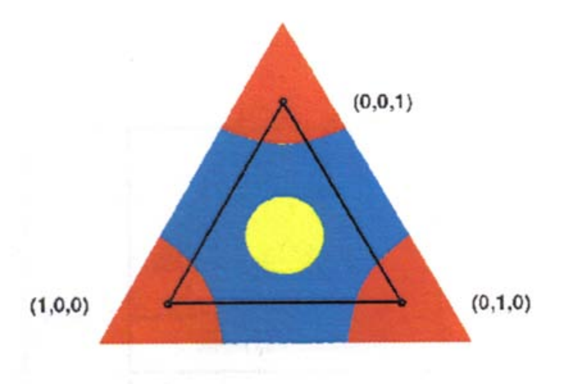
$$\lambda = \frac{1}{\epsilon^2}$$
$$\alpha = \frac{(u_0+v_0)}{2}$$
$$\beta = \frac{(u_0-v_0)}{2}$$

Initial Values

$$\text{u} = \alpha + \beta$$
$$\text{v} = \alpha \text{ - } \beta$$
$$\text{w} = 1 \text{ - u} + \text{v}$$

Gibbs Simplex

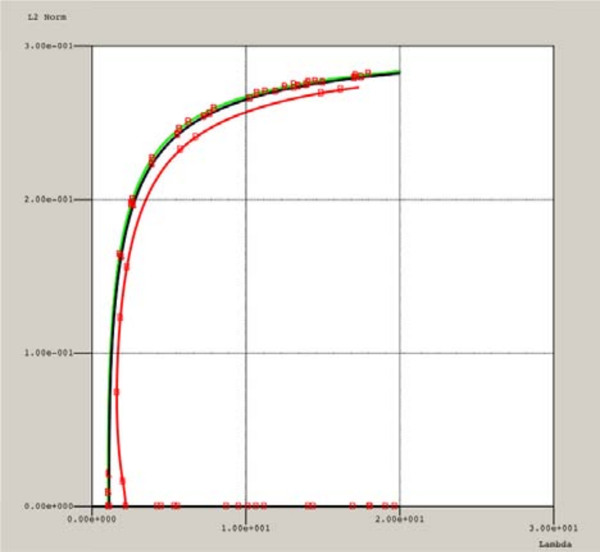
Plane in $\mathbb{R}^n$ (n=3 in our case) where the sum of the positive components is equal to 1



*D. Blömker, S. Maier-Paape, T. Wanner

Bifurcation Theory

Used in dynamical systems to qualitatively study solutions of a differential equation



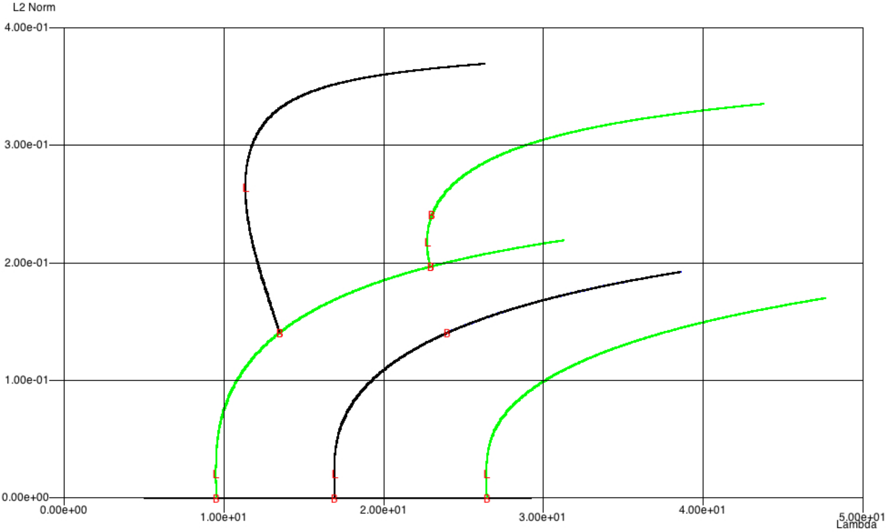
Numerical Methods

- We simulate the Cahn-Morral system in 1-D and 2-D as a system of ODE's
- The system is modeled using the spectral method (implemented in FFTW)
- C code interfaces with the AUTO bifurcation and continuation software

Results

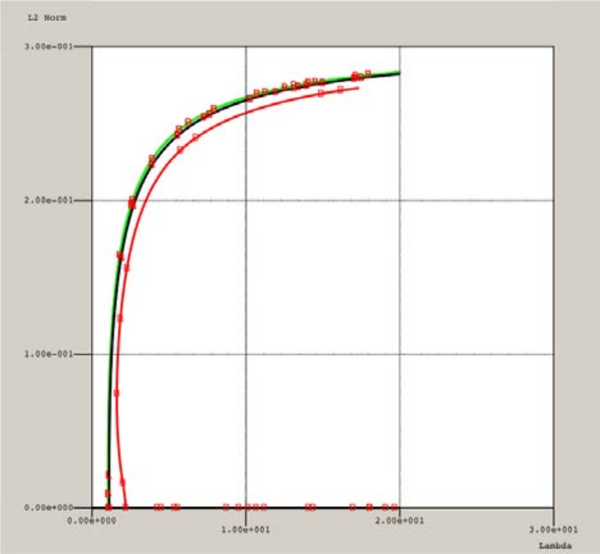
We're interested in varying λ as ϵ goes to 0. We find the solutions in the nucleation region by using the nontrivial solutions in the spinodal region and then vary in α. Then we vary λ to view the solutions in the nucleation region.

Results – 1-D



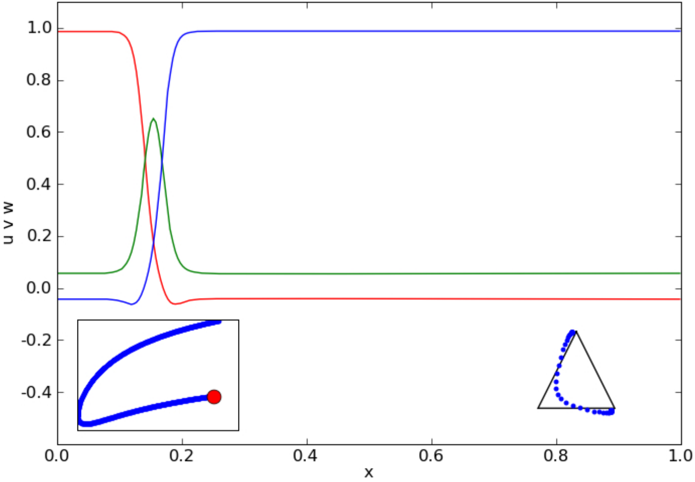
L2 Norm
4.00e-01
3.00e-01
2.00e-01
1.00e-01
0.00e+00
0.00e+00
1.00e+01
2.00e+01
3.00e+01
4.00e+01
5.00e+01
Lambda
L
B

Results – 2-D

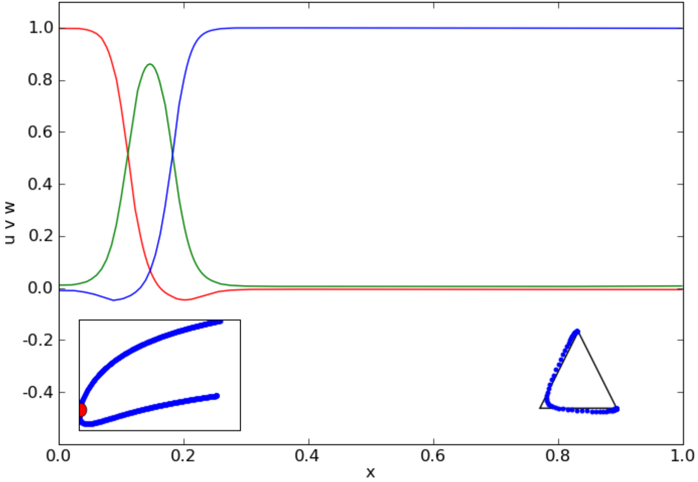


L2 Norm
3.00e-001
2.00e-001
1.00e-001
0.00e+000
0.00e+000
1.00e+001
2.00e+001
3.00e+001
Lambda

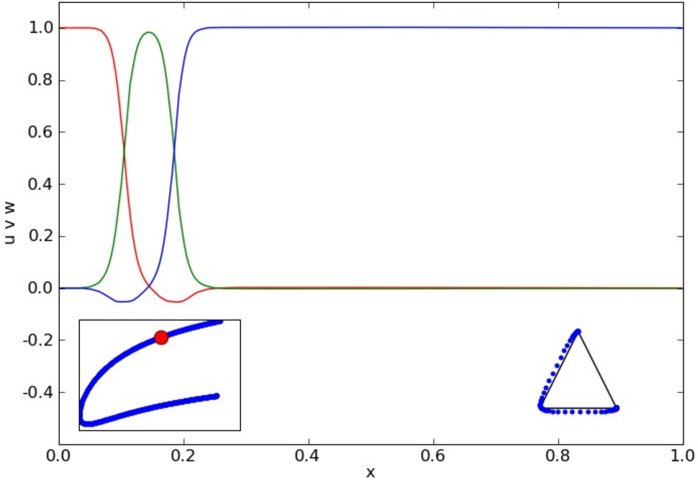
Results – 1-D



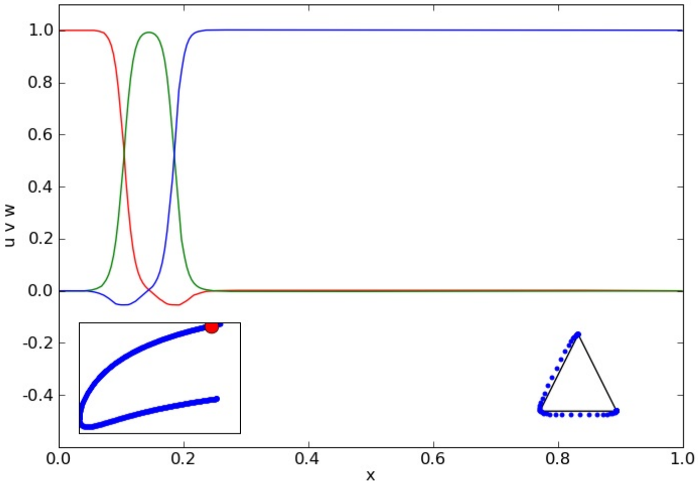
Results – 1-D



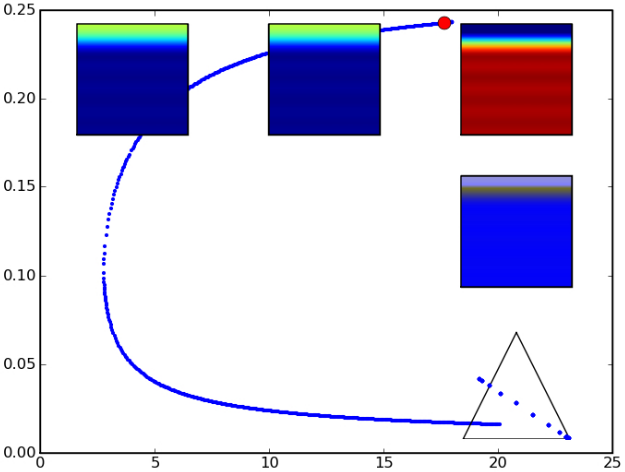
Results – 1-D



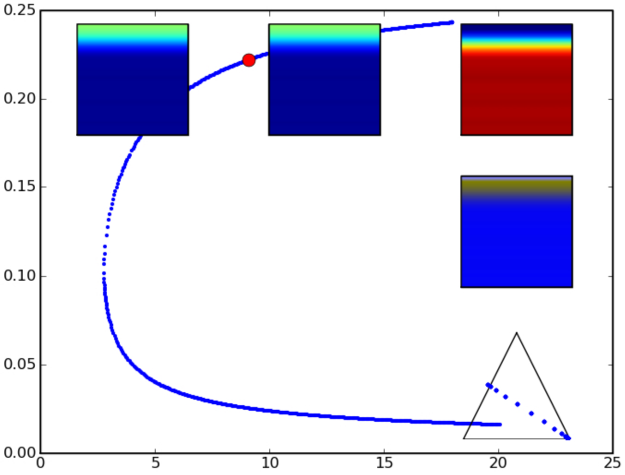
Results – 1-D



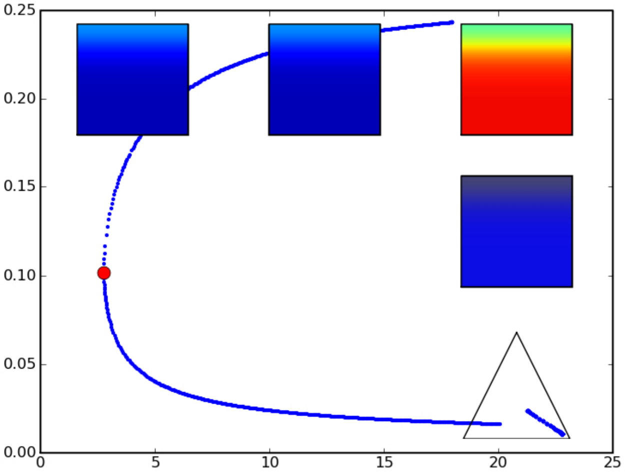
Results – 2-D



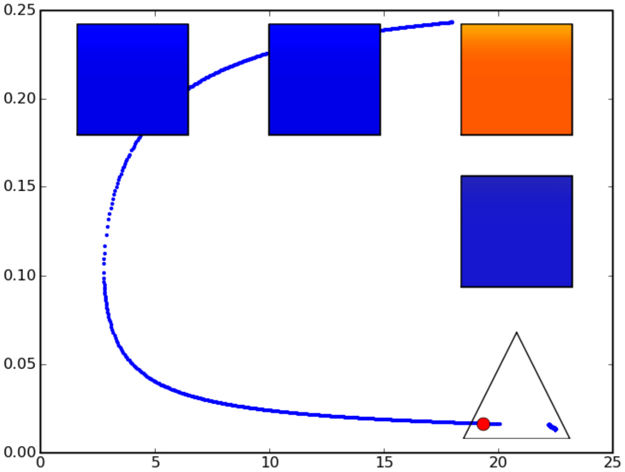
Results – 2-D



Results – 2-D



Results – 2-D



Future Goals/Research

- Examining solutions along other branches of bifurcation diagrams
- Computing stability of these solutions

References:

- Preprint: J. Desi, T. Wanner, *The Dynamics of Nucleation in Stochastic Cahn-Morral Systems.* July 2004.
- D. Blömker, S. Maier-Paape, T. Wanner, *Phase Separation in Stochastic Cahn-Hilliard Models.* May 2004.
- Y. Nishiura, *Translations of Mathematical Monographs: Far-from-Equilibrium Dynamics.* American Mathematical Society, March 2002.
- P. Fife, *Models for phase separation and their mathematics.* Electronic Journal of Differential Equations, 2000.
- D. Duncan, M. Grinfeld, I. Stoleriu, *Coarsening in an integro-differential model of phase transitions.* European Journal of Applied Mathematics, 2000.

THANK YOU!!

- Dr. Thomas Wanner and Dr. Evelyn Sander
- Robert Allen
- National Science Foundation
- URCM
- George Mason University Math Department
- Our Audience
- Did we forget to thank anyone?