Nucleation and Spinodal Decomposition in Multi-component Alloys

Applying the Cahn-Morral System to Ternary Alloys

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July 30, 2009

Acknowledgements

- Dr. Eveyln Sander

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- Dr. Thomas Wanner

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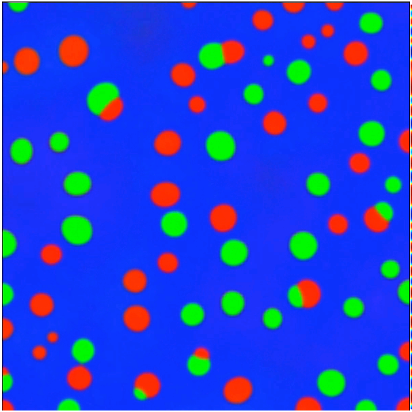
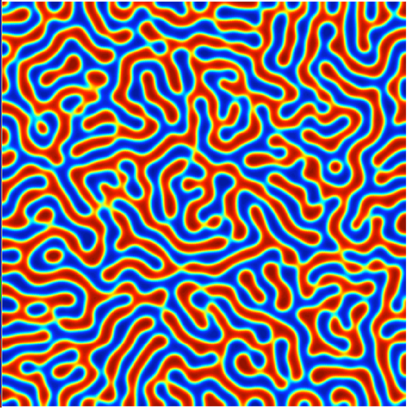
- The Department of Defense

Outline

The Problem

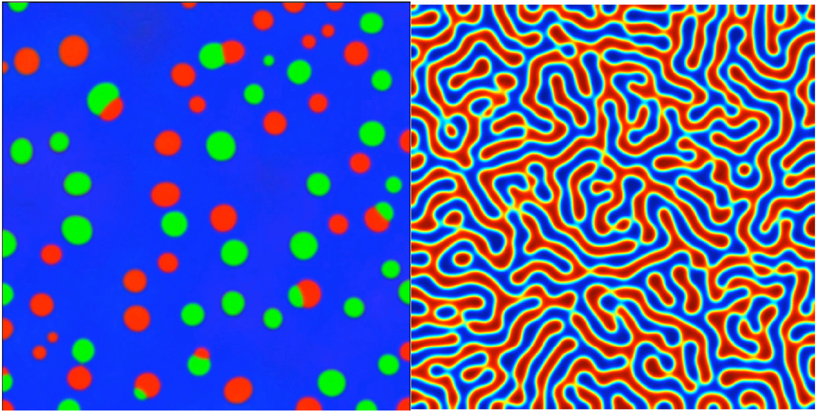
Metals are heated and then mixed to create alloys. However after they undergo rapid cooling they may not remain homogeneous. Often they exhibit undesirable properties including nucleation and spinodal decomposition.

Nucleation and Spinodal Decomposition

Nucleation Region stable, disconnected, bubblelike patterns

Nucleation and Spinodal Decomposition



Nucleation Region stable, disconnected, bubblelike patterns

Spinodal Region unstable, connected, snakelike patterns

The Equations

The Cahn Morral System

$$\vec{u}_t = -\Delta(\varepsilon^2 \Delta \vec{u} + f(\vec{u})) \quad \text{on} \quad \Omega$$
$$\frac{\partial \vec{u}}{\partial \nu} = \frac{\partial \Delta \vec{u}}{\partial \nu} = 0 \quad \text{on} \quad \partial\Omega$$

Van der Waals

$$E_\varepsilon[\vec{u}] = \int_\Omega \left(\frac{\varepsilon^2}{2} \cdot |\nabla \vec{u}|^2 + F(\vec{u}) \right) dx$$

Objectives

- Attempting to better understand droplet formation

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- Time invariant

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- Time invariant
- Different nonlinearities

Past Research

- time dependent analysis

Past Research

- time dependent analysis
- on large domains

Past Research

- time dependent analysis
- on large domains
- no comparison between different nonlinearities

Current Research

- time independent solutions

Current Research

- time independent solutions
- on small 1-D domains

Current Research

- time independent solutions
- on small 1-D domains
- comparing and contrasting the nonlinearities

The Quadratic Nonlinearity

$$F(u, v, w) = \frac{u^2 v^2 + (u^2 + v^2)(w^2)}{4}$$

The Nonlinearities

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The Logarithmic Nonlinearity

$$F(u, v, w) = 3.5(uv + uw + vw) + u \ln u + v \ln v + w \ln w$$

Determining $f(\vec{u})$

Let $f(\vec{u}) : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ be given by,

$$f(\vec{u}) = -P\nabla F(\vec{u})$$

where,

$$P\vec{u} = \vec{u} - \frac{< \vec{u}, e >}{3} \cdot e \qquad \text{with} \qquad e = (1,1,1)$$

The Gibbs Simplex

$$\mathcal{G} = \{(u, v, w) \in \mathbb{R}^3 \, : \, u + v + w = 1 \, , u \geq 0 \, , v \geq 0 \, , w \geq 0\}.$$

where $\vec{u}(t, x) \in \mathcal{G} \, \forall \, t$

Stability Analysis

$$B = J_f(\bar{u}, \bar{v}, \bar{w})$$

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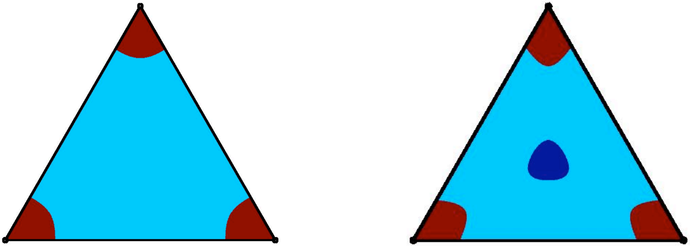
- if B has no positive eigenvalues, then $(\bar{u}, \bar{v}, \bar{w})$ is stable

The Gibbs Triangle



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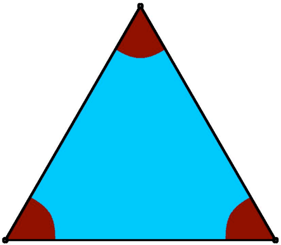

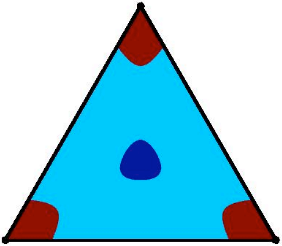

- red area depicts nucleation region

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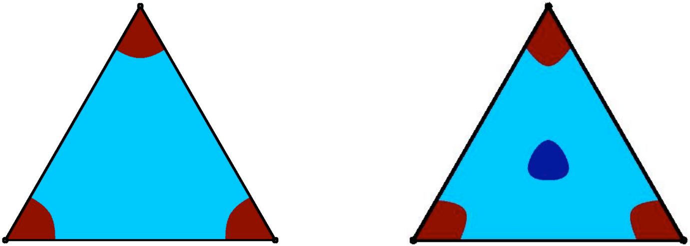

- red area depicts nucleation region
- blue and dark blue areas depict spinodal region

The Parameters

- $\lambda = 1/\varepsilon^2$ is varied inside the spinodal region

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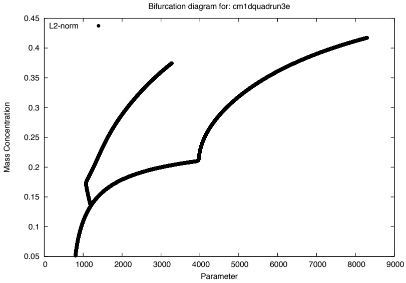
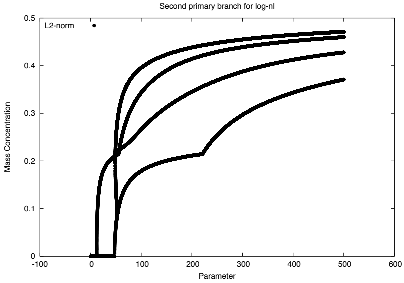
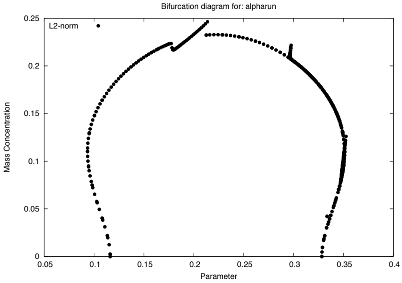
- $\alpha = (\bar{u} + \bar{v})/2$ is varied to reach the nucleation region
- $\beta = (\bar{u} - \bar{v})/2$ is varied within the nucleation region

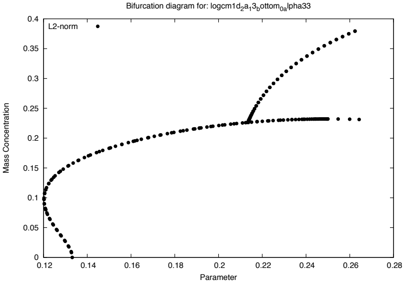
Varying λ



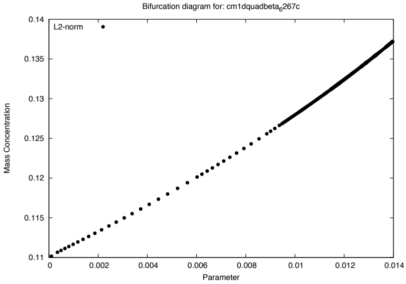


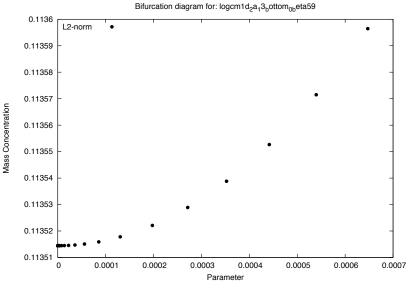
Varying α



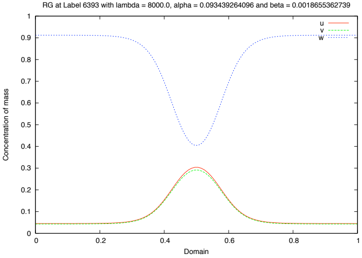


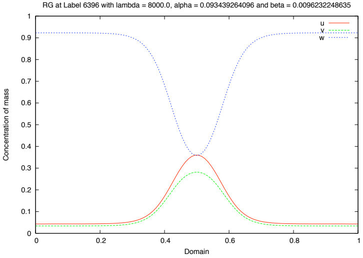
Varying β

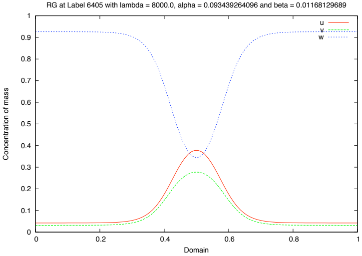


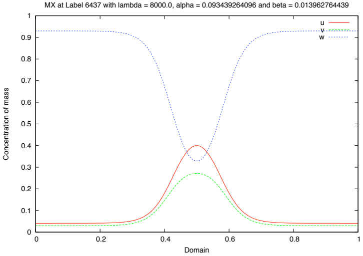


Quadratic β Nucleation Plots

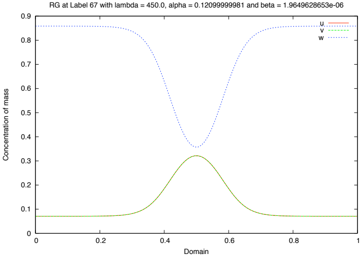


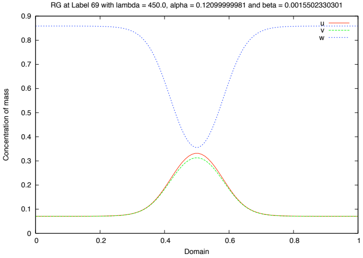


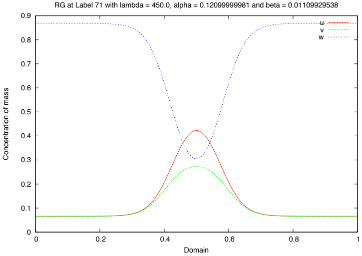


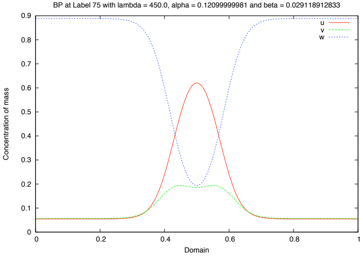


Log β Nucleation Plots









Conclusions

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- could mean the choice of nonlinearity is not significant

Future Work

- further investigating droplet patterns

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- higher dimensional domains

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- different nonlinearities
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- more than three components

Questions?