Viscoelastic dynamics for a scalar two-dimensional continuum model for microstructure formation at an austenite-martensite interface

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Outline

• Motivation
• Mathematical model
• Exact traveling wave solutions
• Numerical method
• Numerical results
  – connections to acoustic emission
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Motivation

• Is nonlinear viscoelasticity with capillarity a good model for austenite-martensite phase transformations?

• Can this dynamic model result in the formation of self-similar microstructure?

• Can we find a good way of obtaining a numerical solution to this model?
Examples of twinning in a model for a cubic to tetragonal phase transition

From Kohn and Müller, 1992
Dynamical Mathematical model

Nonlinear viscoelasticity with capillarity

\[ U_{tt} = \nabla \cdot \sigma(\nabla U) + \nabla \cdot \tau(\nabla U, \nabla U_t) - \epsilon \Delta^2 U \]
Scalar one and two dimensional models

\[ U_{tt} - \nabla \cdot \tau(\nabla U, \nabla U_t) = \nabla \cdot \sigma(\nabla U) - \epsilon \Delta^2 U \]

\[ u_{tt} - \beta \Delta u_t = (u_x^3 - u_x)x + u_{yy} - \epsilon \Delta^2 u \]

\[ u_{tt} - \beta u_{xxt} = (u_x^3 - u_x)x - \alpha u - \epsilon u_{xxxx} \]

Dissipative systems with Lyapunov function

\[ L[u] = \int_\Omega \epsilon \frac{(\Delta u)^2}{2} + \frac{u_y^2}{2} + \frac{(u_x^2 - 1)^2}{4} + \frac{u_t^2}{2} \]

\[ L[u] = \int_\Omega \epsilon \frac{u_{xx}^2}{2} + \alpha \frac{u^2}{2} + \frac{(u_x^2 - 1)^2}{4} + \frac{u_t^2}{2} \]

With \( \alpha, \beta, \) and \( \epsilon \geq 0. \) Interested in small \( \epsilon. \)
Exact traveling wave solutions

\[ u_{tt} - \beta u_{xx} = (u^3_x - u_x)x - \epsilon u_{xxxx} \]
\[ u_{tt} - \beta \Delta u_t = (u^3_x - u_x)x + u_{yy} - \epsilon \Delta^2 u \]

Use \( u(x, y, t) = u(\zeta) \)
where \( \zeta = x\kappa_x + y\kappa_y - ct \) and \( \kappa^2_x + \kappa^2_y = 1 \)

Substitute \( r = u_\zeta \)

\[ \epsilon r_{\zeta\zeta} + \omega \beta r_\zeta + (\rho \omega^2 + \kappa^2_x - \kappa^2_y)r - \kappa^4_x r^3 = A_1 \]

Use the ansatz \( r = A_2 \tanh(A_3\zeta) + A_4 \)
Exact traveling wave solutions

One dimensional solution when

\[ c^2 \left(1 - \frac{\beta^2}{6\epsilon}\right) + 1 \geq 0 \]

\[ u = \sqrt{2\epsilon} \log \left( \cosh \left[ (x - ct) \sqrt{\frac{c^2}{2\epsilon} \left(1 - \frac{\beta^2}{6\epsilon}\right) + \frac{1}{2\epsilon}} \right] \right) \]

\[ - \frac{c\beta(x - ct)}{3\sqrt{2\epsilon}} \]

Video with \( c = 1, \epsilon = 0.01 \) and \( \beta = 0.1 \)
Exact traveling wave solutions

Two dimensional solution when

\[ c^2(1 - \beta^2/6\epsilon) + \kappa_x^2 - \kappa_y^2 \geq 0 \]

\[ u = \frac{\sqrt{2\epsilon}}{\kappa_x^2} \log \left( \cosh \left( (x\kappa_x + y\kappa_y - ct) \sqrt{\frac{c^2}{2\epsilon} \left( 1 - \frac{\beta^2}{6\epsilon} \right) + \frac{\kappa_x^2 - \kappa_y^2}{2\epsilon}} \right) \right) \]

\[ - \frac{c\beta(x\kappa_x + y\kappa_y - ct)}{3\kappa_x^2 \sqrt{2\epsilon}} \]

Video with \( c = 1, \kappa_x = 2/3, \kappa_y = \sqrt{5}/3, \epsilon = 0.01 \)
and \( \beta = 0.1 \)
Requirements of numerical scheme

• Resolve a wide range of length scales
• Resolve a wide range of time scales
• Be able to solve semi-linear equations
• Be able to solve equations with fourth order spatial derivatives
• Be able to solve equations with second order temporal derivatives
• Be able to satisfy boundary conditions on the displacement not the velocity
• Be able to satisfy a wide variety of displacement boundary conditions
Why use a spectral method?

• Advantages of typical spectral methods
  1. Fast spatial convergence for smooth solutions
  2. Can capture wide range of length scales

• Disadvantages of typical spectral methods
  1. Differentiation is ill-conditioned
  2. Standard spectral collocation methods are difficult to use for irregular domains
Chebyshev Integration matrix formulation for a linear boundary value problem

Differentiation

\[ Au_{xxxx} + Bu_{xx} + Cu = f(x) \]
\[ AD^4 u + BD^2 u + Cu = f(x) \]

Integration matrices

Let \( w = u_{xxxx} \)

\[ Aw + B \int \int w + C \int \int \int \int w = f(x) \]
\[ Aw + BS^2 w + CS^4 w + BCL = f(x) + BCR \]
Nonlinear time dependent boundary value problems

• Semi-implicit finite difference method in time

• Spectral integration method in space
Time stepping scheme

\[u_{tt} - \beta u_{xxt} = (u^3_x - u_x)_x - \epsilon u_{xxxx} - \alpha u\]

\[
\frac{2u^{n+1} - 5u^n + 4u^{n-1} - u^{n-2}}{\delta t^2} - \beta \frac{3u_{xx}^{n+1} - 4u_{xx}^n + u_{xx}^{n-1}}{2\delta t} = 2((u_x^n)^3 - u_x^n)_x - ((u_x^{n-1})^3 - u_x^{n-1})_x - \epsilon u_{xxxx}^{n+1} - \alpha u^{n+1}
\]
Relation to linear boundary value problem

\[ Au_{xxxx} + Bu_{xx} + Cu = f(x) \]

\[ \epsilon u_{xxxx}^{n+1} - \frac{3\beta u_{xx}^{n+1}}{2\delta t} + \frac{2u_{n+1}^{n+1}}{\delta t^2} + \alpha u_{n+1}^{n+1} = \]

\[ = \frac{5u^n - 4u^{n-1} + u^{n-2}}{\delta t^2} - \beta \frac{4u_{xx}^n - u_{xx}^{n-1}}{2\delta t} + 2 \left( (u_x^n)^3 - u_x^n \right)_x - \left( (u_x^{n-1})^3 - u_x^{n-1} \right)_x \]
Temporal convergence to traveling wave solution

\begin{figure}
\centering
\includegraphics[width=\textwidth]{temporal_convergence.png}
\caption{Maximum error during run against time step}
\end{figure}

\[ \beta = 0.1, \ \epsilon = 10^{-2}, \ c = 1 \ \text{and} \ 1024 \ \text{modes} \]
Spatial convergence to traveling wave solution

\[ \beta = 0.1, \; \epsilon = 10^{-2}, \; c = 1 \text{ and a timestep of } 10^{-5} \]
Movie of microstructure formation in one dimension

\[ u_{tt} - \beta u_{xxt} = (u_x^3 - u_x)_x - \epsilon u_{xxxx} - \alpha u \]

with boundary conditions

\[ u(x = 1) = 0, \quad u(x = -1) = 0 \]
\[ u_{xx}(x = 1) = 0, \quad u_{xx}(x = -1) = 0 \]

and parameters

\[ \beta = 1, \quad \epsilon = 10^{-4}, \quad \alpha = 100 \]

with 1024 modes and a timestep of \(10^{-4}\)
Preliminary movie of microstructure formation in two dimensions

\[ u_{tt} - \beta \Delta u_t = (u_y^3 - u_y)_y + u_{xx} - \epsilon \Delta^2 u \]

with boundary conditions

\[ u(x = 1, y) = 0, \quad u(x = -1, y) = 0 \]
\[ u_{xx}(x = 1, y) = 0, \quad u_{xx}(x = -1, y) = 0 \]

and periodic boundary conditions in \( y \).

With parameters

\[ \beta = 0.5 \quad \text{and} \quad \epsilon = 2 \times 10^{-6}. \]

With 128 modes in \( x \), 256 modes in \( y \)

and a timestep of 0.05
Energy during microstructure formation

Energy against time

- Total energy
- Strain energy
- Interfacial energy
- Kinetic energy

Time axis: 0 to 10,000
Energy axis: $10^{-20}$ to $10^5$
Figure 1: Initial Iterate A, $t = 0$.
Figure 2: Initial Iterate B, $t = 0$.
Figure 3: Final Iterate A, $t = 400$.
Figure 4: Final Iterate B, $t = 400$.
Figure 5: Energy evolution for run A.
Figure 6: Energy evolution for run B.
Conclusions

• A numerical method to investigate models for microstructure formation in martensite

• Exact traveling wave solution in two dimensions

• Links to acoustic emission when interfaces are formed
Further Work

- Prove spatial convergence of numerical scheme
- Adaptive and corrective time stepping for numerical scheme
- Further analysis of traveling wave solutions
- Use experimental fitted parameters to try and relate to acoustic emission
- Implement numerical scheme in a lower level programming language to obtain self-similar branching
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References


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