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
- Conclusions
- Further work

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

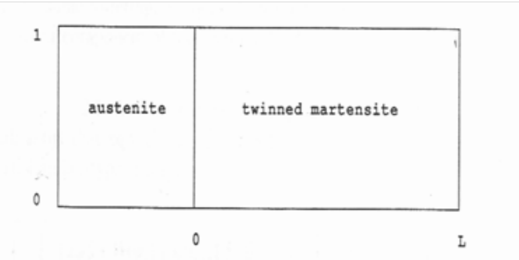
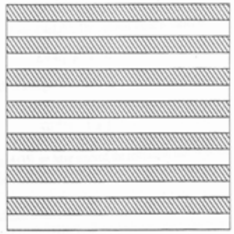
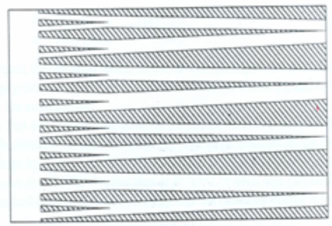


Fig. 2



The standard construction: 2N twins of width 1/2N.



The self-similar construction. Two generations of refinement are shown.

From Kohn and Müller, 1992

Dynamical Mathematical model

Nonlinear viscoelasticity with capillarity

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

Scalar one and two dimensional models

$$
\begin{aligned}
U_{tt} - \ \nabla\cdot\boldsymbol{\tau}(\nabla U, \nabla U_t) &= \nabla\cdot\boldsymbol{\sigma}(\nabla U) - \epsilon\Delta^2 U \\
u_{tt} - \qquad\qquad\qquad \beta\Delta u_t &= (u_x^3 - u_x)_x + u_{yy} - \epsilon\Delta^2 u \\
u_{tt} - \qquad\qquad\qquad \beta u_{xxt} &= (u_x^3 - u_x)_x - \alpha u - \epsilon u_{xxxx}
\end{aligned}
$$

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 α, β, and $\epsilon \geq 0$. Interested in small ϵ.

Exact traveling wave solutions

$$u_{tt} - \beta u_{xxt} = (u_x^3 - u_x)_x - \epsilon u_{xxxx}$$
$$u_{tt} - \beta \Delta u_t = (u_x^3 - u_x)_x + u_{yy} - \epsilon \Delta^2 u$$

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

Substitute $r = u_\zeta$

$$\epsilon r_{\zeta\zeta} + \omega\beta r_\zeta + (\rho\omega^2 + \kappa_x^2 - \kappa_y^2)r - \kappa_x^4 r^3 = A_1$$

Use the ansatz $r = A_2 \tanh(A_3\zeta) + A_4$

Exact traveling wave solutions

One dimensional solution when

$$c^2(1-\beta^2/6\epsilon)+1\geq 0$$

$$u=\sqrt{2\epsilon}\log\left(\cosh\left[(x-ct)\sqrt{\frac{c^2}{2\epsilon}\left(1-\frac{\beta^2}{6\epsilon}\right)+\frac{1}{2\epsilon}}\right]\right) - \frac{c\beta(x-ct)}{3\sqrt{2\epsilon}}$$

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

$$
\begin{aligned}
&Au_{xxxx} &&+Bu_{xx} &&+Cu &&=f(x)\\
&AD^4u &&+BD^2u &&+Cu &&=f(x)
\end{aligned}
$$

Integration matrices
Let $w = u_{xxxx}$

$$
\begin{aligned}
&Aw &&+B\iint w &&+C\iiiint w &&=f(x)\\
&Aw &&+BS^2w &&+CS^4w + BCL &&=f(x) + BCR
\end{aligned}
$$

Nonlinear time dependent boundary value problems

- Semi-implicit finite difference method in time

- Spectral integration method in space

Time stepping scheme

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

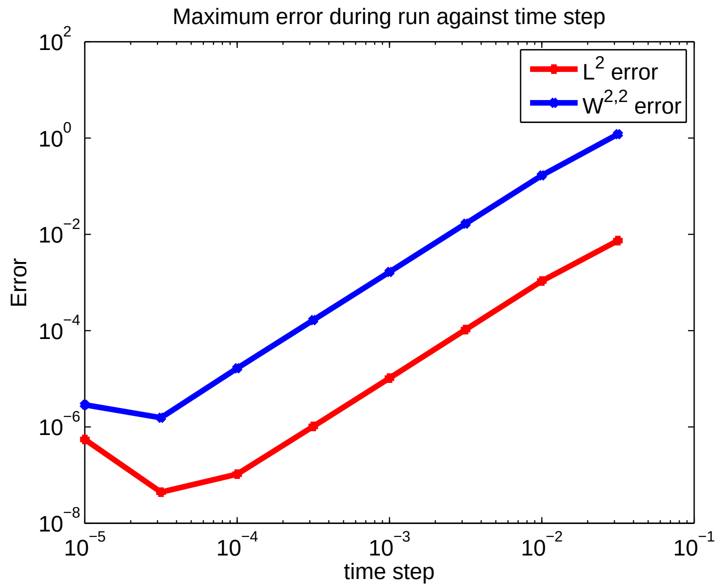
$$\frac{2u^{n+1} - 5u^n + 4u^{n-1} - u^{n-2}}{\delta t^2}$$
$$- \beta \frac{3u_{xx}^{n+1} - 4u_{xx}^n + u_{xx}^{n-1}}{2\delta t}$$
$$= 2((u_x^n)^3 - u_x^n)_x - ((u_x^{n-1})^3 - u_x^{n-1})_x$$
$$- \epsilon u_{xxxx}^{n+1} - \alpha u^{n+1}$$

Relation to linear boundary value problem

$$Au_{xxxx} \quad + Bu_{xx} \quad + Cu$$
$$= f(x)$$

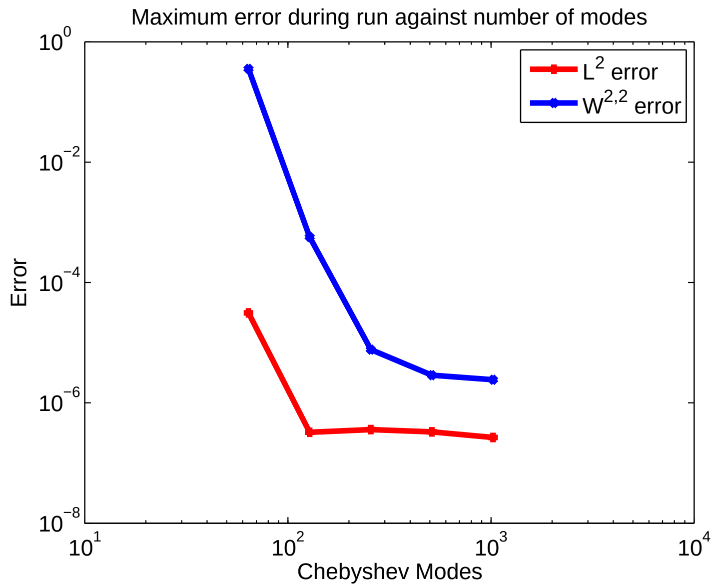
$$\epsilon u_{xxxx}^{n+1} \quad - \frac{3\beta u_{xx}^{n+1}}{2\delta t} \quad + \frac{2u^{n+1}}{\delta t^2} + \alpha u^{n+1}$$
$$= \frac{5u^n - 4u^{n-1} + u^{n-2}}{\delta t^2} - \beta \frac{4u_{xx}^n - u_{xx}^{n-1}}{2\delta t}$$
$$+ 2\left((u_x^n)^3 - u_x^n\right)_x - \left((u_x^{n-1})^3 - u_x^{n-1}\right)_x$$

Temporal convergence to traveling wave solution



$\beta = 0.1$, $\epsilon = 10^{-2}$, $c = 1$ and 1024 modes

Spatial convergence to traveling wave solution



$\beta = 0.1$, $\epsilon = 10^{-2}$, $c = 1$ 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

$$\begin{aligned} u(x=1) &= 0, & u(x=-1) &= 0 \\ u_{xx}(x=1) &= 0, & u_{xx}(x=-1) &= 0 \end{aligned}$$

and parameters

$$\beta = 1 \qquad \epsilon = 10^{-4} \qquad \alpha = 100$$

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

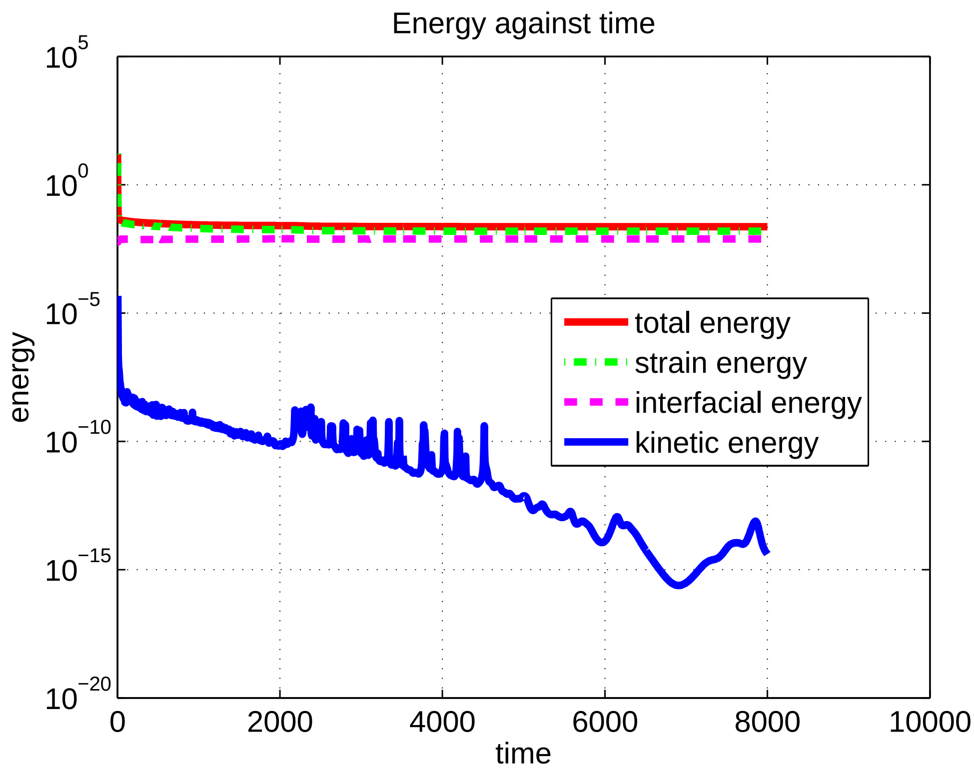
$$\begin{aligned} u(x=1,y) &= 0, & u(x=-1,y) &= 0 \\ u_{xx}(x=1,y) &= 0, & u_{xx}(x=-1,y) &= 0 \end{aligned}$$

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



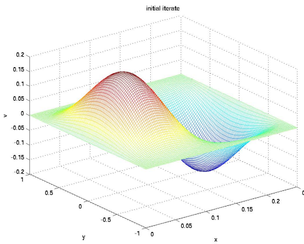


Figure 1: Initial Iterate A, $t = 0$.

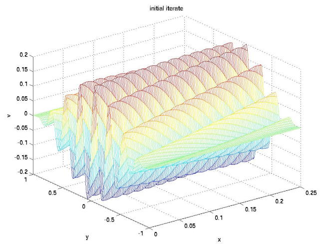


Figure 2: Initial Iterate B, $t = 0$.

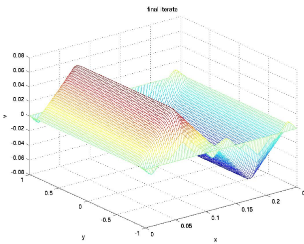


Figure 3: Final Iterate A, $t = 400$.

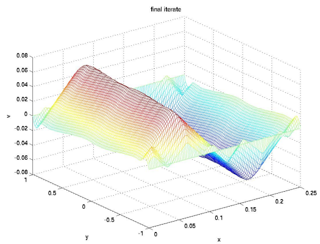


Figure 4: Final Iterate B, $t = 400$.

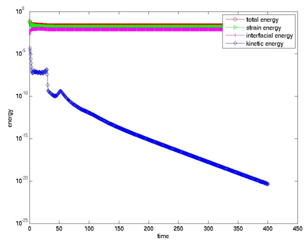


Figure 5: Energy evolution for run A.

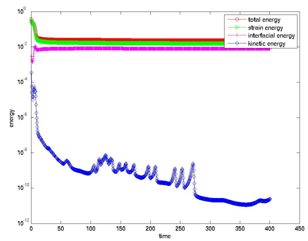


Figure 6: Energy evolution for run B.

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

Acknowledgements

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