Spectral methods for investigating solutions to partial differential equations

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Acknowledgements

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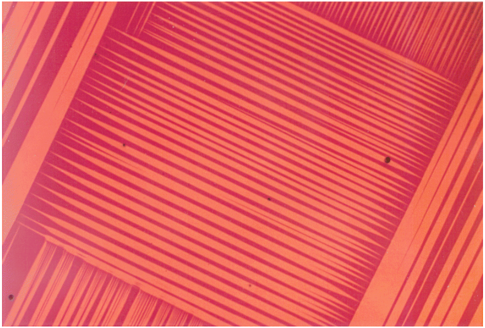
Outline

- The Kohn-Müller functional
- The Aviles-Giga functional
- The 2D Navier Stokes equation
- Klein-Gordon equation
- Conclusion

Section 1: Computations of the Kohn-Müller model

- The sharp interface Kohn-Müller model
- The smooth interface Kohn-Müller model
- Computational results

Simplified model which may capture twinning at a boundary



Twinning in Copper Aluminum Nickel (picture by Chu and James)

The Kohn-Müller model

- Conjectured correspondence

$$\int_\Omega \tfrac{\gamma}{2} w_y^2 + \tfrac{15}{4}\left(w_x^2 - 1\right)^2 + \tfrac{\epsilon^2}{2} w_{xx}^2 \mathrm{d}x\mathrm{d}y$$
$$\approx \int_\Omega \tfrac{\gamma}{2} w_y^2 \mathrm{d}x\mathrm{d}y + \int_{J_{w_x}} 2\epsilon\sqrt{\tfrac{10}{3}}\,|[w_x]|^3\,\mathrm{d}\mathcal{H}^1.$$

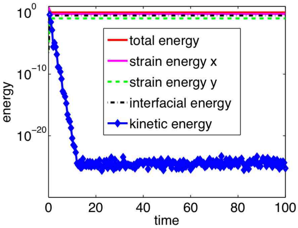
- Smooth interface

$$\int_\Omega \frac{5}{2} w_y^2 + \frac{15}{4}\left(w_x^2 - 1\right)^2 + \frac{\epsilon^2}{2} w_{xx}^2 \mathrm{d}x$$

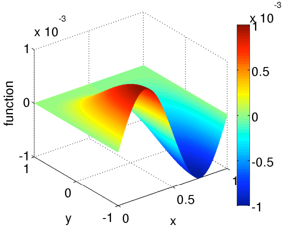
- Equation of motion

$$\rho w_{tt} - \beta\Delta w_t = 15(3w_x^2 - 1)w_{xx} + 5w_{yy} - \epsilon^2 w_{xxxx}$$

Numerical Results for the Kohn-Müller model



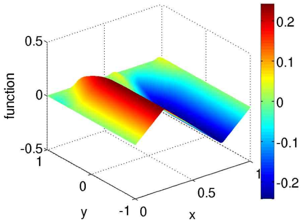
(a) A plot showing the evolution of the different energy components.



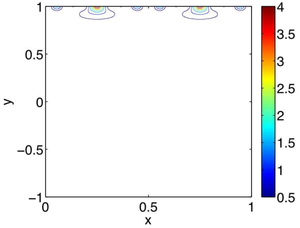
(b) Initial Iterate Contour plot of $\frac{\epsilon^2}{2} w_{xx}^2$.

A local minimum for the Kohn-Müller energy functional with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.0316$.

Numerical Results for the Kohn-Müller model



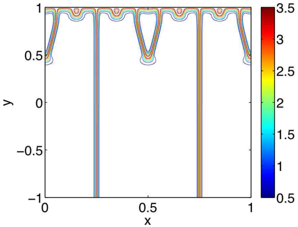
(c) Final iterate. Colours show the function, w.



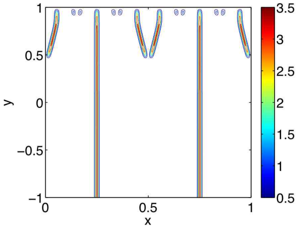
(d) Contour plot of $\frac{5}{2}w_y^2$ in the final iterate.

A local minimum for the Kohn-Müller energy with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.0316$.

Numerical Results for the Kohn-Müller model



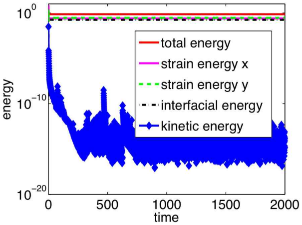
(e) Contour plot of $\frac{15}{4}(w_x^2 - 1)^2$ in the final iterate.



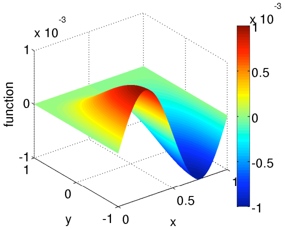
(f) Contour plot of $\frac{\epsilon^2}{2} w_{xx}^2$ in the final iterate.

A local minimum for the Kohn-Müller energy functional with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.0316$.

Numerical Results for the Kohn-Müller model



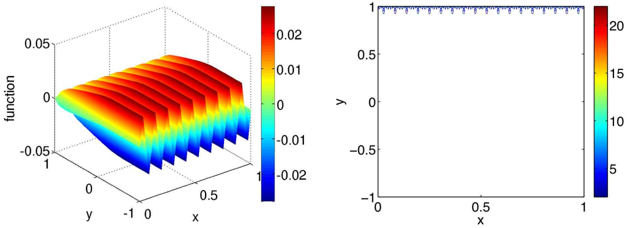
(g) A plot showing the evolution of the different energy components.



(h) Initial Iterate Contour plot of $\frac{\epsilon^2}{2} w_{xx}^2$.

A local minimum for the Kohn-Müller energy functional with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.001$.

Numerical Results for the Kohn-Müller model

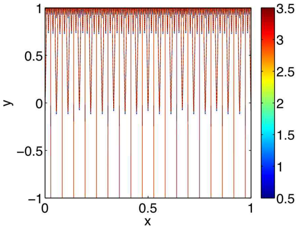


(i) Final iterate. Colours show the function, w.

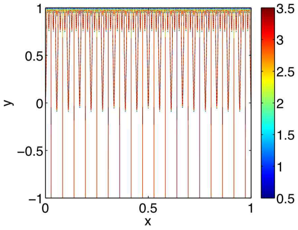
(j) Contour plot of $\frac{5}{2}w_y^2$ in the final iterate.

A local minimum for the Kohn-Müller energy with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.001$.

Numerical Results for the Kohn-Müller model



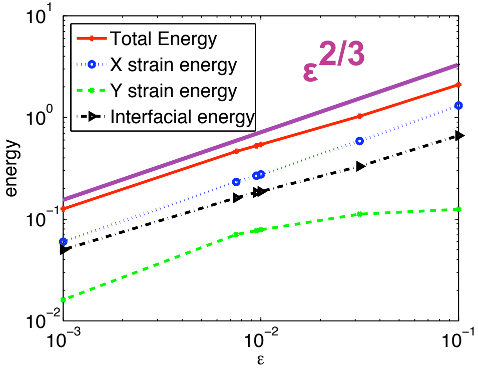
(k) Contour plot of $\frac{15}{4}(w_x^2 - 1)^2$ in the final iterate.



(l) Contour plot of $\frac{\epsilon^2}{2} w_{xx}^2$ in the final iterate.

A local minimum for the Kohn-Müller energy functional with $\rho = 1$, $\beta = 0.1$ and $\epsilon = 0.001$.

Scaling law predicted by Kohn and Müller for the total energy



Energy scaling, reference line drawn for ease of comparison.
For small ϵ good agreement with theoretical predictions.

Section 2: Computations of the Aviles-Giga model

- The model
- The conjecture
- Computational results

The model

- The energy to minimise

$$\int \frac{1}{4\epsilon}(w_x^2 + w_y^2 - 1)^2 + \frac{\epsilon}{2}(\Delta w)^2 \, \mathrm{d}x\mathrm{d}y$$

- limiting solution as $\epsilon \to 0$,

$$w_x^2 + w_y^2 = 1$$

and minimise

$$\int_{J_{\nabla w}} \frac{\sqrt{2}}{12} |[\nabla w]|^3 \, \mathrm{d}\mathcal{H}^1$$

- Remarks:
  1. Assume a one dimensional interface
  2. The above assumption leads to equipartition of energy

Points which need to be demonstrated for the conjecture to hold

- The Γ–limit is infinite unless $w_{xx} + w_{yy} = 1$ almost everywhere
- The proposed sharp interface limit $|\nabla w|/3$ is correct
- The asymptotic energy lives on a one dimensional defect set, and lower dimensional singularities carry no energy

DeSimone, Kohn, Müller and Otto

Equation of motion

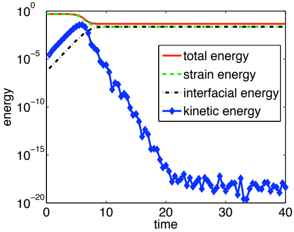
- The energy to minimise

$$\int \frac{1}{4}(w_x^2 + w_y^2 - 1)^2 + \frac{\epsilon^2}{2}(\Delta w)^2 \, \mathrm{d}x\mathrm{d}y$$

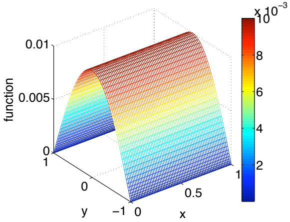
- Viscoelastic dynamics

$$\begin{aligned} &\rho w_{tt} - \beta \Delta w_t \\ &= \left[w_x (w_x^2 + w_y^2 - 1) \right]_x + \left[w_y (w_x^2 + w_y^2 - 1) \right]_y - \epsilon^2 \Delta^2 w \end{aligned}$$

Numerical Results for the Aviles-Giga model 1



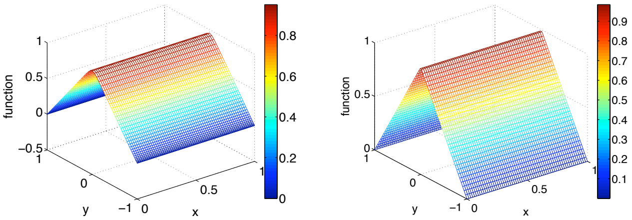
(m) A plot showing the evolution of the different energy components.



(n) Initial Iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.05$, $w(y = \pm 1) = 0$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 1

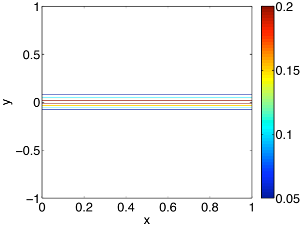


(o) Final Iterate

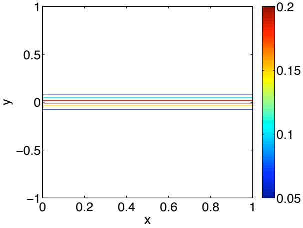
(p) Viscosity solution assuming equipartition of energy

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.05$, $w(y = \pm 1) = 0$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 1



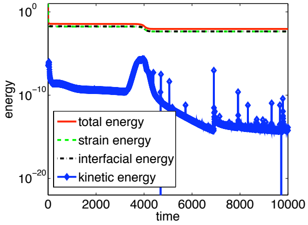
(q) Contour plot of interface energy term $\frac{\epsilon^2}{2}(\Delta w)^2$ in the final iterate.



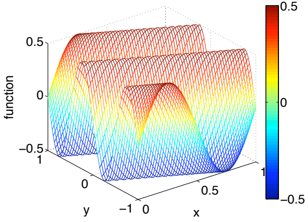
(r) Contour plot of $\frac{1}{4}(w_x^2 + w_y^2 - 1)^2$ in the final iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.05$, $w(y = \pm 1) = 0$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 2



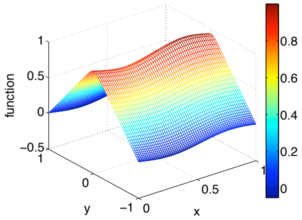
(s) A plot showing the evolution of the different energy components.



(t) Initial Iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.01$, $w(y = \pm 1) = -0.05 \sin(2\pi x)$ and $w_{yy}(y = \pm 1) = 0$.

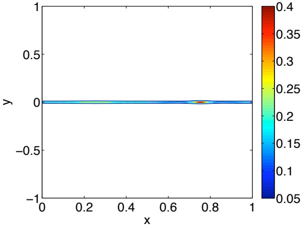
Numerical Results for the Aviles-Giga model 2



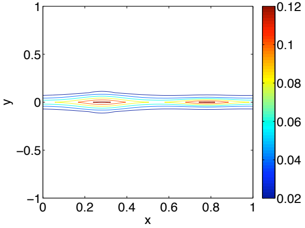
(u) Final Iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.01$, $w(y = \pm 1) = -0.05 \sin(2\pi x)$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 2



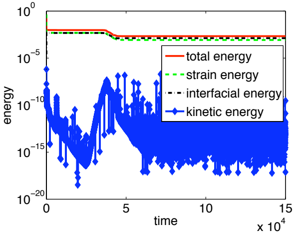
(v) Contour plot of interface energy term $\frac{\epsilon^2}{2}(\Delta w)^2$ in the final iterate.



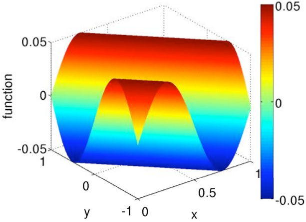
(w) Contour plot of $\frac{1}{4}(w_x^2+w_y^2-1)^2$ in the final iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.05$, $w(y = \pm 1) = 0$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 3



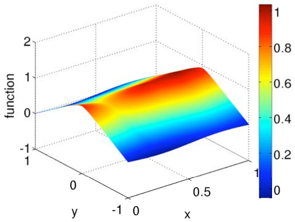
(x) A plot showing the evolution of the different energy components.



(y) Initial Iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.0025$,
$w(y = \pm 1) = -0.05 \sin(2\pi x)$ and $w_{yy}(y = \pm 1) = 0$.

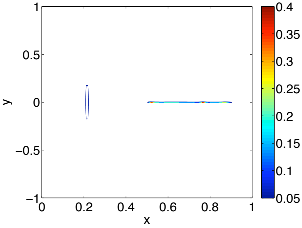
Numerical Results for the Aviles-Giga model 3



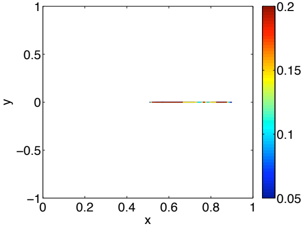
(z) Final Iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.0025$, $w(y = \pm 1) = -0.05 \sin(2\pi x)$ and $w_{yy}(y = \pm 1) = 0$.

Numerical Results for the Aviles-Giga model 3



() Contour plot of interface energy term $\frac{\epsilon^2}{2}(\Delta w)^2$ in the final iterate.



() Contour plot of $\frac{1}{4}(w_x^2 + w_y^2 - 1)^2$ in the final iterate

Numerically computed minimizer for the Aviles-Giga energy functional with $\rho = 1$, $\beta = 1.0$, $\epsilon = 0.0025$, $w(y = \pm 1) = 0$ and $w_{yy}(y = \pm 1) = 0$.

Result Summary

$w(y=\pm 1)$	ϵ	$\int \frac{1}{4}(w_x^2 + w_y^2 - 1)^2$	$\int \frac{\epsilon^2}{2}(\Delta w)^2$	$\frac{\text{Total Energy}}{\epsilon}$
0	0.05	0.0235	0.0236	0.944
0	0.01	0.00471	0.00471	0.942
$-0.005\sin(2\pi x)$	0.05	0.0235	0.0237	0.942
$-0.005\sin(2\pi x)$	0.01	0.00471	0.00471	0.942
$0.05\sin(2\pi x)$	0.05	0.0217	0.0261	0.956
$0.05\sin(2\pi x)$	0.01	0.00451	0.00458	0.909
$0.05\sin(2\pi x)$	0.0025	0.000846	0.00132	0.868

Prediction that (Total Energy)/$\epsilon = 2\sqrt{2}/3 \approx 0.943$ if Aviles-Giga conjecture holds and zero boundary conditions.

Conclusions

- Simulations can be a useful tool to test scaling assumptions
- For the Kohn-Müller model, the simulations are in agreement with the model
- For the Aviles-Giga model, the conjecture may not hold when non-zero boundary conditions are applied

The 2D Navier-Stokes Equation

Introduction

- Consider incompressible case only
- Model for dynamics in a uniform and thin layer of water
- $$\begin{aligned} \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) &= -\nabla p + \mu\Delta\mathbf{u} \\ \nabla\cdot\mathbf{u} &= 0. \end{aligned}$$
- $\mathbf{u}(x,y) = (u(x,y), v(x,y))$, p pressure, μ viscosity, ρ, density

Vorticity-Streamfunction Formulation

- $$\omega = \nabla \times \mathbf{u} = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = -\Delta\psi$$

- $$\rho\left(\frac{\partial \omega}{\partial t} + u\frac{\partial \omega}{\partial x} + v\frac{\partial \omega}{\partial y}\right) = \mu\Delta\omega$$

  and

  $$\Delta\psi = -\omega.$$

Time Discretization

- $$\rho \left[\frac{\omega^{n+1,k+1} - \omega^n}{\delta t} \right.$$
  $$\left. + \frac{1}{2} \left(u^{n+1,k} \frac{\partial \omega^{n+1,k}}{\partial x} + v^{n+1,k} \frac{\partial \omega^{n+1,k}}{\partial y} + u^n \frac{\partial \omega^n}{\partial x} + v^n \frac{\partial \omega^n}{\partial y} \right) \right]$$
  $$= \frac{\mu}{2} \Delta \left(\omega^{n+1,k+1} + \omega^n \right),$$
  and
  $$\Delta \psi^{n+1,k+1} = -\omega^{n+1,k+1},$$
  $$u^{n+1,k+1} = \frac{\partial \psi^{n+1,k+1}}{\partial y}, \quad v^{n+1,k+1} = -\frac{\partial \psi^{n+1,k+1}}{\partial x}.$$
- Fixed point iteration used to obtain nonlinear terms

Example Videos

- `http://www-personal.umich.edu/~cloutbra/research.html`
- Simulations on a single NVIDIA Fermi GPU about 20 times faster than a 16 core CPU

The Real Cubic Klein-Gordon Equation

The Real Cubic Klein-Gordon Equation

- $$u_{tt} - \Delta u + u = |u|^2 u$$

- $$E(u, u_t) = \int \frac{1}{2}|u_t|^2 + \frac{1}{2}|u|^2 + \frac{1}{2}\left|\nabla u\right|^2 - \frac{1}{4}\left|u\right|^4 \mathrm{d}\boldsymbol{x}$$

- $$\frac{u^{n+1} - 2u^n + u^{n-1}}{(\delta t)^2} - \Delta \frac{u^{n+1} + 2u^n + u^{n-1}}{4} + \frac{u^{n+1} + 2u^n + u^{n-1}}{4}$$
  $$= \pm \left|u^n\right|^2 u^n$$

- Parallelization done using 2decomp library for FFT and processing independent loops

Relevant Previous Work

- Donninger and Schlag (2010) - Study of blowup of radially symmetric solutions, 2^{nd} order symplectic schemes
- Bao and Yang (2006) and Yang (2007) 2D simulations
- Chen (2006) 4^{th} order symplectic schemes
- Hamaza and Zaag (2010) Solutions can only blow up in an ODE like manner

Relevant Previous Work

- Nakanishi and Schlag (2011) Characterization of behavior of solutions near ground state
    (i) Scattering to zero in both forward and backward time
    (ii) Blow up in finite forward and backward time
    (iii) Scattering to zero in forward time and blow up in backward time
    (iv) Blow up in forward time and scattering to zero in backward time
    (v) Trapping by the ground state $\pm Q$ in forward time and scattering to zero in backward time
    (vi) Scattering to 0 in forward time and trapping by the ground state $\pm Q$ in backward time
    (vii) Trapping by the ground state $\pm Q$ in forward time and blow up in backward time
    (viii) Blow up in forward time and trapping by the ground state $\pm Q$ in backward time
    (ix) Trapping by $\pm Q$ in both forward and backward time

What is Q?

- $$\Delta Q - Q = Q^3.$$

Example Videos

- Dispersion 1
- Dispersion 2
- Blow up

Interaction of 2 Solitons

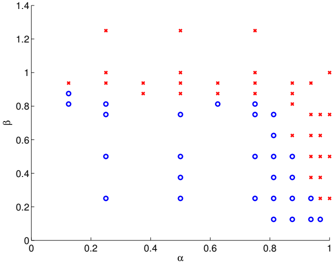
- Initial Conditions

$$u(t=0) = \alpha Q_1 + \beta Q_{-1}$$

$$u_t(t=0) = 2\beta \exp\left(-x^2 - y^2 - z^2\right)\cos(4x)\cos(6y)\cos(8z)$$

where $\alpha \in (0,1]$ and $\beta \in (0,1]$.

Interaction of 2 Solitons



-

- The $\times$ indicate numerical experiments in which there was blowup and the o indicate numerical experiments for which the solution dispersed. As predicted from theory, here is a surface separating solutions which blow up and those which disperse.

- Work in reasonable agreement with previous work by Donninger and Schlag
- Again, exact criteria to examine for distinguishing between blow up and global existence is unclear

Simulations and Videos by Brian Leu, Albert Liu, and Parth Sheth

- http://www-personal.umich.edu/~alberliu/
- http://www-personal.umich.edu/~pssheth/

Conclusion

- Easy to program numerical method which can be used to study semilinear partial differential equations
- Method parallelizes well on hardware with good communications so a good tool to introduce parallel programming ideas
- Research tool to investigate and provide conjectures for behavior of solutions to partial differential equations
- Research tool to investigate computer hardware performance and correctness
- Better user interface and integration with visualization would help make it easier for those without strong programming backgrounds

Acknowledgements and References

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- Hopper at the National Energy Research Scientific Computing Center
- SCREMS NSF DMS-1026317
- The Blue Waters Undergraduate Petascale Education Program administered by the Shodor foundation
- The Division of Literature, Sciences and Arts at the University of Michigan

- B.K. Muite, D.Phil. Thesis, University of Oxford 2010
- G. Chen, B. Cloutier, N. Li, B.K. Muite, P. Rigge and S. Balakrishnan, A. Souza, J. West, "Parallel Spectral Numerical Methods" `http://en.wikibooks.org/w/index.php?title=Parallel_Spectral_Numerical_Methods`