# Nuemrical Simulation of Two-Dimensional Martensitic Phase Transition and Microstructure

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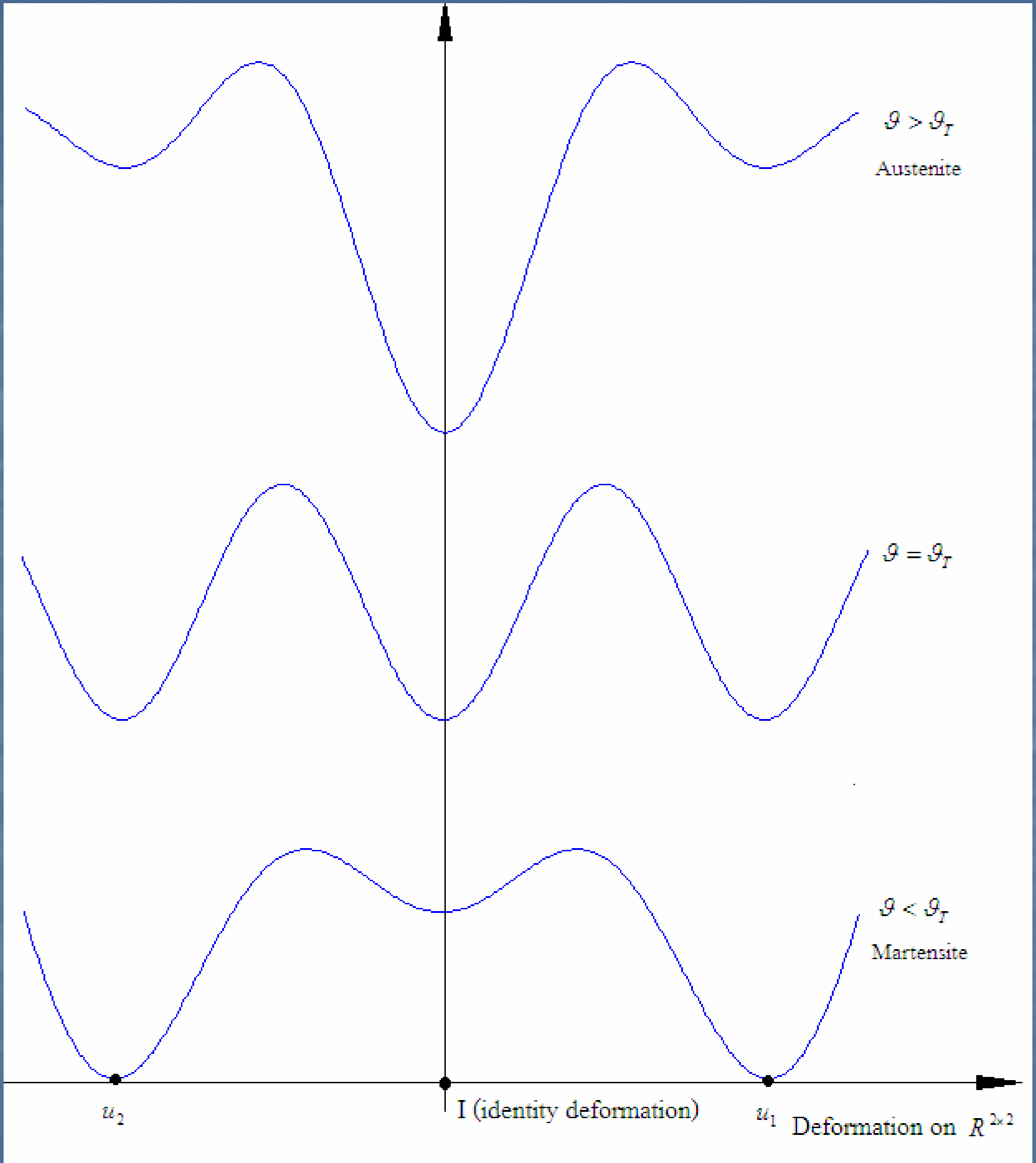
# Outline

- Background Problem Description
- Finite Element Discretization
- Numerical Optimization
- Some Preliminary Results
- Future Work

# Background Problem Description

- Two-Dimensional (2D) martensitic phase transition and microstructure
  - Martensitic microstructure is a low-temperature phase with fine-scale mixture of different martensitic variants
  - Austenitic microstructure is a high-temperature phase with one phase stable lattice structure

- Minimize the bulk energy
- Energy-minimizing sequences can model fine-scale martensitic microstructure


$\vartheta > \vartheta_T$
Austenite
$\vartheta = \vartheta_T$
$\vartheta < \vartheta_T$
Martensite
$u_2$
I (identity deformation)
$u_1$
Deformation on $R^{2\times 2}$

# Background Problem Description Con'd

- A two-dimensional energy model I am working on

The total energy is associated with a deformation *y(x)*, of the reference domain

$$\Omega = [0,1]^2, y : \Omega \to R^{2\times 2}$$

I consider Lipschitz continuous functions which satisfy the boundary condition

*y(x) = F(x)*.

The energy function is given by

$$E(y) = \int_\Omega W(\nabla y(x))dx$$

Energy Density

$$W(F) = \Phi(F^T F) = \Phi(C) \qquad \Phi(C) = \kappa_1 (trC - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3 \left( \left( \frac{C_{11} - C_{12}}{2} \right)^2 - \varepsilon^2 \right)^2$$

with constants $\kappa_i > 0$ and $\varepsilon > 0$

# Finite Element Discretization

- Finite-element approximation of the space of admissible deformations

$$\Omega_{ij} = [ih, (i+1)h] \times [jh, (j+1)h]$$

- Bilinear Finite Element $\quad u_h = (u_h^1, u_h^2)$

$$u_h^k = \sum_{i,j=0}^{N} u_{ij}^k \phi_{ij} \qquad k = 1 \text{ or } 2$$

where $\phi_{ij}$ are the bilinear basis functions.

- Discretization form of energy function

$$E(y) = h^2 \sum_{i,j=0}^{N-1} W(\nabla u_h(m_{ij}))$$

where $m_{ij}$ is the midpoint of $\Omega_{ij}$

# Finite Element Discretization Con'd

- Deformation Gradient $\nabla u_h$

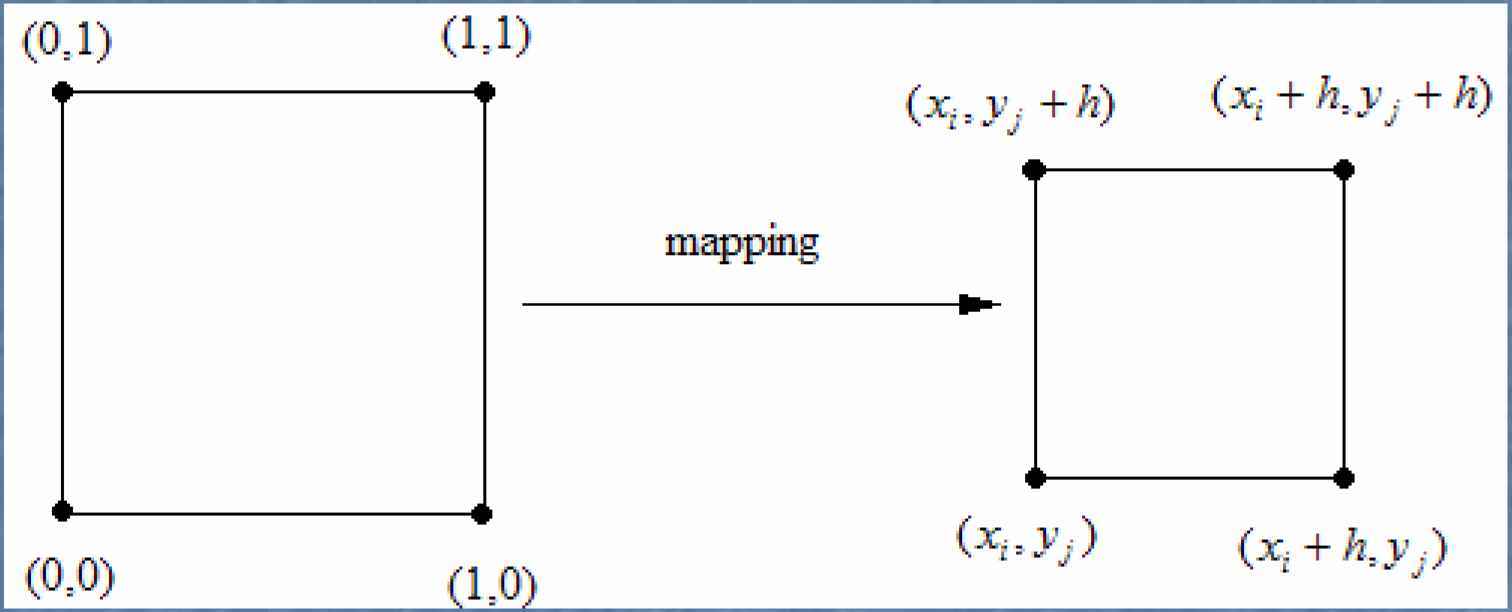
$$\frac{\partial u_h^k}{\partial x}(m_{ij}) = \frac{1}{2h}\left(u_{i+1j}^k + u_{i+1j+1}^k - u_{ij}^k - u_{ij+1}^k\right)$$

$$\frac{\partial u_h^k}{\partial y}(m_{ij}) = \frac{1}{2h}\left(u_{ij+1}^k + u_{i+1j+1}^k - u_{ij}^k - u_{i+1j}^k\right)$$

- First Derivative of energy function $\nabla E$

  - Use ADIC, generate the derivative functions automatically. (Give up)

  - Do it by hand. Basic idea is to use the bilinear basis function in each element. There is a mapping from the unitary square to an arbitrary element.


(0,1)
(1,1)
(0,0)
(1,0)
mapping
$(x_i, y_j + h)$
$(x_i + h, y_j + h)$
$(x_i, y_j)$
$(x_i + h, y_j)$

# Numerical Optimization

- One-Dimensional Function
  - Bracket Method (Golden Section Search)
- Multidimensional Function
  - Method with the computation of first derivatives
    - Conjugate Gradient Method
  - Method without the computation of first derivatives
    - Downhill Simplex method (Nelder-Mead's method)

# Some Preliminary Work

- Study a Two-Well problem with the energy density

$$\Phi(C) = \kappa_1 (trC - 2)^2 + \kappa_2 C_{12}^2 + \kappa_3 \left( \left( \frac{C_{11} - C_{12}}{2} \right)^2 - \varepsilon^2 \right)^2$$

- Build the discretization  format of the problem

- Study the numerical methods of optimization

# Some Preliminary Work con’d

- Programming
  - Configuration class that sets up domain, boundary condition, discretized energy density, and the first derivative of the energy function.
  - Optimization class that handles the iterative descent method for my energy function. Currently I finished 1-D optimization part, and conjugate gradient method. I am taking codes in Numerical Recipe as reference.

    Bugs in my optimization module.

# Some Preliminary Work con'd

- Test ADIC (Automatic Differentiation Tool for ANSI-C ), but finally found that its code is very inefficient.
- I transform the definition part of C code to Matlab, then use Nelder-Meade method in Matlab to test my problem.
- Initially I linked the SUN library for some basis functions. After I switched to UMIACS Linux cluster, I rewrote them by myself.
- Use CVS to manage the code

# Future Work

- During the winter break
  - Finish optimization framework using conjugate gradient method
  - Investigate Nelder-Meade method
  - Explore the parallel scheme for my project.

- In next semester
  - Solve the problem with the surface energy.
  - Deal with different boundary condition
  - Explore the adaptive FMM
  - Visualization

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