

A Numerical and Analytical Study of Modeling Techniques for Solidification Problems

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Abstract

Solidification is a phenomenon of paramount importance in various areas of industry; its understanding is critical for designing materials with superior properties. The nonlinear and metastable nature of this mesoscale phenomenon has given rise to various numerical models that attempt to describe it. In this talk we provide a comparison of several computational models that describe solidification based on their ability to predict statistical properties of different materials. The results of numerical experiments and several extensions of the known modeling techniques are discussed.

Introduction

Solidification is the process of a substance transitioning from solid to liquid. Two popular models for describing this are the Phase-Field Model and the Monte Carlo Metropolis algorithm.

Phase-Field Model

Let $\phi(x, t)$ describe the state of matter of a substance. ϕ is a continuous function defined to be 0 if the substance is solid at a given point and 1 if the substance is liquid at a given point. A physical interpretation of ϕ is to let ϕ be a curve drawn along the damped wave that represents the probability of an atom existing at a given position (Figure 1). [1] This concept explains the non-integral values of ϕ and will also be useful in comparing with atomistic methods. We will be assuming that a pure substance is being modeled, that the energy functional for ϕ is a "double well", and that the temperature, T is constant. Our model is:

Cahn-Allen Equation

$$\frac{\partial \phi}{\partial t} = \epsilon^2 \nabla^2 \phi - 2W\phi(1-\phi)(1-2\phi) - \frac{30L}{T_M}(T_M - T)\phi^2(1-\phi)^2$$

Where W is a constant that scales our "double well", T_M is the melting temperature, L is the latent heat, and ϵ is the gradient energy coefficient. We will only be considering the static solution to this model.



Metropolis Algorithm

To perform this computer simulation, first we create a virtual block of atoms to represent some substance. Then we perform the following:

1. Select a random particle and calculate its energy, E_1
2. Randomly move the particle and recalculate its energy, E_2
3. Accept or reject the change
 - If $E_2 - E_1 < 0$, accept the change
 - otherwise
 - Compute $p = \exp\left[\frac{E_2 - E_1}{-k_B T}\right]$
 - Randomly generate $r \in [0, 1]$
 - If $r \leq p$, accept the change
4. Repeat

Metropolis Algorithm Results

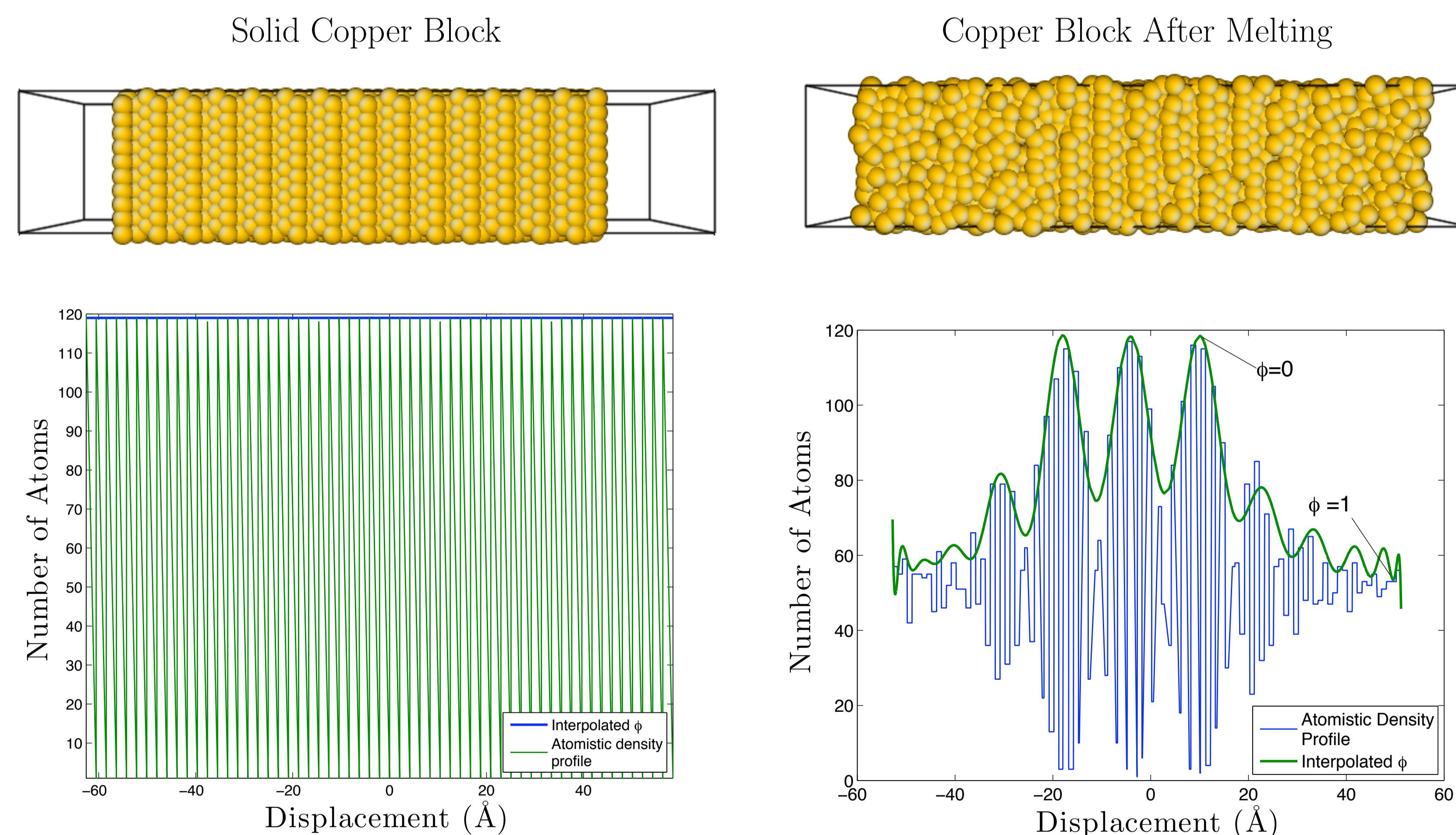


Figure 3: Upper Left: A solid copper block visualized atomistically. Upper Right: A partially melted copper block at equilibrium as simulated by the Metropolis Algorithm. The simulation was conducted at the melting point, 1327 K. Lower Left: Green Line: The number of atoms in a 1Å vertical 'slice' of the block above it. Blue Line: Value for ϕ interpolated from the atomistic data (Here ϕ is constant and always equal to 0). Lower Right: Blue Line: The number of atoms in a 1Å vertical 'slice' of the block above it. Green Line: Value for ϕ interpolated from the atomistic data by a degree 25 polynomial (The implications of this interpolation are discussed in the Comparison of Results section.)

Phase-Field Results

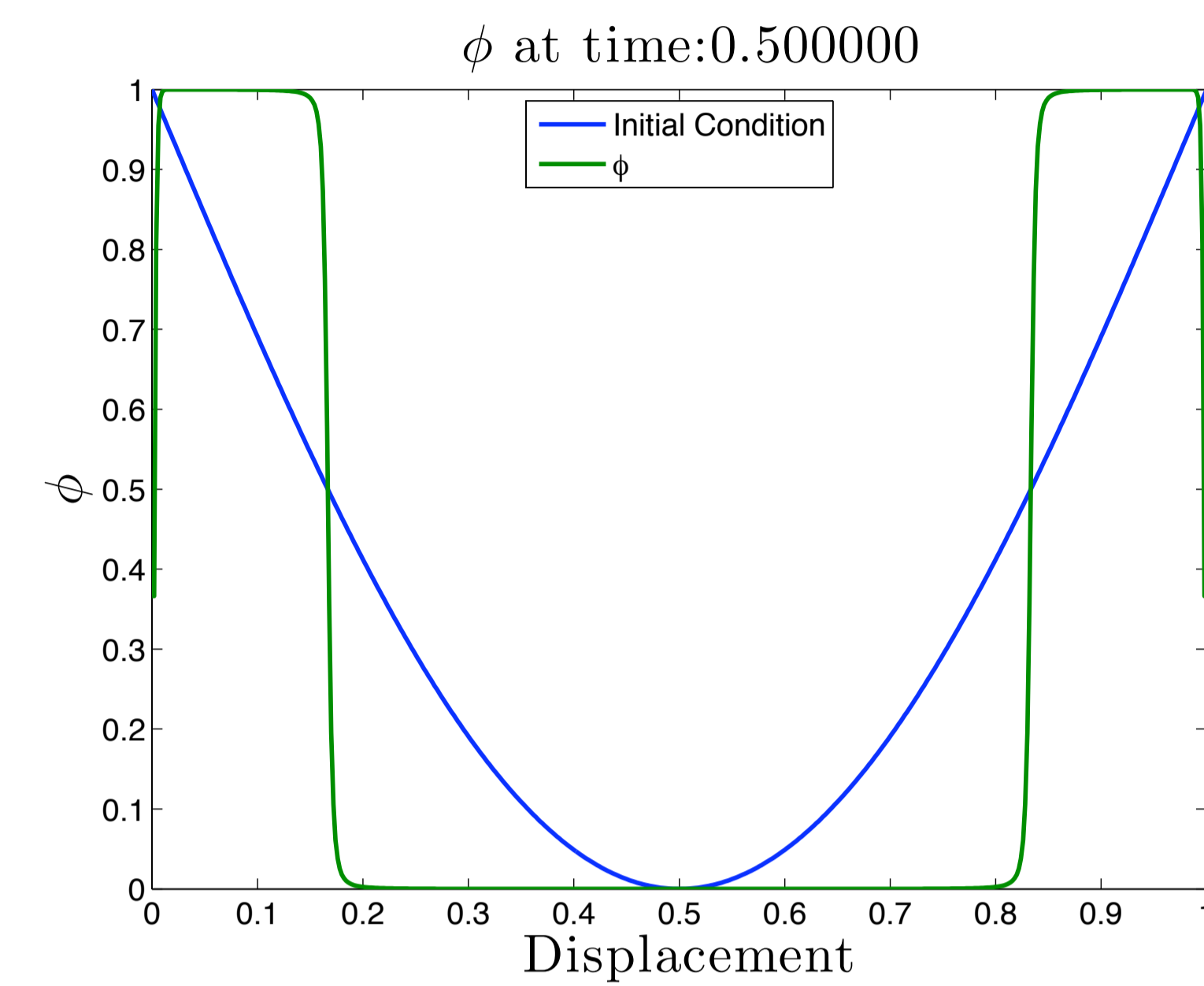


Figure 2: Blue Line: Initial Condition, Green Line: Static, numerical solution of the phase field model with homogeneous Neumann boundary conditions

Comparison of Results

Based on our physical understanding of ϕ , we would expect the curve drawn along the maxima of damped wave (Figure 3: Lower Right) that represents atomic density to correspond exactly with the static solution we have obtained for ϕ . This, however, is not the case. There are several reasons for this:

- Incorrect parameters for Phase-Field Model
- Polynomial interpolation
- Crude method for generating density profile [4]
- Unknown differences in the two models

References

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<http://www.ctcms.nist.gov/fipy>

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