Simple phase field model of martensitic transformation written in ANSYS APDL

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1 Introduction

In this post, we illustrate a simple implementation of a phase field model using APDL (Ansys Parametric Design Language). We assume that we are looking for the solution on a rectangular domain with a regular mesh. This assumption allows us to solve the phase field equations using the finite difference scheme. Meantime, the displacement field is solved using the finite element method of the ANSYS's solver without any restriction on the underlying material model (elastic, elasto-plastic, etc.). Both implicit or explicit solvers can be used. Such implementation provides ample opportunities for testing the behaviour of various material models or loading conditions on the process of phase transformation.

2 Governing equations

Here, we consider a simple phase field model presented by [1]. In this model, the total energy of the system Ψ can be written as

$$\Psi = \int_\Omega \left[\frac{A}{2}\phi^2 + \frac{B}{3}\phi^3 + \frac{C}{4}\phi^4 + \frac{\kappa}{2}|\vec{\nabla}\phi|^2 + \frac{1}{2}\boldsymbol{\varepsilon}^e : \mathbb{C} : \boldsymbol{\varepsilon}^e \right] d\Omega \tag{1}$$

where A, B, and C are material constants related to the double-well energy landscape defining the thermodynamics of the phase transformation, ϕ is the scalar order parameter which is a continuous function typically in the range between 0 and 1, where 0 represents the parent phase and 1 represents the product phase. The symbol : indicate the tensor contraction. κ is a material parameter related to the interface energy between the parent and the product phase.

$$|\vec{\nabla}\phi|^2 = \left(\frac{\partial\phi}{\partial x}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2 + \left(\frac{\partial\phi}{\partial z}\right)^2 \tag{2}$$

$\mathbb{C}$ is the tensor of elastic constants, and $\boldsymbol{\varepsilon}^e$ is the elastic strain tensor. Depending on the choice of the constitutive model, the elastic strain can be additively decomposed into

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^t \tag{3}$$

where the total strain tensor $\boldsymbol{\varepsilon}$ is defined by

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\vec{\nabla}\boldsymbol{u} + \left(\vec{\nabla}\boldsymbol{u}\right)^T\right) \tag{4}$$

and $\boldsymbol{\varepsilon}^t$ is the transformation strain associated with the phase transformation, therefore

$$\boldsymbol{\varepsilon}^t = \phi\boldsymbol{\varepsilon}^0 \tag{5}$$

Other strain components can be considered together with the transformation strain, such as plastic strain for instance, if dealing with elasto-plastic material model.

The kinetics of the phase transformation is typically captured by the Ginzburg-Landau theory where the rate of the change in the order parameter becomes

$$\frac{\partial\phi}{\partial t} = -\mathcal{M}\frac{\delta\Psi}{\delta\phi} \tag{6}$$

Here, the right term of the equation represents a variational derivative of the energy function with respect to the function $\phi(\vec{x})$

The right hand side of this equation can be obtained from the Euler-Lagrange equation where

$$\frac{\delta\Psi}{\delta\phi} = \frac{\partial\Psi}{\partial\phi} - \sum_i \frac{\partial}{\partial x_i}\left(\frac{\partial\Psi}{\partial\phi_i'}\right) \tag{7}$$

which can be easily evaluated in the following steps

$$\begin{aligned} \frac{\partial\Psi}{\partial\phi} &= A\phi + B\phi^2 + C\phi^4 - \boldsymbol{\varepsilon}^0\mathbb{C} : \boldsymbol{\varepsilon}^e \\ \sum_i \frac{\partial}{\partial x_i}\left(\frac{\partial\Psi}{\partial\phi_i'}\right) &= \kappa\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2}\right) \end{aligned} \tag{8}$$

Therefore

$$\frac{\delta\Psi}{\delta\phi} = A\phi + B\phi^2 + C\phi^4 - \boldsymbol{\varepsilon}^0\mathbb{C} : \boldsymbol{\varepsilon}^e - \kappa\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial z^2}\right) \tag{9}$$

We have therefore obtained a non-linear differential equation of the order parameter function ϕ. In addition to this equation, it is also necessary to consider the evolution of the displacement field which can be solved through

$$\rho\ddot{\boldsymbol{u}} = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} + \boldsymbol{b} \tag{10}$$

Neglecting the inertial forces (considering instantaneous mechanical equilibrium), and neglecting the body forces, the displacement field can be obtained by solving

$$\boldsymbol{\nabla}\cdot\boldsymbol{\sigma} = \mathbf{0} \tag{11}$$

Here, we use ANSYS to deal with the mechanical solver and write an APDL script to solve the phase field differential equation. The numerical implementation and the APDL script is presented below.

3 Numerical solution

On a regular grid, we can solve the equations using explicit finite difference scheme

$$\frac{\Delta t}{\mathcal{M}}\phi_{ijk}^{t+\Delta t} = \phi_{ijk}^{t} + A\phi_{ijk}^{t} + B\left(\phi_{ijk}^{t}\right)^{2} + C\left(\phi_{ijk}^{t}\right)^{3} - \boldsymbol{\varepsilon}^{0}\mathbb{C} : \left(\boldsymbol{\varepsilon} - \phi_{ijk}^{t}\boldsymbol{\varepsilon}^{0}\right) - \kappa \sum_{\xi=i,j,k} \frac{\phi_{\xi-1}^{t} - 2\phi_{\xi} + \phi_{\xi+1}}{\Delta x_{\xi}^{2}} \tag{12}$$

Here, Δt is the simulation time step, and Δx_{ξ} is the grid spacing.

4 APDL script

In order to solve these equations in ANSYS, we write a APDL script. In the first illustration, we consider a 2D simulation.

We identify a rectangular domain with 100^2 quadrilateral elements of the element type 42.

We consider the isotropic material model defined by Young's modulus and Poisson's ratio.

In order to prescribe the transformation strain $\boldsymbol{\varepsilon}^0$, we will be using the in-built thermal strain option, where the anisotropic tensor can be prescribed.

With such settings, we then use temperature field to represent the order parameter ϕ, where the temperature values near zero will define the parent phase while temperature values near one will define the product phase. Values in between will represent the diffused interfaces.

The overall finite difference implementation is written within a loop in which the order parameter evolves in time by a time step Δt.

5 Simulations

References

[1] Hemantha Kumar Yeddu, Amer Malik, John Ågren, Gustav Amberg, and Annika Borgenstam. Three-dimensional phase-field modeling of martensitic microstructure evolution in steels. *Acta Materialia*, 60(4):1538–1547, 2012.