NON-LINEAR FINITE ELEMENT METHODS

ASSIGNMENT – SUMMER TERM 2022

TECHNICAL DOCUMENTATION

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CODED IN : MATLAB (v2022a)
VARIANT : 7

INTRODUCTION

The task is to solve the weak form of the Cahn-Hilliard equation shown in figure 1 and obtain the following results:

$$0 = \delta W = \int_0^L \left[\dot{c}\delta c + M(c)\,\partial^2_{cc}\Psi(c)\,c'\delta c' + \partial_c M(c)\,\lambda c'' c'\delta c' + M(c)\,\lambda c''\delta c'' \right] \mathrm{d}x$$
$$+ \left[\bar{H}^c \delta c + \left[M(c)\,\lambda c' - \bar{H}^\xi \right] \delta c'' - r\delta c' \right]_{x=0}^{L}$$

Figure 1. Weak form of Cahn-Hilliard equation

- Extracting and plotting the stationary distributions of the concentration field together with the initial conditions.
- Visualizing the evolution of the total energy defined in figure 2 for t > 100000[1] (value assigned to the individual).

$$\bar{\Psi} = \int_0^L \Psi(c) + \frac{1}{2}\lambda |c'|^2 \mathrm{d}x \; .$$

Figure 2. Stationary solution of the Cahn-Hilliard equation obtained in the case of constant mobility

- Extracting the Newton-Raphson iterations for each time history.

THEORY

The solution of the weak form is to be obtained for *n* number of elements and *t* time steps for a total time as indicated in the reference[1]. The weak form consists of three parts namely: mass matrix, internal force vector and external force vector. Applying the Neumann and Dirichlet boundary conditions to figure 1 lead to the internal force vector becoming zero, leaving only the mass matrix and internal force vector. This remaining equation is discretized by using Euler implicit time integration and 4-point Gauss quadrature, together with the constants. The obtained Δ*c* value is decided based on the convergence criteria shown in figures 3 and 4. Then the required plots are obtained as declared in the introduction section.

$$\left\| \blacktriangle \underline{\hat{\mathbf{c}}}_k \right\|_\infty < 10^{-5} * \left\| \underline{\hat{\mathbf{c}}} \right\|_\infty$$

Figure 3. Convergence criterion 1

$$\left\| \underline{\hat{\mathbf{R}}} \right\|_\infty < 0.005 * \max\left(\left\| \underline{\hat{\mathbf{F}}}_{\mathrm{int}}|_{k=0} \right\|_\infty , 10^{-8} \right)$$

Figure 4. Convergence criterion 2

PROGRAM STRUCTURE AND INSTRUCTIONS ON HOW TO RUN IT

The structure of the program is described in the following:

1. Starting section:

   The constants are assigned. The user enters the following values: *n* = number of elements (based on heuristic condition), *del_t* = time step**, *t_tot* = total time in seconds. Then the global c matrix is constructed.

2. Main function:

   The main function starts with the time step loop. Then the WHILE loop is placed (condition = convergence). Inside this loop, first lies the element routine together with the Galerkin method to iterate over the 4-point Gauss quadrature. After the element routine, lies the material routine, thereby ending the elementwise looping. Then comes the computing of Δc and related values such as c_{m+1}. The convergence criteria as shown in figures 3 and 4 are checked using IF... ELSE condition and corresponding block is run. Then the sub-routine for computing the total energy is run in a similar fashion corresponding to element routing. The obtained values are stored in suitable vectors and plotted automatically for the user to visualize the results.

3. Functions:

   The first function computes the residual and tangent stiffness matrices together with the internal force vector in the elemental form. It accepts the constants declared in (1) and calculates the corresponding internal variables required to compute the residual and tangent stiffness matrices. The second function computes the elementwise total energy. It accepts the constants declared in (1) along with the result of the Newton-Raphson loop.

VERIFICATION AND RESULTS:

This program runs based on the values according to variant 7 (check *assignment_2022.pdf* for the values). After running the program for several test cases, the following is inferred:

- **The convergence criteria are not met for time step > 1 second.
- $\tilde{c} \sim 0.1$ which is close to the stationary solution.
- $\breve{c} \sim 0.85$ which is close to the stationary solution.
- $c'\left(\frac{L}{2}\right) \sim 0.54$ is obtained which is close to the stationary solution.
- The number of Newton-Raphson iterations before convergence is reached is high during the initial condition and reduces approximately to 2 – 3 iterations.

The obtained numerical results only approximately meet the expected stationary solution results. After running several test cases, the results lead to conclusion that these deviations are arising from how Δc is calculated i.e., the method by which the linear system of equations are solved (backslash operator, cgs, pcg). This is because the values obtained after each different method were different by a noticeable margin.