Identification of deteriorated nanostructures

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Abstract

The methodology for corroded nanostructure density identification using non-local fractional continuum model is presented. The starting point is reference displacement measurement. The structure is loaded with gravity load and linear relation between stiffness and density is assumed. The inverse problem is formulated and solved for various configuration of non-local model parameters. The final results provide also contrasting of distribution of density with one obtained from the classical local model.

Keywords: inverse problem, non-local model, fractional continuum mechanics

1. Introduction

Problem of deteriorated nanostructures is under consideration. It is assumed that the nanostructure is constant during progressive corrosion whereas change in the nanostructure density is observed – cf. Fig.1. Next, one looks for methodology of finding the density distribution based on displacement measurements.

The overall problem is described in terms of non-local fractional continuum model (FCM) proposed in [7]. This model bases on the classical continuum mechanics model generalised utilising fractional calculus [4]. The model introduces new material parameters: order and intrinsic length scale of a body.

In the most simple case of 1D isotropic elastic body [8] the inverse problem mentioned above includes single order and single length scale. Final results are contrasted with the classical local 1D continuum model (special case of presented FCM) to present the meaningful role of non-local action.

2. Material and methods

2.1. Structure

The 1D body of total length equals L=1.0 and constant cross section area is analyzed (Fig. 1). The body is fixed at the left side while on the right there is a free end. Mass load b (gravity) is assumed. For a non-local model, length scale l_f and order α can vary, whereas nanostructure is constant as mentioned.

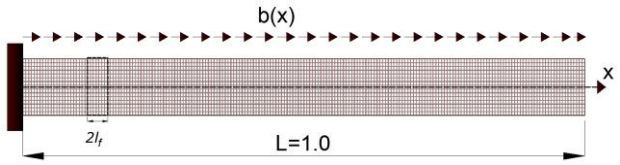

Figure 1: The analyzed structure view with representative cell assumed (dimensions proportion changed for image clarity)

2.2. Numerical model

Due to 1D assumption bar model was used with the governing equation as follows:

$$\frac{d}{dx}\left(EA\frac{\rho(x)}{\rho_0}\hat{\varepsilon}(x)\right)+b(x)=0\,,$$

$$u(0)=0 \quad \varepsilon(L)=0\,, \tag{1}$$

where $\rho(x)$ denotes a density distribution along axis x in the corroded nanostructure while ρ_0 is the initial value of density. E and A are Young modulus and cross section area, respectively. Body force $b(x)$ comes from mass load, which converted to linearly distributed load is defined as follows:

$$b(x)=gA\rho(x) \tag{2}$$

where g denotes gravitational acceleration. For simplicity purpose, values g, A and E are assumed to be 1.

Two types of strains definition is considered, classical ($\alpha=1$) and fractional. Therefore for a 1D case the classical infinitesimal Cauchy strain is ($\alpha=1$):

$$\hat{\varepsilon}(x)\,|_{\alpha=1}=\bar{\varepsilon}(x)=\frac{du}{dx}, \tag{3}$$

and fractional one with assumption that parameter $0<\alpha<1$ can be presented in the form [1,3,4,6,7]:

$$\hat{\varepsilon}(x)=l_f^{\alpha-1}\frac{1}{2}\frac{\Gamma(2-\alpha)}{\Gamma(2)}\left({}_{x-l_f}{}^{C}D_x^{\alpha}u-{}_{x}{}^{C}D_{x+l_f}^{\alpha}u\right), \tag{4}$$

$${}_{x-l_f}{}^{C}D_x^{\alpha}u(\chi)=\frac{1}{\Gamma(1-\alpha)}\int_{x-l_f}^{x}\frac{u'(\tau)}{(\chi-\tau)^{\alpha}}\,d\tau\,, \tag{5}$$

$${}_{x}{}^{C}D_{x+l_f}^{\alpha}u(\chi)=\frac{1}{\Gamma(1-\alpha)}\int_{x}^{x+l_f}\frac{u'(\tau)}{(\tau-\chi)^{\alpha}}\,d\tau\,, \tag{6}$$

where u denotes displacement, α is the real order of the derivative.

Finite difference method was used to solve the problem. The domain was discretized using 100 intervals. For each node governing equation (Eq. 1) was build assuming central difference and numerical approximation of Caputo's derivatives given in Eqs (5, 6) [4,5]. Backward difference was used for the last node. At the both ends virtual nodes were created [9]. It was assumed that displacement in the virtual nodes is the same as for

the closest boundary node. A specially prepared Python library was used to solve the problem.

2.3. Optimization problem formulation

In order to find the density distribution, the inverse problem was defined as follows:

$$\min_{P} \left| U(P) - U_{Test} \right| \tag{6}$$

where U represents function of displacements along axis x for the test data and a current distribution of density while vector $P=[P_1, P_2 P_3, P_4, P_5, P_6]$ consists of positive values representing density for six points uniformly distributed along axis x from 0 to L. Density in the intermediate points is interpolated using spline function of order 3. The initial elements of vector P are assumed as 1.

3. Results

The optimization problem was solved for various values of parameter α (see Eqn (4-6)) using Limited-memory BFGS concept [2]. The obtained density distribution is presented in Fig. 2 while $U(P_{optimal})$ for various alpha parameter in Fig. 3.

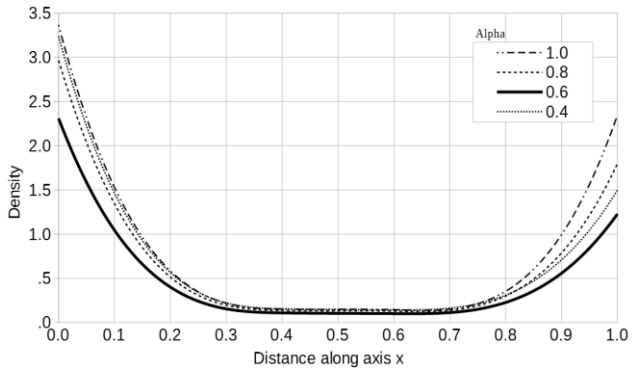

Figure 2: Density distribution obtained in the optimization for various value of parameter alpha

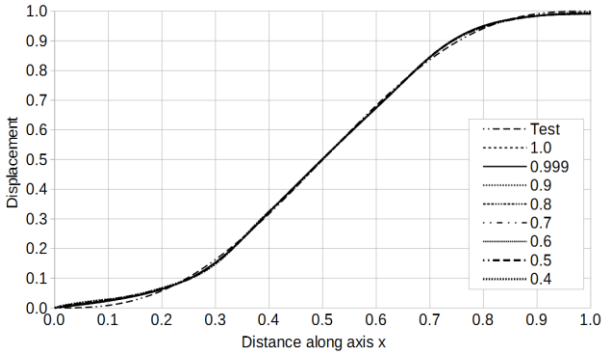

Figure 3: Displacement comparison for test data and various value of parameter alpha

4. Summary

The methodology for corroded nanostructure density identification using non-local fractional continuum model was presented. The obtained results demonstrated, that the non-local model used in the study, can lead to different solutions dependently of nanostructure (fractional parameters) properties. Classical local solution appears as a special case in the presented study and can lead to significant change in density distribution.

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