Computing of Nano Holes in Piezoelectric Materials

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Abstract—In this paper we shall study the modeling and solution of two-dimensional in-plane (P- SV) and anti-plane (SH) wave propagation problems in piezoelectric anisotropic solids containing multiple nano holes. For this purpose we shall apply new approach via cellular nonlinear networks architecture. We shall present the modeling of some reaction-diffusion problems and the accuracy of the method. For piezoelectric material with nano holes we shall state 2D dynamic problem and study the stress concentration near the nano holes. Extensive simulations will be provided in order to show the advantages of the proposed technique.

Keywords— nano holes, piezoelectric material, computing, cellular nonlinear networks, modeling, approximation

1. INTRODUCTION

Mathematical macro-scale modelling and its applications for solution of complex mechanical problems concerning new multifunctional materials, hi-tech technologies and based on them smart structures is a very challenging field of mechanics. The topic for wave scattering, diffraction and stress concentration near nano holes in composite materials is a modern, interesting and important for nanotechnologies, but an absolutely new research field with lack of results as models and accompanying computational tools.

The knowledge of both the scattered wave field and dynamic stress concentration near nano defects may provide useful information concerning damage and fracture of these materials and structures made by them. For this reason we shall study 2D dynamic problem for the bounded piezoelectric solid with a set of nano holes. The problem under consideration is described by a boundary value system of second order differential equations. The investigations of the solutions of two-dimensional in-plane and anti-plane dynamical problems arising in piezoelectric solids with nano-hole are done in a few works [1,2,3] till now. This is because this study involves multidisciplinary knowledge from different fields as piezoelectricity, continuum mechanics, equations of mathematical physics, and of course numerical methods.

Nanoscale mechanics applies multi-scale approach in order to extend the theory of continuum mechanics by presenting its basic principles at the molecular level. The work of Gurtin and Murdoch [2] is providing the general theory in this direction under both surface and interface stresses. They develop a model in which the interface between nano-heterogeneities and the surrounding matrix is made of thin membranes with their own mechanical properties and surface tension. The residual stresses around the surface and the interface is obtained even when there is the absence of external loading. This effect is not depending on the size and for that reason, it is very significant in nanomaterials in which the ratio between the surface and volume is high. This is because the molecules near the surfaces and interfaces have equilibrium positions and energy which are different from the same in the bulk materials. When the size of the material is greater than 100 nm the ratio between the surface and volume is very small and can be neglected. Then the material properties are described by classical bulk elastic strain energy via a fourth-order elastic stiffness tensor. But when the size goes smaller, then the strain energy can be changed by the surface effects, and therefore, the local and macroscopic properties of this material are different in order to be considered as the basis of nanotechnology. The methods which are used in computational nano mechanics for pure elastic homogeneous isotropic solids are mainly analytical or semi-analytical and they are applied for the cases of simple geometry, for example, finite element method (see [2]).

In this paper we shall apply a new approach in studying of two-dimensional in-plane (P- SV) and anti-plane (SH) wave propagation problems in piezoelectric anisotropic solids containing multiple nano-holes. It is based on cellular nonlinear network architecture which will allow us to study more precisely the dynamics of the problem under consideration. This approach has many advantages – it is based on the fundamental solution of the considered problem; the accuracy of obtained simulation results is very high and the numerical scheme is directly applied to the boundary value system under investigation; the cellular nonlinear network method is mesh reducing because the discretization is made only along the surface of certain range; the considered model contains heterogeneities of different geometry; the size of the dimensionality is reduced to the algebraic system of equations unlike the other numerical methods. The applications of cellular nonlinear networks include many disciplines, starting from classical and sophisticated image filtering, to signal processing solution of nonlinear partial differential equations, physical systems and nonlinear phenomena modeling, generation of nonlinear and chaotic dynamics, associative memories, robotics, etc.
In sum, the originality and innovative character of the proposed research work lies in a detail and effective combination of five stages: (a) mechanical modeling based on the classical elastodynamic and piezoelectricity in the bulk solid, theory of linear wave propagation with established relation between the scattered and total wave field, non-classical boundary conditions on the surface/interface and local constitutive equation on the surface/interface in the frame of surface elasticity theory of Gurtin and Murdoch [2]; (b) development of new computational tool and its validation; (c) simulations and new and extended knowledge in understanding of surface stress effects when sizes of the holes are in nano-scale and influence of these new effects on the wave scattered field inside the solid and local stress concentrations near nano holes.

In Section 2 we shall introduce cellular nonlinear networks and we shall present the main equations describing their dynamics. In Section 2 we shall present the cellular nonlinear networks modeling showing how the main types of reaction-diffusion equations can be approximated by this new architecture. Section 4 deals with the computing of the nano holes in 2D piezoelectric solid applying cellular nonlinear networks approach.

II. CELLULAR NONLINEAR NETWORKS

Many complex computational tasks can be solved by using a 2- or 3-D grid consisting of signal values that are directly connected within a finite local neighborhood. Cellular Nonlinear Networks (CNN) [4] present such an architecture, namely the processing elements are arranged in a grid with local interconnections. CNN works as an analog dynamic processor and has many applications in information processing, bioinspired mechatronics, robotics, mechanics, electrical engineering, etc. Moreover, the equations describing the dynamics of CNN can be considered as a very accurate approximation of nonlinear partial differential equations, for instance, reaction-diffusion systems.

CNN can represent complex dynamics in real-time and that is why a lot of mechatronic structures were developed in [5,6,7,8]. It was built in bioinspired walking machines for their locomotion having many joints of the basic circuits. Sometime after the invention of CNN, Universal Machine was built [9] and CNN technology has grown very fast, and successful chips were developed together with cellular software [10].

CNN can solve many problems and a lot of researchers work in this field since its discovering using different computational tools [9,10,11]. This network is operating as an analog dynamic processor which is made of the simple circuits made of linear resistors, linear capacitors, and linear and nonlinear controlled sources.

We shall give the following definition of CNN:

**Definition 1.** CNN is arranged as a 2-, 3- or n-dimensional grid consisting of cells that are connected locally to each other. The state variables of CNN are continuous-valued signals.

In Figure 1 below the architecture of CNN is given. The squares are the simple circuits - cells and the connections of each cell with its neighborhood cells are shown.

In this section we shall show how the CNN architecture can be applied for modelling the three well-known equations from physics – heat equation, reaction-diffusion equation, and Burgers’ equation.

In Figure 1 below the architecture of CNN is given. The squares are the simple circuits - cells and the connections of each cell with its neighborhood cells are shown.
\( w_{xx} + w_{yy} = \frac{1}{p} w_t, \)  \hspace{1cm} (3)

where \( p = \text{const.} \) is thermal conductivity. The solution, \( w(x,y,t) \) of (3) is a continuous function. We shall map function \( w(x,y,t) \) by the functions \( w_{ij}(t) \), which are defined in the following way

\[ w_{ij}(t) = w(ih_x, jh_y, t), \]  \hspace{1cm} (4)

where \( h_x \) and \( h_y \) are steps in the \( x \) and \( y \) coordinates of the 2D grid. Then the partial derivatives of \( w(x,y,t) \) with respect to \( x \) and \( y \) can be approximated by:

\[ w_{xx} + w_{yy} \approx \frac{1}{4} \left[ w_{ij-1}(t) + w_{ij+1}(t) + w_{i-1j}(t) + w_{i+1j}(t) \right] - w_{ij}, \]  \hspace{1cm} (5)

Therefore, equation (3) can be discretized by the following equations:

\[ \frac{1}{\Delta x^2} \frac{\partial w_{ij}}{\partial t} = f(w) + D \nabla^2 w, \]  \hspace{1cm} (6)

The above models we usually call reaction-diffusion CNN since they are described by the approximation of the well-known system of nonlinear partial differential equations—reaction-diffusion system which can be presented in the following form

\[ \frac{\partial w}{\partial t} = f(w) + D \nabla^2 w, \]  \hspace{1cm} (7)

where \( w \in \mathbb{R}^n, f \in \mathbb{R}^n \), \( D \) is a \( n \times n \) diagonal matrix consisting of the diffusion coefficients, and

\[ \nabla^2 w_i = \frac{\partial^2 w_i}{\partial x^2} + \frac{\partial^2 w_i}{\partial y^2}, i = 1, 2, ..., n, \]  \hspace{1cm} (8)

is 2D Laplacian operator.

We shall model the Laplacian operator (8) in discrete space by discretized feedback A template [11]. We shall use in this paper the following discretized A templates.

a) 1D feedback template:

\[ A_1: (1, -2, 1); \]

b) 2D feedback template:

\[ A_2: \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -4 \end{pmatrix}, \]

\[ A_2: \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -4 \end{pmatrix}. \]

being actually equivalent to (5).

Now we shall approximate the Burgers' equation given by:

\[ \frac{\partial w(x,t)}{\partial t} = \frac{1}{R} \frac{\partial^2 w(x,t)}{\partial x^2} - w(x,t) \frac{\partial w(x,t)}{\partial x} + F(x,t). \]  \hspace{1cm} (9)

The solution of (9) when \( F(x,t) = 0 \), is obtained in [12] by the following formula

\[ w(x,t) = \int_{-\infty}^{0} \left. \int \frac{R}{2 \pi} (x-y)^2 - \frac{R}{2} \int w(x',t) dy' \right| dy \]

\[ + \int_{0}^{\infty} \frac{R}{2 \pi} (x-y)^2 - \frac{R}{2} \int w(x',t) dy' \right| dy, \]

\[ f_{-\infty}^{\infty} w(y,0) dy < \infty. \]  \hspace{1cm} (10)

We shall use difference terms in order to approximate the derivatives of (9): \( w_{ij}(t) = w(x_i,t), F_i(t) = F(x_i,t), \) \( \Delta x = x_{i+1} - x_i \). Therefore (9) is modeled by the system of ordinary differential equations given below:

\[ \frac{dw_{ij}(t)}{dt} = \frac{1}{\Delta x^2} \left[ w_{ij+1}(t) - 2w_{ij}(t) + w_{ij-1}(t) \right] - w_{ij}(t) \frac{w_{ij+1}(t) - w_{ij-1}(t)}{2\Delta x} + F_i(t), \]

\[ i = 1, ..., M - 1 \text{ for 1D CNN array.} \]  \hspace{1cm} (11)

We take \( w_{0}(t) = w(0,t) \) and we assume that \( w(x,t) \) is zero outside the interval \([x_0, x_M]\). When we compare the coefficients of (11) with the state equation of a nonlinear CNN we obtain the following templates:

\[ A_{LIN} = \left( \frac{1}{R(\Delta x)^2}, \frac{1}{R} - \frac{2}{R(\Delta x)^2} \right), \]

\[ A_{NLIN} = \left( \frac{1}{2(\Delta x)}, 0, -\frac{1}{2(\Delta x)} \right). \]  \hspace{1cm} (12)

Therefore the discretized template is equal to \( A = A_{LIN} + A_{NLIN} \).

We calculated the solutions of Burgers' equation by applying the CNN architecture taking into account various values of \( R, \Delta x \), and different initial conditions \( w(x,0) \). Then we estimated the accuracy of CNN approximation by comparing these solutions to the explicit solutions given by (10). We obtain the relative error:

\[ e^{rel}_i = \left| \frac{w^\text{CNN}_i(t) - w^\text{LIN}_i(t)}{w^\text{LIN}_i(t)} \right|, \]  \hspace{1cm} (13)

where \( w^\text{CNN}_i(t) \) corresponds to the CNN approximation and \( w^\text{LIN}_i(t) \) is the approximation by (11). We calculated the relative error \( e^{rel}_i \) of all cells for different step sizes \( \Delta x \) and for the initial state condition

\[ w(x,0) = \frac{1}{\sqrt{2\pi}} \left( e^{-(x-3)^2/2} + e^{-(x+3)^2/2} \right). \]

The obtained simulation results give us the following information: CNN solutions are accurate approximation of \( w^\text{LIN}_i(t) \) for step sizes \( \Delta x < 0.02 \) with the error calculated by (13) of less than 10^-4. The following simulations are derived.
Remark 1. The solution of the CNN model of the Burgers’ equation is (a) continuous in time, (b) continuous and bounded in value, (c) continuous in the parameters of the interaction, and (d) discrete in space.

IV. CNN COMPUTING OF NANO HOLES IN PIEZOELECTRIC MATERIAL

In this section we shall present the application of the CNN approach for the problem solving the case of a single nano hole of arbitrary shape in a piezoelectric solid subjected to time-harmonic mechanical/electric load. We shall approximate 2D boundary value problem via CNN architecture and we shall provide a computation of stress concentration and scattered wave field [2].

In Figure 3 we consider 2D bounded piezoelectric solid with different nano scale heterogeneities $I \in G$ like nano-holes, cracks, etc. We shall evaluate the field and stress concentration at every point of the matrix $M$ around these holes.

![Fig. 3. Piezoelectric material with nano inhomogeneities.](image)

In order to state the problem we shall apply the theory of continuum mechanics [2]. Let us consider the following system of second order partial differential equations describing the dynamics of the above model:

\[
\begin{align*}
\frac{\partial^2 w_N}{\partial t^2} + e_{15}^N \frac{\partial w_N}{\partial x_3} - e_{11}^N \frac{\partial w_N}{\partial x_1} &= 0 \\
\rho_N \frac{\partial^2 w_N}{\partial t^2} - e_{33}^N \frac{\partial^2 w_N}{\partial x_1^2} &= 0
\end{align*}
\]  

where $x = (x_1, x_2)$, the Laplace operator is $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$, $N = M$, for $x \in M$ and $N = I$ for $x \in I$, the variable $w_N^3$ states for the mechanical displacement, the variable $w_N^4$ states for the electric potential. The parameters in (14) are mass density $\rho_N$, shear stiffness $c_{15}^N > 0$, piezoelectric constant $e_{15}^N \neq 0$ and dielectric permittivity $e_{11}^N > 0$. The frequency $\omega$ is applied on the boundary $\partial G$.

The interface between each nano hole $I$ and its surrounding matrix $M$ is supposed to have its own mechanical parameters $c_{14}^N$, $e_{15}^N$, $e_{11}^N$. In our case these parameters are equal to zero and therefore the boundary conditions on the boundary $S$ of the matrix are given by:

\[ t_{ij}^M = \frac{\partial \sigma_{ij}^M}{\partial n} \]  

According to [2] $\sigma_{ij}^M$ is the general stress and $t_{ij}^N$ is the generalized traction, $j = 3, 4$, $l$ is the tangential vector. We shall now apply the CNN approach to the boundary value problem (14), (15) defined above.

In the literature there are few results concerning the numerical study of the dynamic behavior of the piezoelectric solid having nano holes. Validation of infinite piezoelectric plane with a hole is presented in [1]. In [3] isotropic bounded domain is considered and numerical simulations are provided in the cases of holes and inclusions.

We shall approximate the system (14) by the CNN 2D-grid architecture in the following way:

\[ \begin{align*}
c_{14}^N A_1 \ast w_N^3 + e_{15}^N A_1 \ast w_N^4 - \rho_N \frac{\partial^2 w_N^3}{\partial t^2} &= 0 \\
e_{15}^N A_1 \ast w_N^3 - e_{11}^N w_N &= 0,
\end{align*} \]  

where $A_1$ is 1D feedback template, $1 \leq i \leq n$.

The Stress Concentration Field $(\sigma / \sigma_0)$ is the characteristic that is of interest in nano-structures [7] and it is normalized calculated by the following formula:

\[ \sigma = -\sigma_{13} \sin(\varphi) + \sigma_{23} \cos(\varphi). \]  

The polar angle is $\varphi$ and it is at the observing point, $\sigma_{ij}$ is the stress [2] near $S$. Solution at each internal point in the domain is expressed in terms of boundary values without recourse to domain discretization and this main facility is very important when wave propagation problems are being solved in heterogeneous solids, because only the boundaries of heterogeneities are discretized, not their volumes as it is when domain discretization methods as finite element or finite difference methods are used.

We shall provide the simulation of our CNN model for the piezoelectric material with nano-holes PZT4 with the following material parameters:

- $c_{44}^M = 2.56 \times 10^{10} \frac{N}{m^2}$
- $e_{15}^M = 12.7 \frac{C}{m^2}$
- $e_{11}^M = 64.6 \times 10^{-10} \frac{C}{V m}$
\[ \rho M = 7.5 \times 10^3 \text{kg/m}^3. \]

In our extensive simulations we take the following boundary conditions (15) for the 2D PZT4 material shown in Figure 4:

- on \( G_1G_2 \): \( t^M_3 = -\sigma_0, t^M_4 = -D_0 \);
- on \( G_2G_3 \): \( t^M_3 = t^M_4 = 0 \);
- on \( G_3G_4 \): \( t^M_3 = \sigma_0, t^M_4 = D_0 \);
- on \( G_4G_1 \): \( t^M_3 = t^M_4 = 0 \),

where \( \sigma_0 = 400 \times 10^6 \text{N/m}^2 \) is the amplitude of the mechanical traction and \( D_0 = k \frac{e_{13}M}{e_{15}} \sigma_0 \) is the amplitude of electrical displacement.

Remark 2. In Figure 5 we present numerical simulations of Stress Concentration Field very near the nano hole (see Fig. 4) for different values of the parameters. We obtain high accuracy and efficiency for the evaluation because not mesh discretization is used close to the nano hole applying the CNN approach. The fundamental solution at infinite makes the method very appropriate to be used when infinite and semi-infinite ranges are considered. In engineering, the sensors from piezoelectric nanocomposites are often subjected to all kinds of loadings. The strength of these sensors will greatly influence their function in the serving life.

V. CONCLUSION

CNN architecture is a very accurate approximation for many models arising in physics, chemistry, mechanics and biology. It is possible to have real-time signal processing with high precision due to the continuous-time analog operation with CNN. One very important feature is the local interconnection between cells which enables to perform of several digital and analog implementations of CNN and to obtain very large-scale integrated chips. For this reason there are many applications of CNN in mechatronics, electrical engineering, locomotion, robotics, etc.

In this paper we present CNN computing with applications. First we introduce CNN and their architecture as well as the dynamic system of equations. We show how CNN can approximate some equations of physics, such as reaction-diffusion equation, heat equation and Burgers’ equation. As an application we present CNN computing of nano holes in piezoelectric material. Validation of the CNN model is given as well.

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REFERENCES


