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DYNAMICS OF PEM WITH NANO-INHOMOGENEITIES VIA CELLULAR NANOSCALE NETWORKS*

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In this paper we study the dynamics of piezoelectrical material (PEM) with nano-inhomogeneities. The boundary value model defined by the system of two partial differential equations and the boundary conditions for the generalized stress is mapped into Cellular Nanoscale Networks architecture. We study the dynamics of the obtained CNN model via harmonic balance technique. Validation and simulations are provided which illustrate the theoretical results.

1. Introduction

Cellular Nanoscale Networks (CNN) present a new class of information processing systems which shows important potential applications (Fig. 1). The concept of CNN is based on some aspects of neurobiology and adapted to integrated circuits. CNN are defined as spatial arrangements of locally coupled dynamical systems, referred to as cells. The CNN dynamics are determined by a dynamic law of an isolated cell, by the coupling laws between the cells and by boundary and initial conditions. The cell coupling is confined to the local neighborhood of a cell within a defined sphere of influence. The dynamic law and the coupling laws of a cell are often combined and described by nonlinear ordinary differential- or difference equations (ODE), respectively, referred to as the state equations of cells.

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Key words: piezoelectric solid, Cellular Nanoscale Networks (CNN), dynamic behaviour, harmonic balance method.

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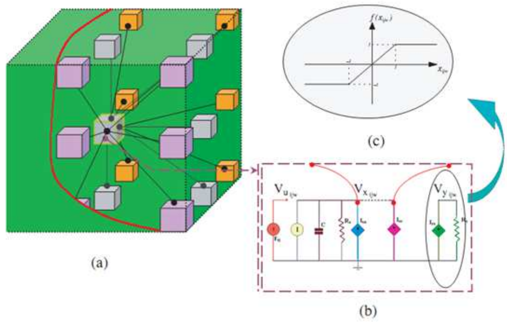

Figure 1: a) CNN architecture; b) cell circuit; c) output function of CNN

Thus a CNN is given by a system of coupled ODE with a very compact representation in the case of translation invariant state equations. Despite of having a compact representation, CNN can show complex dynamics like chaotic behavior, self-organization, and pattern formation or nonlinear oscillation and wave propagation. Furthermore, Reaction-Diffusion Cellular Nonlinear/Nanoscale Networks (RD-CNN) have been applied for modeling complex systems [8]. These networks are not representing a paradigm for complexity only but also establishing novel approaches to information processing by the dynamics of nonlinear complex systems.

In this paper we shall study piezoelectric material (PEM) with nano-inhomo-

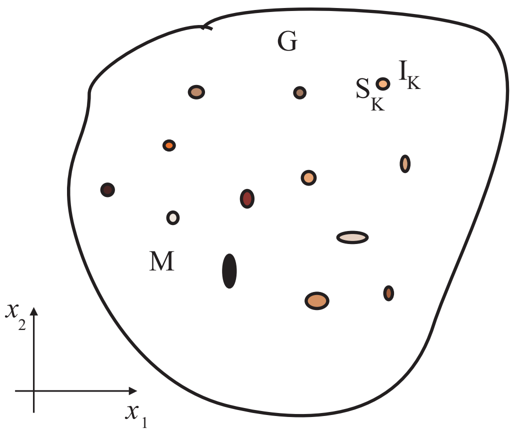

Figure 2: PEM with nano-inhomogeneities

geneities (see Figure 2). PEM active composites are anisotropic dielectrics, where the electric, magnetic and elastic fields are coupled. The demand for smaller and faster devices has encouraged technological advances resulting in the ability to manipulate matter at nano-scales that have enabled the fabrication of nano-scale electromechanical systems. With the advances in materials synthesis and device processing capabilities, the importance of developing and understanding nano-scale engineering devices has dramatically increased over the past decade. 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.

In Section 2 we shall present the application of CNN in modeling partial differential equations (PDE). In Section 3 we shall state the mechanical problem. We shall map the boundary value problem under consideration into CNN architecture in Section 4. Harmonic balance technique will be presented and the dynamics of the CNN model will be studied. Validation and simulations will be provided in Section 5.

2. CNN modeling of PDE

Some autonomous CNN represent an excellent approximation to the nonlinear PDE. Although the CNN equations describing reaction-diffusion systems are with the large number of cells, they can exhibit new phenomena that can not be obtained from their limiting PDE. This demonstrates that an autonomous CNN is in some sense more general than its associated nonlinear PDE.

In this section we shall present the derivation of the CNN implementations through spatial discretization, which suggests a methodology for converting a PDE to CNN templates and vice versa. The CNN solution of a PDE has four basic properties – it is

i) continuous in time;

ii) continuous and bounded in value;

iii) continuous in interaction parameters;

iv) discrete in space.

We shall demonstrate how an autonomous CNN can serve as a unifying paradigm for active wave propagation. Several well-known examples chosen from different disciplines will be modeled. Moreover, we shall show how the three basic types of PDE: the diffusion equation, the Laplace equation, and the wave equation, can be solved via CNN.

In [8] it was shown how a typical PDE, the heat equation, can be approximated, on a finite spatial grid, by a CNN with a given simple cell and cloning templates. This is possible, because PDE and CNN share a common property; namely, their dynamics behavior depends only on their spatial local interactions.

The well known heat equation from physics is:

$$u_{xx} + u_{yy} = \frac{1}{k} u_t, \tag{1}$$

where k is a constant, called the thermal conductivity. The solution, $u(x, y, t)$ of the heat equation is a continuous function of the time t, and the space variables x, y. If the function $u(x, y, t)$ is approximated by a set of functions $u_{ij}(t)$, which are defined as

$$u_{ij}(t) = u(ih_x, jh_y, t), \tag{2}$$

where h_x and h_y are the space intervals in the x and y coordinates, then, the partial derivatives of $u(x, y, t)$ with respect to x and y can be replaced approximately by:

$$u_{xx} + u_{yy} \approx \frac{1}{4}[u_{ij-1}(t) + u_{ij+1}(t) + u_{i-1j}(t) + u_{i+1j}(t)] \\ -u_{ij}(t), \quad for \ all \ i, j. \tag{3}$$

Thus, the heat equation (1) can be approximated by a set of equations

$$\frac{1}{k}\frac{du_{ij}}{dt} = \frac{1}{4}[u_{ij-1}(t) + u_{ij+1}(t) + u_{i-1j}(t) + u_{i+1j}(t)] \\ -u_{ij}(t), \quad for \ all \ i, j. \tag{4}$$

By adding a capacitor across the output of a simple cell, wave type equations have been also generated. Moreover, at the equilibrium, we recover the Laplace equation. These CNN will be called reaction-diffusion CNNs because they are described mathematically by a discretized version of the following well-known system of nonlinear PDE - reaction-diffusion equations [8]:

$$\frac{\partial u}{\partial t} = f(u) + D\nabla^2 u, \tag{5}$$

where $u \in \mathbf{R}^m$, $f \in \mathbf{R}^m$, D is a $m \times m$ diagonal matrix whose diagonal elements D_i are called the diffusion coefficients, and

$$\nabla^2 u_i = \frac{\partial^2 u_i}{\partial x^2} + \frac{\partial^2 u_i}{\partial y^2}, \quad i = 1, 2, \ldots, m, \tag{6}$$

is the Laplacian operator in $\mathbf{R}^2$.

There are several ways to approximate the Laplacian operator (6) in discrete space by a CNN synaptic law with an appropriate A-template [8]. For example we can have:

a) one-dimensional discretized Laplacian template:

$$A_1 : (1, -2, 1); \tag{7}$$

b) two-dimensional discretized Laplacian template:

$$A_2 : \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{8}$$

which is in fact the approximation for the heat equation (1).

2.1. One dimensional CNN and PDE

Let us consider a one-dimensional CNN, described by the space-invariant A-template $A = [r\,p\,s]$ with no B-template and no independent term ($I = 0$). The equation describing the cell C_i of such a CNN is thus given by

$$\dot{u}_i = -u_i + rf(u_{i-1}) + pf(u_i) + sf(u_{i+1}) = -u_i + [r\,p\,s] * f(u_i), \tag{9}$$

where the nonlinearity $f(u)$ is the piecewise linear function and the symbol $*$ denotes a discrete spatial convolution. If $|u_i| \leq 1$, cell C_i will be called a linear cell, whereas, if $|u_i| > 1$, it will be called saturated cell. The template $[r\,p\,s]$ can be decomposed as follows

$$[r\,p\,s] = (p + s + r)[0\,1\,0] + (s + r)/2[1\;-2\,1]+ \tag{10}$$
$$+(s - r)[-1/2\,0\,1/2].$$

Notice that the template $[1\;-2\,1]$ corresponds to the discrete version of the second spatial derivative, while $[-1/2\,0\,1/2]$ is the discrete central spatial derivative. Consequently equation (9) can be written in the following form

$$\dot{u}_i = -u_i + (p + r + s)f(u_i) + (s + r)/2\hat{\partial}^2 * f(u_i) + (s - r)\hat{\partial} * f(u_i), \tag{11}$$

where $\hat{\partial} = [-1/2\,0\,1/2]$ and $\hat{\partial}^2 = [1\;-2\,1]$. Equation (11) indicates that equation (9) is the spatially discrete analog of the PDE

$$\partial_t u(z,t) = -u + af(u(z,t)) + d\partial_z^2 f(u(z,t)) + c\partial_z f(u(z,t)), \tag{12}$$

where z is the spatial variable, ∂_t, ∂_z are the partial derivatives with respect to t and z and a, d, c are three constants. The three last terms of the right hand side of equation (12) are respectively the active reaction, diffusion and convection terms. Moreover, by comparing equation (11) and (12), the following correspondence can be stated among the parameters of the two equations:

$$(s+r)/2 \to d,\ (s-r) \to c,\ p+s+r \to a. \tag{13}$$

The correspondence (13) can be used to compare the qualitative dynamics of equation (9) with that of equation (12). In particular it is shown that, whenever the spatial discrete nature of CNN has not a critical influence on dynamics, PDEs are an useful tool to explain properties proved or simply shown by means of numerical simulations for CNN. Interesting is that, when this is the case, CNNs can be used as analog simulators of physical and biological continuous systems.

3. Statement of the boundary value problem

Let $G \in R^2$ is a bounded piezoelectric domain with a set of inhomogeneities $I = \cup I_k \in G$ (holes, inclusions, nano–holes, nano–inclusions) subjected to time–harmonic load on the boundary ∂G, see Figure 2. Note that heterogeneities are of macro size if their diameter is greater than $10^{-6}m$, while heterogeneities are of nano–size if their diameter is less than $10^{-7}m$.

The aim is to find the field in every point of $M = G\backslash I$, I and to evaluate stress concentration around the inhomogeneities.

Using the methods of continuum mechanics [9] the problem can be formulated in terms of boundary value problem for a system of 2-nd order differential equations:

$$\left| \begin{array}{l} c_{44}^N \Delta u_3^N + e_{15}^N \Delta u_4^N - \rho^N u_{3,tt} = 0, \\ e_{15}^N \Delta u_3^N - \varepsilon_{15}^N \Delta u_4^N = 0, \end{array} \right. \tag{14}$$

where $x = (x_1, x_2)$, $\Delta = \dfrac{\partial^2}{\partial x_1^2} + \dfrac{\partial^2}{\partial x_2^2}$ is Laplace operator with respect to t, $N = M$ for $x \in M$ and $N = I$ for $x \in I$; u_3^N is mechanical displacement, u_4^N is electric potential, ρ^N is the mass density, $c_{44}^N > 0$ is the shear stiffness, $e_{15}^N \neq 0$ is the piezoelectric constant and $\varepsilon_{11}^N > 0$ is the dielectric permittivity.

Assume that the interface between the nano-inhomogeneity I and its surrounding matrix M is regarded as thin material surface S that possesses its own mechanical parameters c_{44}^I, e_{15}^I, ε_{11}^I.

We shall consider that constants in I to be $c_{44}^I = 0$, $e_{15}^I = 0$, $\varepsilon_{11}^I = 0$ and boundary conditions on S to be

$$t_j^M = \frac{\partial \sigma_{lj}^S}{\partial l} \quad \text{on} \quad S \tag{15}$$

where σ_{lj}^S is generalized stress [2, 5], $j = 3, 4$, l is the tangential vector. Then we shall study boundary value problem (BVP) (14) with boundary conditions (15).

There are only few numerical results for dynamic behavior of bounded piezoelectric domain with nano-inhomogeneities under anti-plane load. For instance, validation is done in [1, 6] for infinite piezoelectric plane with a hole, in [4] for isotropic bounded domain with holes and inclusions and in [3] for piezoelectric plane with nano-hole or nano-inclusion.

4. CNN model of boundary value problem and its dynamics

Following Section 2, CNN model of the BVP (14), (15) which consists of $n = L.L$ cells can be written in the following form:

$$\begin{aligned} &c_{44}^N A_1 * u_{3i} + e_{15}^N A_1 * u_{4i} - \rho^N \frac{d^2 u_{3i}}{dt^2} = 0 \\ &e_{15}^N A_1 * u_{3i} - \varepsilon_{11}^N A_1 * u_{4i} = 0, 1 \le i \le n, \end{aligned} \tag{16}$$

where A_1 is 1-dimensional discretized Laplacian template [8], $*$ is convolution operator, $1 \le i \le n$. Boundary conditions (15) can be written in terms of CNN architecture are as follows:

$$\begin{aligned} &t_j^M = \frac{\partial \sigma_{lij}^M}{\partial l}, j = 3, 4, \\ &\sigma_{l3i}^M = c_{44}^M \frac{\partial u_{3i}^l}{\partial x_l} + e_{15}^M \frac{\partial u_{4i}^l}{\partial x_l}, \\ &\sigma_{l4i}^M = e_{15}^M \frac{\partial u_{3i}^l}{\partial x_l} - \varepsilon_{11}^M \frac{\partial u_{4i}^l}{\partial x_l}, 1 \le i \le n. \end{aligned} \tag{17}$$

We express from the second equation of (16), $A_1 * u_{4i}$ and substitute in the first equation. So we obtain the following equation for u_{3i}:

$$\tilde{C} A_1 * u_{3i} - \rho^N \frac{d^2 u_{3i}}{dt^2} = 0, \tag{18}$$

where $\tilde{C} = c_{44}^N + \dfrac{(e_{15}^N)^2}{\varepsilon_{11}}$.

We shall take the output of the CNN model (17), (18) as a piecewise linear function [8].

We shall apply approximative method in order to study the dynamics of our CNN model (17), (18). This method is based on a special Fourier transform and is known in electrical engineering as harmonic balance method [7].

4.1. Harmonic balance technique

The frequency response method is a powerful tool for the analysis and design of linear control systems. It is based on describing a linear system by a complex-valued function, the frequency response, instead of differential equation. The power of the method comes from a number of sources. First, graphical representations can be used to facilitate analysis and design. Second, physical insights can be used, because the frequency response functions have clear physical meanings. Finally, the method's complexity only increases mildly with system order. Frequency domain analysis, however cannot be directly applied to nonlinear systems because frequency response functions cannot be defined for nonlinear systems.

For some nonlinear systems an extended version of the frequency response method, called the **harmonic balance technique** (HBT), can be used to approximately analyze and predict nonlinear behaviour. Even though it is only an approximation method, the desirable properties it inherits from the frequency response method, and the shortage of other systematic tools for nonlinear system analysis, make it an indispensable component of the bag of tools of practicing control engineers. The main use of HBT is for the prediction of limit cycles in nonlinear systems, although the method has a number of other applications such as predicting sub-harmonics, jump phenomena, and the response of nonlinear systems to sinusoidal inputs.

It is well-known that the presence of limit cycles in nonlinear autonomous systems which admit a Lur'e representation [7] but have no spatial dependence can be investigated by resorting to the HBT. Such technique consists of two fundamental steps:

1. The signal entering through the nonlinear block of the Lur'e scheme [7] is approximated by means of a suitable sinusoidal term whose frequency and amplitude are unknown.

2. The higher-order harmonics in the output of the nonlinear block are neglected, i.e. the nonlinear block is replaced by a constant gain having the same input, which minimizes the mean squared error between the output from the nonlinearity and that from the gain itself.

We shall consider a basic Lur'e scheme [7], with $\mathcal{L}$ – linear time- invariant dynamic system and $\mathcal{N}$ – nonlinear time-invariant static and memoryless system.

The block $\mathcal{L}$ can be described by its transfer function

(19) $$L(s) = \frac{p(s)}{q(s)}$$

where s is the complex variable and $p(.)$ and $q(.)$ are polynomial operators, while the block $\mathcal{N}$ is represented by the nonlinear single-valued function $n(.)$. In terms of differential equation the system is governed by the form

(20) $$q(D)y(t) + p(D)n[y(t)] = 0$$

where D is the differential operator.

The feedback structure in study is an important class of representation of circuits and systems also with regard to their chaotic dynamics.

Since the methods presented in this section are based on a first harmonic study, assume for the system output the form

(21) $$y_0(t) = \mathcal{A} + \mathcal{B}\cos\omega t,\ \ \mathcal{B}, \omega > 0$$

and assume that the corresponding nonlinearity output $n[y_0(t)]$ is expanded in Fourier series as

(22) $$n[y_0(t)] = N_0(\mathcal{A},\mathcal{B})\mathcal{A} + N_1(\mathcal{A},\mathcal{B})\mathcal{B}\cos\omega t + \cdots$$

The nonlinear system $\mathcal{N}$ is characterized, in an approximate form related to the (steady state) periodic regime, by the bias and ω frequency real gains

(23) $$N_0(\mathcal{A},\mathcal{B}) = \frac{1}{2\pi\mathcal{A}}\int_{-\pi}^{\pi} n[y_0(t)]d\omega t$$

(24) $$N_1(\mathcal{A},\mathcal{B}) = \frac{1}{\pi\mathcal{B}}\int_{-\pi}^{\pi} n[y_0(t)]\cos\omega t d\omega t$$

which are the well-known describing function terms. As an extension, one can define higher frequency complex gains $N_k(\mathcal{A},\mathcal{B})$, $k = 2, 3, \ldots$, which describe the remaining terms of (22).

Definition 1. Predicted Limit Cycles *The approximative periodic solutions* $y_0(t)$ *of the system derived by the HBT. According to* (22), (23) *and* (24) *the predicited limit cycles conditions are:*

(25) $$\mathcal{A}[1 + N_0(\mathcal{A},\mathcal{B})]L(0) = 0$$

(26) $$1 + N_1(\mathcal{A},\mathcal{B})L(j\omega) = 0.$$

Such equations follow by imposing the HBT [7] along the system loop of the Lur'e scheme, where the transfer function L and the nonlinearity n have been evaluated at their steady state gains of zero and ω frequency. Equations (25) and (26) must be solved with respect to the parameters $\mathcal{A}$, $\mathcal{B}$ and ω. In general, when $\mathcal{B}$ tends to zero the relation (26) expresses the Hopf bifurcation existence and the relation (25) leads to a bias value $\mathcal{A} = E_j$, being E_j the equilibrium points where the bifurcation occurs. Such a point can be viewed as the generator of a family of periodic solutions.

Any periodic solution $y_0(t)$ indicates in the state space a limit cycle which is called predicted since it derives from a heuristic analysis and its exact shape and even existence are uncertain. The reliability of the prediction depends on the distortion along the system loop.

4.2. Dynamics of CNN model (17), (18)

Following harmonic balance method we introduce double Fourier transform:

$$F(s,z) = \sum_{k=-\infty}^{k=\infty} z^{-k} \int_{-\infty}^{\infty} f_k(t) exp(-st) dt. \tag{27}$$

where $z = \exp(i\Omega)$, Ω is continuous spatial frequency, $s = i\omega$, ω is continuous temporal frequency.

We apply the above transform (27) to (18) and obtain the following transfer function:

$$H(s,z) = \frac{\rho^N s^2}{\tilde{C}(z^{-1} - 2 + z)}. \tag{28}$$

According to harmonic balance method we shall look for the solution of (17), (18) in the form:

$$\begin{aligned} u_{3i} &= U_3 \sin(\omega t + i\Omega), \\ u_{4i} &= U_4 \sin(\omega t + i\Omega), \end{aligned}$$

where U_3, U_4 are amplitudes, $0 \leq \Omega \leq 2\pi$, $\omega = \dfrac{2\pi}{T}$, T being the minimal period.

We shall express the transfer function (28) in terms of $s = i\omega$ and $z = \exp(i\Omega)$ and we obtain:

$$H_\Omega(\omega) = \frac{-\rho^N \omega^2}{\tilde{C}(2\cos\Omega - 2)}. \tag{29}$$

Following harmonic balance method the following constraints hold:

$$
\begin{aligned}
Re(H_\Omega(\omega)) &= \frac{U_3}{U_4} \\
Im(H_\Omega(\omega)) &= 0.
\end{aligned} \tag{30}
$$

Now according to the method [7], if for a given value of Ω, we can find a solution $(\omega, U_3 U_4)$ of (30), then we can predict the existence of periodic solutions with amplitudes U_3, U_4 and period of approximately $T = \frac{2\pi}{\omega}$. The following proposition hold:

Proposition 1. *CNN model* (17), (18) *consisting of* $n = L.L$ *cells has periodic state solutions* u_{3i}, u_{4i} *with a finite set of spatial frequencies* Ω *and a period* $T = \frac{2\pi}{\omega}$.

S k e t c h o f t h e P r o o f. Following harmonic balance method [7], we first approximate the output of our CNN model (17), (18), the fundamental component of its Fourier expansion

$$
y = Y \sin(\omega t + i\Omega) \tag{31}
$$

with

$$
Y = \frac{1}{\pi} \int_{-\pi}^{\pi} N(V \sin \psi) \sin \psi d\psi.
$$

Then we substitute real and imaginary part of the transfer function $H_\Omega(\omega)$ (28) in (30) and we obtain the system of algebraic equations for the unknowns $(\omega, U_3 U_4)$. We solve this system and find the unknowns.This is the end of the proof. □

Remark. In order to validate the accuracy of the obtained results we apply possible initial conditions from which the network will reach, at steady state, a steady state solution characterized by the desired value of Ω. In our case we propose the initial conditions of the form: $u_{ji}(0) = \sin(\Omega i)$, $j = 3, 4$,$1 \leq i \leq n$.

Consider the square PEM domain $G_1 G_2 G_3 G_4$ with a side α, containing a single circular inhomogeneity with a radius $r = \beta\alpha$ and center at the square center. Note that if $\beta < 0.05$ the influence of the exterior boundary G on the solution is expected to be small, while if $\beta > 0.2$ it is expected significant influence. In our case of inhomogeneities at nano-scale, we shall take the material parameters inside I to be: $c_{44}^I = 0.1$, c_{44}^M,$e_{15}^I = 0.1$, e_{15}^M, ${}_{11}^I = 0.1$, ${}_{11}^M$, ${}^I = {}^M$. Spatial frequency is defined as $\Omega = c\sqrt{(\frac{M}{c_{44}^M})}\omega$. For this parameter set we present below on Figure 3 the obtained solution of our CNN model (17), (18).

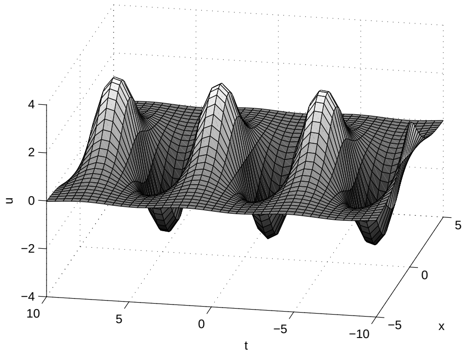

Figure 3: Simulations of CNN model (17), (18)

5. Simulations and validation

The characteristic that is of interest in nano-structures is normalized Stress Concentration Field (SCF) (σ/σ_0) and it is calculated by the following formula [2, 5]:

$$\sigma = -\sigma_{13}\sin(\varphi) + \sigma_{23}\cos(\varphi), \tag{32}$$

where φ is the polar angle of the observed point, σ_{ji} is the stress near S.

Material parameters of the matrix are for transversely isotropic piezoelectric material PZT4 are:

– Elastic stiffness: $c_{44}^M = 2.56 \times 10^{10}$ N/m^2;
– Piezoelectric constant: $e_{15}^M = 12.7$ C/m^2;
– Dielectric constant: $\varepsilon_{11}^M = 64.6 \times 10^{-10}$ C/Vm;
– Density: $\rho^M = 7.5 \times 10^3$ kg/m^3.

The applied load is time harmonic uni-axial along vertical direction uniform mechanical traction with frequency ω and amplitude $\sigma_0 = 400 \times 10^6$ N/m^2 and electrical displacement with amplitude $D_0 = k\dfrac{\varepsilon_{11}^M}{e_{15}^M}\sigma_0$. This means that the boundary conditions (15) are:

– on $G_1G_2 : t_3^M = -\sigma_0$, $t_4^M = -D_0$;
– on $G_2G_3 : t_3^M = t_4^M = 0$;
– on $G_3G_4 : t_3^M = 0$, $t_4^M = D_0$;
– on $G_4G_1 : t_3^M = t_4^M = 0$.

The validation of our model is provided below on Figure 4 for the parameter sets given above.

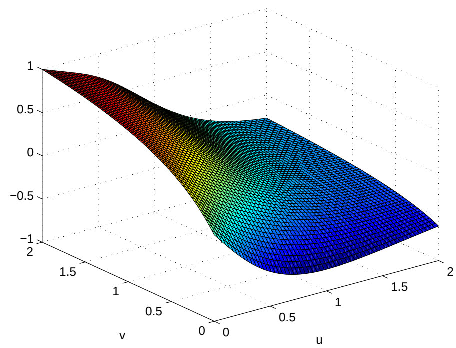

Figure 4: Validation – dynamic SCF at observed point

6. Conclusions

In this paper we consider homogeneous or functional graded piezoelectric material with heterogeneities of different type (hole, crack, inclusion, nano-hole, nano-inclusion) subjected to time-harmonic wave. There is a certain lack of work for solution of 2D ant-plane dynamic problems for piezoelectric and magnetopiezoelectric solids with nanoinclusions or nano-cavities. The reason is that such a goal requires multidisciplinary knowledge and skills.

In this paper we propose CNN approach for numerical study of the dynamics of the boundary value model (14), (15). We study the dynamics of the obtained CNN architecture by means of harmonic balance technique. We provide simulations and validation in order to illustrate the theoretical results.

Computational nanomechanics has a high priority in Europe, because it concerns the development and creation of new smart materials and devices based on them. The present paper addresses the vital component of accurate description and computation of the wave motions and stress concentrations that are developed in the multifunctional materials with nano-structures.

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