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A LOW COMPLEXITY FINITE DIFFERENCES-NEURAL NETWORK COMBINED APPROACH FOR THE MODELING OF P-N JUNCTION ELECTRICAL PROPERTIES

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ABSTRACT

Our aim in this work, is to develop a low complexity approach compared to classical methods used in the establishment of numerical solution of partial differential equations. The proposed approach is suitable for situations where it's necessary to increase the number of nodes in the mesh scheme. The reduction of complexity is guaranteed through the combination of a finite differences model and an artificial neural network approach, obtained results reflect theoretical predictions and are in our opinion very satisfactory.

Keywords— *p-n Junction, Radial Basis Function Network, Finite Differences approach.*

1. INTRODUCTION

It's widely believed now, that the technological evolution in microelectronics field cannot reach this advanced level of maturity without the exploration of electrical effects generated initially by p-n junctions (illustrated in figure 1), [1]. Consequently, the developments of this type of components have been an industrial concern for many years. The original resolution tools were based on numerical methods, which are of high complexity cost in term of calculation time. The numerical solution of partial differential equations governing the electrical behavior of p-n junctions has been dominated by either finite difference methods, finite element methods, and finite volume methods. These methods can be derived from the assumptions of the local interpolation schemes. These methods require a mesh to support the localized approximations; the construction of a mesh in three or more dimensions is a non-trivial problem. In practice, only low order approximations are used because of the notorious polynomial snaking problem, while higher order schemes are necessary for more accurate approximations of the spatial derivatives [2]. Because of the low order schemes typically employed, the spatial truncation errors can only be controlled by using progressively smaller meshes. The mesh spacing, *h*, must be sufficiently fine to capture the functions partial derivative behavior and to avoid unnecessarily large amounts of numerical artifacts contaminating the solution.

Thanks to the advent of new methods such as artificial intelligence methods .i.e., neural networks technique. This novel paradigm has shown to be very efficient in approximating nonlinear and multivariable functions when the sample training set is selected in a rigorous manner [3].

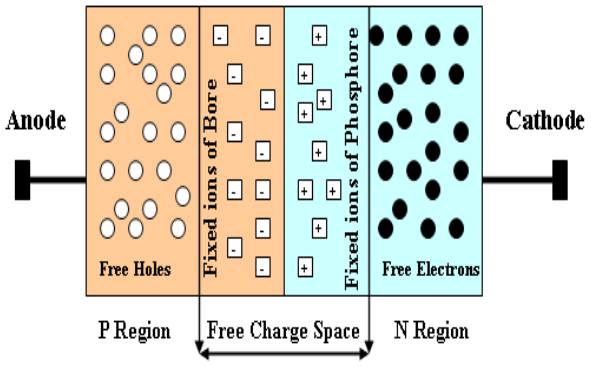


Figure. 1. Illustration of p-n Junction at equilibrium.

The aim of this paper is to develop a hybrid approach based on finite differences scheme and a neural network model. The proposed approach exhibits low computational complexity compared to classical methods. First, we give the mathematical formulation for both parameters: the electrical potential and the electrical field. Then the architecture of the proposed approach is presented and finally we validate our results via simulation which are in good accordance with theoretical findings.

2. PROBLEM FORMULATION

2.1. Electrical Potential Modeling

The electrical potential in both parts of the p-n junction is modeled through Poisson law which is a special case of boundary partial differential equations and is expressed by the following formula:

$$\begin{cases} -u''(x) = f(x), & x \in]a,b[\\ u(a) = \alpha \quad et \quad u(b) = \beta \end{cases} \qquad (1)$$

where f is a continuous function and the last two equalities describe the boundary equations of Newman type.

It should be noted that for each side of the p-n junction we have an appropriate equation characterized not only by a specific charge density but also by a different boundary conditions. In our case we assimilate u to the electrical potential V and f to the reduced charge density $\rho(x)/\varepsilon$.

2.2. Electrical Field Modeling

The electrical field is related to the electrical potential by the relation $\vec{E} = -gradV$ which when combined with Poisson law allow us to get the following model describing E in both parts of the p-n junction:

$$\begin{cases} u'(x) = f(x), & x \in]a,b[\\ u(a) = \eta \quad et \quad u(b) = \mu \end{cases} \qquad (2)$$

In our case we assimilate u to the electrical field E and f to the reduced charge density $\rho(x)/\varepsilon$.

3. PROPOSED APPROACH

The architecture of the proposed approach is given by the following figure :

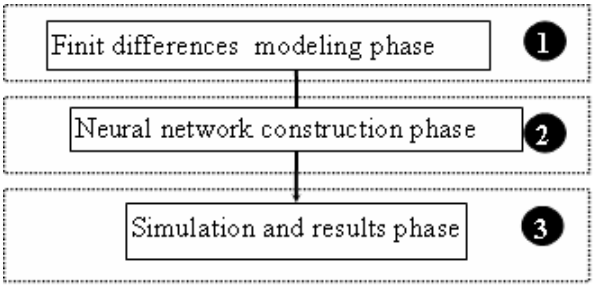


Figure. 2. Architecture of the proposed approach

3.1. Finite Differences Modeling Phase

The modeling process is applied for each equation related to p and n sides of the junction. The mesh scheme is created by

introducing N +1 nodes x_i with i = 0, 1,..,N, regularly spaced with a distance Δx.
The quantity u_i symbolizes the value of the function $u(x)$ at node x_i.
Then, the equation to be resolved is written in discreet form at each node as [4]:

$$-\left(\frac{d^2u}{dx^2}\right)_i = f(x_i) = f_i \quad (3)$$

The second derivative for u can be approximated through a centered scheme of order 2:

$$\left(\frac{d^2u}{dx^2}\right)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \quad (4)$$

and we get finally the set of equations for $i = 1$ to $N-1$:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = f_i \quad (5)$$

It's more comfortable to use a matrix based formulation in order to appear the vector of discreet variables u_i as given below:

$$\frac{1}{\Delta x^2}\begin{bmatrix} 2 & -1 & 0 & .. & 0 \\ -1 & 2 & -1 & .. & 0 \\ . & . & . & . & . \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ . \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 + \alpha/\Delta x^2 \\ f_2 \\ . \\ f_{N-2} \\ f_{N-1} + \beta/\Delta x^2 \end{bmatrix} \quad (6)$$

For the electrical field, we have the discreet equation at each node x_i :

$$\left(\frac{du}{dx}\right)_i = f(x_i) = f_i \quad (7)$$

The first derivative for u can be approximated through a centered scheme of order 1:

$$\left(\frac{du}{dx}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} \quad (8)$$

So, the final discreet equation for i = 1 to N-1 is:

$$\frac{u_{i+1} - u_i}{\Delta x} = f_i \quad (9)$$

Or, equivalently, in a matrix based formulation :

$$\frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & 0 & .. & 0 \\ 0 & -1 & -1 & .. & 0 \\ . & . & . & . & . \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ . \\ u_{N-2} \\ u_{N-1} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ . \\ f_{N-2} \\ f_{N-1} \end{bmatrix} \quad (10)$$

3.2. Neural Network Construction Phase

Radial basis function (RBF) networks are feed-forward networks trained using a supervised training algorithm. They are typically configured with a single hidden layer of units whose activation function is selected from a class of functions called basis functions. While similar to back propagation in many respects, radial basis function networks have several advantages. They usually train much faster than back propagation networks. They are less susceptible to problems with non-stationary inputs because of the behavior of the radial basis function hidden units [5].

3.2.1. Structure of the RBF networks

Radial Basis Functions are first introduced in the solution of the real multivariable interpolation problems [6]. The structure of an RBF networks in its most basic form involves three entirely different layers (Figure 3).

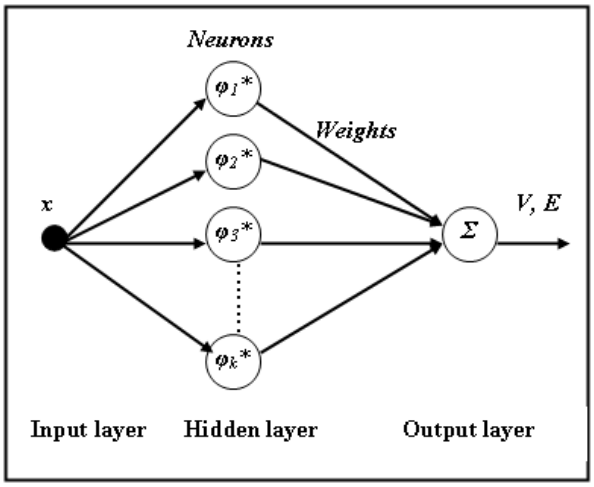


Figure. 3. Optimized RBF structure considered in this study.

The input layer is made up of source nodes (sensory units) whose number is equal to the dimension *p* of the input vector *u*.

The second layer is the hidden layer which is composed of nonlinear units that are connected directly to all of the nodes in the input layer.

The transformation from the input space to the hidden unit space is nonlinear, whereas the transformation to the hidden unit space to the output space is linear. The j^{th} output is computed as :

$$y = f(x) = w_0 + \sum_{i=1}^{i=m} w_i h_i \qquad (11)$$

3.2.2. Mathematical model

In summary, the mathematical model of the RBF network can be expressed as:

$$\begin{cases} f: \ \Re^N \rightarrow \Re^M \\ x_j = f_j(u) = w_{0j} + \sum_{i=1}^{L} w_{ij} G(\|u - c_i\|) \end{cases} \qquad (12)$$

where $\| \ \|$ is the Euclidean distance between *u* and c_i

3.2.3. Function approximation

Let $y=g(u)$ be a given function of *u*, $y \in R$, $u \in R$, $g: R \rightarrow R$, and let G_i $i=1..L$, be a finite set of basis functions. The function *g* can be written in terms of the given basis functions as:

$$y = g(u) = \sum_{i=1}^{L} w_i G_i(u) + r(u) \qquad (13)$$

where r(*u*) is the residual. The function *y* can be approximated as [7]:

$$y \cong \sum_{i=1}^{L} w_i G_i(u) \qquad (14)$$

The aim is to minimize the error by setting the parameters of G_i appropriately. A possible choice for the error definition is the L^2 norm of the residual function *r(u)* which is defined as [8]:

$$\|r(u)\|_{L^2} = \int r^2(u) \qquad (15)$$

3.2.4. Training RBF networks

The training of a RBF network can be formulated as a nonlinear unconstrained optimization problem given below :

Given input output training patterns (u^k, y^k), $k=1,2, ..K$, choose $w_{i,j}$ and c_i,, $i=1,2...L$, $j=1,2...M$ so as to minimize

$$J(w,c) = \sum_{i=1}^{i=K} \| y - f(x) \|^2$$

Note that the training problem becomes quadratic once if c_i's (radial basis function centers) are known. In general we have to pass through the following steps [9]:

a) Adjusting the widths

In its simplest form, all hidden units in the RBF network have the same width or degree of sensitivity to inputs. However, in portions of the input space where there are few patterns, it is sometime desirable to have hidden units with a wide area of reception. Computing these individual widths increases the performance of the RBF network at the expense of a more complicated training process.

b) Adjusting the centers

In radial basis function networks, the weights into the hidden layer basis units are usually

set before the second layer of weights is adjusted. As the input moves away from the connection weights, the activation value falls off. This behavior leads to the use of the term "center" for the first-layer weights. These center weights can be computed using Kohonen feature maps, statistical methods such as K-Means clustering, or some other means.

c) Adjusting the weights

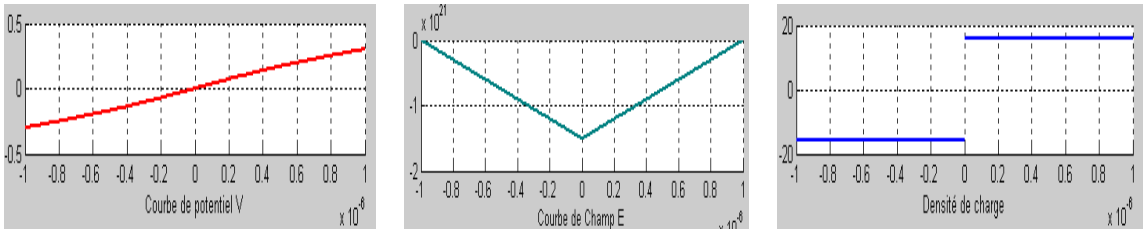
Once the hidden layer weights are set, a second phase of training is used to adjust the output weights. This process typically uses the standard steepest descent algorithm. Note that the training problem becomes quadratic once if c_i's (radial basis function centers) are known.

4. SIMULATION AND RESULTS

In order to evaluate the performances of the proposed approach, we have applied the different steps to three well known prototypes of p-n junctions found in literature [10].

First at all, a finite differences method is used to get the training data set which will be employed later in the creation of the RBF network, that gives the best approximation for electrical properties in each prototype. Input data are presented in tables which precedes curves giving obtained results of simulation.

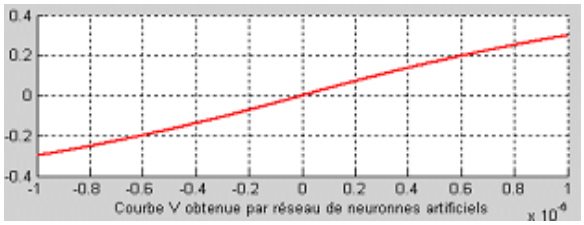
Table.1. Parameters of the abrupt p-n junction			
P side		N side	
Charge density	-10^{20}e	Charge density	10^{20}e
Nodes number	100	Nodes number	100
Boundary conditions		Boundary conditions	
at $x=0$	0	at $x=0$	0
at $x=x_p$	-0.3	at $x=x_n$	0.3
Material permittivity	$12\ \varepsilon_0$	Material permittivity	$12\varepsilon_0$



Electrical potential **Electrical field** **Charge density**

Figure.4. Electrical properties of the abrupt p-n junction

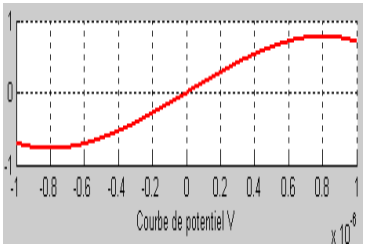
Table.2. RBF network parameters for the abrupt p-n junction			
P side		N side	
error	0.02	error	0.02
Spread factor	1	Spread factor	1
New nodes number	1200	New nodes number	1200

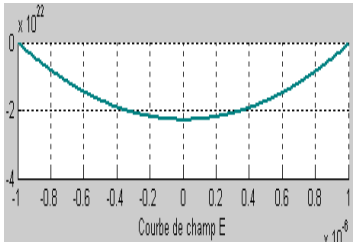


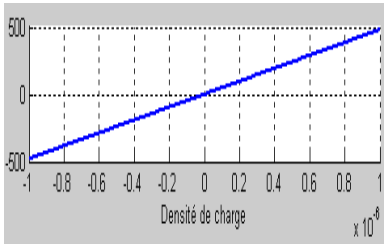
Curve obtained by the RBF network **Curve obtained by the**

Figure.5. Enhancement of the numerical solution using a RBF network

Table.3. Parameters of the gradual p-n junction (linear)			
P side		N side	
Charge density	$-(3\times10^{27}e)x$	Charge density	$(3\times10^{27}e)x$
Nodes number	100	Nodes number	100
Boundary conditions		Boundary conditions	
at $x=0$	0	at $x=0$	0
at $x=x_p$	-0.7	at $x=x_n$	0.7
Material permittivity	$12\varepsilon_0$	Material permittivity	$12\varepsilon_0$



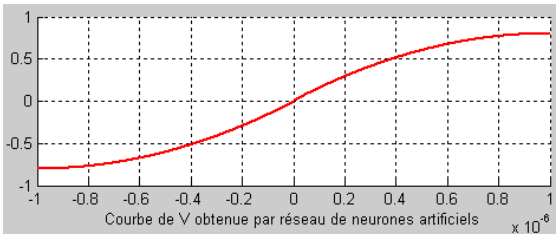


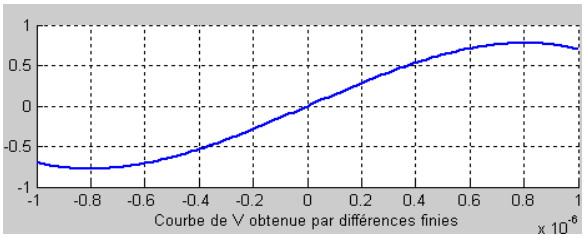


Electrical potentiel **Electrical field** **Charge density**

Figure.6. Electrical properties of the gradual linear p-n junction

Table.4. RBF network parameters for the gradual p-n junction (linear)			
P side		N side	
Goal error	0.2	Goal error	0.2
Spread factor	1	Spread factor	1
New nodes number	1000	New nodes number	1000

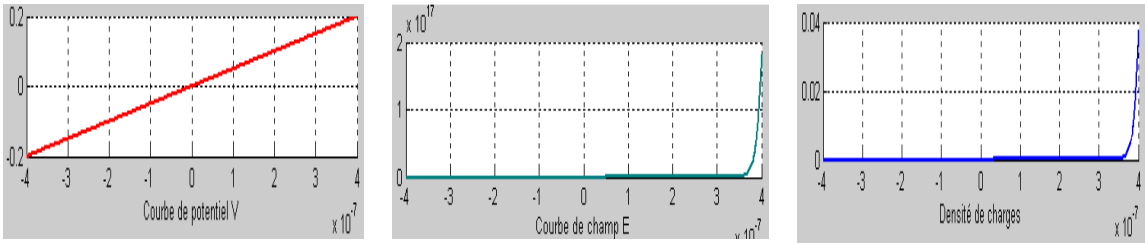




Curve obtained by the RBF network **Curve obtained by the finite differences**

Figure.7. Enhancement of the numerical solution using a RBF network

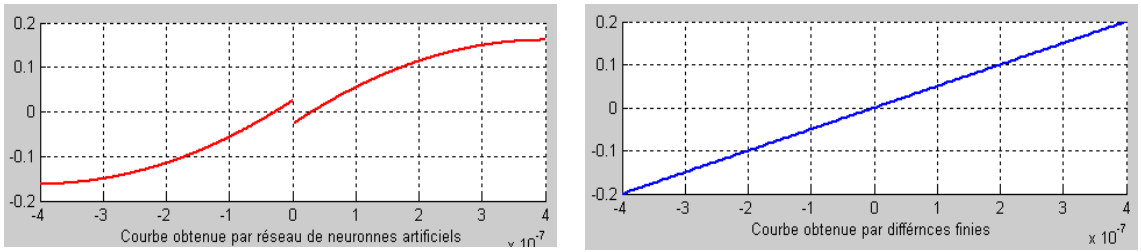
Table.5. Gradual p-n junction (exponential)			
P side		N side	
Charge density	$-\exp(10^8 x)e$	Charge density	$\exp(10^8 x)e$
Nodes number	100	Nodes number	100
Boundary conditions		Boundary conditions	
at $x=0$	0	at $x=0$	0
at $x=x_p$	-0.2	at $x=x_n$	0.2
Material permittivity	$12\varepsilon_0$	Material permittivity	$12\varepsilon_0$



Electrical potential **Electrical field** **Charge density**

Figure.8. Electrical properties of the gradual exponential p-n junction

Table.6. RBF network parameters for the gradual p-n junction (exponential)			
P side		N side	
Goal error	0.2	Goal error	0.2
Spread factor	1	Spread factor	1
New nodes number	10000	New nodes number	10000



Curve obtained by the RBF network **Curve obtained by the finite differences**

Figure.9. Enhancement of the numerical solution using a RBF network

5. CONCLUSIONS

In this paper, we have deduced that a pure discreet modeling of p-n junction electrical properties can lead in some situations to an unacceptable growth in the amount of time required for calculation. Such encountered difficulty was resolved by proposing a tow stages low complexity approach, allowing us to explicitly construct a RBF network that computes the analytical expression giving electrical potential inside the p-n junction with more accurate precision. The main advantage of such formalism consists in getting a lower bound for complexity compared to classical methods used in numerical solutions in partial differential equations.

Further research can be conducted by using Boltzmann near equilibrium equation, in order to support evolutionary states and not only stationary state. On the other hand, fuzzy logic can also be integrated to enhance the performance of the proposed approach.

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