Solution of the Schrodinger-Maxwell equations via Finite Elements and Genetic Algorithms with Nelder-Mead

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Abstract: - In this paper the Numerical Solution of the system of PDEs of Schrodinger-Maxwell equations (with a general nonlinear term) via Finite Elements and Genetic Algorithms with Nelder-Mead is proposed. The method of Finite Elements and Genetic Algorithms with Nelder-Mead that has been proposed by the author recently is also used. (Recently, the existence of a nontrivial solution to the nonlinear Schrodinger-Maxwell equations in R3, assuming on the nonlinearity the general hypotheses introduced by Berestycki & Lions has been proved)

Keywords: - Schrodinger-Maxwell equations, Finite Elements, Genetic Algorithms with Nelder-Mead,.

1 Introduction

Recently many authors have examined the following system of the non-linear Partial Differential Equations (PDEs) in $\mathbb{R}^3$

$$-\nabla^2 u + q\phi u = g(u) \qquad (1)$$

$$-\nabla^2 \phi = qu^2 \qquad (2)$$

with $g(.)$ being a known function. The system of (1) and (2) is called: Schrodinger-Maxwell equations. This system of Equations arises in many mathematical physics contexts, such as in quantum electrodynamics, in nonlinear optics, in nano-mechanics and in plasma physics.

The greatest part of the literature focuses on the study of the previous system for the very special nonlinearity $g(u) = -u + |u|^{p-1} u$ and existence, nonexistence and multiplicity results are provided in many papers for this particular problem (see [18]÷[28]).

In [29], Azzollini, D'Avenia and Pomponio that a solution of a boundary problem of (1) and (2) yields the minimization of some functional.

In this paper solve the problem with the method of finite elements

In this paper we will solve the boundary value problem of

$$-\nabla^2 u + q\phi u = g(u) \qquad (1)$$

$$-\nabla^2\phi = qu^2 \qquad (2)$$

where $g(.)$ is known using Variational Techniques (Finite elements). In Section 2, we produce the appropriate functional for minimization. After finding this functional, the solution of (1) and (2) with the nexesary boundary conditions can be easily reduced to an Optimization problem that can be solved by Genetic Algorithms with Nelder-Mead. An early paper of the author with the title "Solving Differential Equations via Genetic Algorithms" was presented in [1].

The author presented in 1996 the solution of ODE and PDE using Genetic Algorithms optimization, while the author use the same method to solve various problems in [2]÷[9].

The main Results are given in Section 2 and a numerical example illustrates the method in Section 3.

2 Variational Formulation of (1) and (2) and Finite Elements Approach with GA

Consider that our functional is functional of u,ϕ, i.e. $I = I(u,\phi)$

Let the "point" of u_0,ϕ_0 that minimize the $I(u,\phi)$. Then for another point u,ϕ we have

$u = u_0 + \varepsilon_1 u_1, \phi = \phi_0 + \varepsilon_2\phi_1$

So, we must have the first order conditions

$\frac{\partial I(u,\phi)}{\partial \varepsilon_1} = 0$ and $\frac{\partial I(u,\phi)}{\partial \varepsilon_2} = 0$

Working first for (1) we can formulate:

$$I = \frac{1}{2}\iiint_V (\nabla u)^2 dv + \frac{1}{2}\iiint_V q\phi u^2 dv - \iiint_V G(u)dv + B(\phi) \qquad (3)$$

with $G(u) = \int g(u)du$ and $B(\phi)$ a function in ϕ

It is easy to verify by replacing $u = u_0 + \varepsilon_1 u_1$ that the condition $\frac{\partial I(u,\phi)}{\partial \varepsilon_1} = 0$ leads to

$$\iiint_V (\nabla u_0)(\nabla u_1)dv + \iiint_V q\phi u_0 u_1 dv - \iiint_V g(u_0)u_1 dv = 0$$

Now by applying the Green's first identity we have

$$\oiint u_1(\nabla u \cdot \bar{n}) + \iiint_V (-\nabla^2 u_0)u_1 dv +$$

$$+\iiint_V q\phi u_0 u_1 dv - \iiint_V g(u_0)u_1 dv = 0$$

Considering appropriate u_1 we can have $\oiint u_1(\nabla u \cdot \bar{n}) = 0$ which means

$$\iiint_V (-\nabla^2 u_0)u_1 dv + \iiint_V q\phi u_0 u_1 dv - \iiint_V g(u_0)u_1 dv = 0$$

or

$$\iiint_V (-\nabla^2 u_0 + q\phi u_0 - g(u_0))u_1 dv = 0$$

But u_1 is arbitrary which implies

$-\nabla^2 u_0 + q\phi u_0 - g(u_0) = 0$ i.e. we have (1)

Working analogously with (2) we could have

$$I = \frac{1}{2}\iiint_V (\nabla\phi)^2 dv - \iiint_V q\phi u^2 dv + C(u) \qquad (4)$$

with $C(u)$ a function in u

We must compromise (3) and (4). To this end we multiply the right hand member of (4) with the coefficient -1/2 and finally we propose the functional

$$I = \frac{1}{2}\iiint_V (\nabla u)^2 dv - \frac{1}{4}\iiint_V (\nabla\phi)^2 dv +$$

$$+\frac{1}{2}\iiint_V q\phi u^2 dv - \iiint_V G(u)dv$$

So, the solution of the problem of Schrodinger-Maxwell equations

$$-\nabla^2 u + q\phi u = g(u) \qquad (1)$$

$$-\nabla^2\phi = qu^2 \qquad (2)$$

leads to

$$\min_{u,\phi} I$$

where

$$I=\frac{1}{2}\iiint_V (\nabla u)^2 dv-\frac{1}{4}\iiint_V (\nabla \phi)^2 dv+$$

$$+\frac{1}{2}\iiint_V q\phi u^2 dv-\iiint_V G(u)dv \tag{5}$$

We consider that u is written as

$u=\sum_n \lambda_n f_n$ and $\phi=\sum_n \mu_n \tilde{f}_n$

or

$$u=\sum_n f_n \qquad \phi=\sum_n \tilde{f}_n \tag{6}$$

where λ_n have been incorporated in f_n

So, we have the minimization problem of (5). One can select a triangular mesh and appropriate functions f_n and $\tilde{f}_n$ that have non-zero value only in the *n-th* triangle ("finite elements"). So, in a triangular mesh, for example of □ ^{2}, we can have $f_n=a_n x+b_n y+c_n$ and $\tilde{f}_n=\tilde{a}_n x+\tilde{b}_n y+\tilde{c}_n$ for the *n-th* triangle. Without loss of generality we consider the case□ ^{2} here u in (4).

To avoid to write **continuity conditions** on the common vertices of the triangles of the mesh, one can find that in the *n-th* triangle of the points *s,q,r* (see Figure 1)

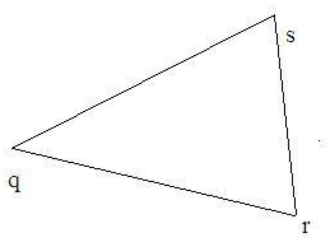

Fig.1 A triangle in a 2-D mesh

$$u_s=a_n x_s+b_n y_s+c_n \tag{7.1}$$

$$u_q=a_n x_q+b_n y_q+c_n \tag{7.2}$$

$$u_r=a_n x_r+b_n y_r+c_n \tag{7.3}$$

$$\phi_s=\tilde{a}_n x_s+\tilde{b}_n y_s+\tilde{c}_n \tag{7.4}$$

$$\phi_q=\tilde{a}_n x_q+\tilde{b}_n y_q+\tilde{c}_n \tag{7.5}$$

$$\phi_r=\tilde{a}_n x_r+\tilde{b}_n y_r+\tilde{c}_n \tag{7.6}$$

These 6 equations can be solved with respect to a_n,b_n,c_n, $\tilde{a}_n,\tilde{b}_n,\tilde{c}_n$ and give

$$a_n=\frac{\begin{vmatrix} u_s & y_s & 1\\ u_q & y_q & 1\\ u_r & y_r & 1\end{vmatrix}}{D} \tag{8.1}$$

$$b_n=\frac{\begin{vmatrix} x_s & u_s & 1\\ x_q & u_q & 1\\ x_r & u_r & 1\end{vmatrix}}{D} \tag{8.2}$$

$$c_n=\frac{\begin{vmatrix} x_s & y_s & u_s\\ x_q & y_q & u_q\\ x_r & y_r & u_r\end{vmatrix}}{D} \tag{8.3}$$

$$\tilde{a}_n=\frac{\begin{vmatrix} \phi_s & y_s & 1\\ \phi_q & y_q & 1\\ \phi_r & y_r & 1\end{vmatrix}}{D} \tag{8.4}$$

$$\tilde{b}_n=\frac{\begin{vmatrix} x_s & \phi_s & 1\\ x_q & \phi_q & 1\\ x_r & \phi_r & 1\end{vmatrix}}{D} \tag{8.5}$$

$$\tilde{c}_n=\frac{\begin{vmatrix} x_s & y_s & \phi_s\\ x_q & y_q & \phi_q\\ x_r & y_r & \phi_r\end{vmatrix}}{D} \tag{8.6}$$

and

$D = \begin{vmatrix} x_s & y_s & 1 \\ x_q & y_q & 1 \\ x_r & y_r & 1 \end{vmatrix}$ (which is by the way 2*E where E is the algebraic area of the triangle)

Hence, from the minimization problem

$$\min_{u,\phi} I$$

where

$$I = \frac{1}{2}\iiint_V (\nabla u)^2 dv - \frac{1}{4}\iiint_V (\nabla \phi)^2 dv +$$

$$+\frac{1}{2}\iiint_V q\phi u^2 dv - \iiint_V G(u) dv$$

we find the equivalent minimization problem

$$\min \int W(a_n, b_n, c_n, \tilde{a}_n, \tilde{b}_n, \tilde{c}_n) dv \quad (9)$$

where $W(a_n, b_n, c_n, \tilde{a}_n, \tilde{b}_n, \tilde{c}_n)$ is the function that we find after replacing $f_n = a_n x + b_n y + c_n$ and $\tilde{f}_n = \tilde{a}_n x + \tilde{b}_n y + \tilde{c}_n$ in the above functional

and a_n, b_n, c_n, $\tilde{a}_n, \tilde{b}_n, \tilde{c}_n$ will be replaces using (8.1), (8.2), (8.3) (8.4), (8.5), (8.6) for each triangle of the mesh.

Equation (9) can be solved now by a variety of techniques. The author uses Genetic Algorithms with Nelder-Meade for Non-linear Problems as in [2], [3], [4], [5], [6], [7], [8].
The same optimization scheme: Genetic Algorithms with Nelder-Meade will be also applied for (9).

Before proceeding in the solution of the problem, some background on GA (Genetic Algorithms) and Nelder-Mead is necessary. In [4], the author has also proposed a hybrid method that includes a) Genetic Algorithm for finding rather the neiborhood of the global minimum than the global minimu itself and b) Nelder-Mead algorithm to find the exact point of the global minimum itself.

So, with this Hybrid method of Genetic Algorithm + Nelder-Mead we combine the advantages of both methods, that are a) the convergence to the global minimum (genetic algorithm) plus b) the high accuracy of the Nelder-Mead method.

If we use only a Genetic Algorithm then we have the problem of low accuracy.

If we use only Nelder-Mead, then we have the problem of the possible convergence to a local (not to the global) minimum.

These disadvantages are removed in the case of our Hybrid method that combines Genetic Algorithm with Nelder-Mead method. We recall the following definitions from the Genetic Algorithms literature:

Fitness function is the objective function we want to minimize.
Population size specifies how many individuals there are in each generation. We can use various Fitness Scaling Options (rank, proportional, top, shift linear, etc), as well as various Selection Options (like Stochastic uniform, Remainder, Uniform, Roulette, Tournament). Fitness Scaling Options: We can use scaling functions. A Scaling function specifies the function that performs the scaling. A scaling function converts raw fitness scores returned by the fitness function to values in a range that is suitable for the selection function.

We have the following options:
Rank Scaling Option: scales the raw scores based on the rank of each individual, rather than its score. The rank of an individual is its position in the sorted scores. The rank of the fittest individual is 1, the next fittest is 2 and so on. Rank fitness scaling removes the effect of the spread of the raw scores.
Proportional Scaling Option: The Proportional Scaling makes the expectation proportional to the raw fitness score. This strategy has weaknesses when raw scores are not in a "good" range.

Top Scaling Option: The Top Scaling scales the individuals with the highest fitness values equally.

Shift linear Scaling Option: The shift linear scaling option scales the raw scores so that the expectation of the fittest individual is equal to a constant, which you can specify as Maximum survival rate, multiplied by the average score.
We can have also option in our Reproduction in order to determine how the genetic algorithm creates children at each new generation.
For example,
Elite Counter specifies the number of individuals that are guaranteed to survive to the next generation.
Crossover combines two individuals, or parents, to form a new individual, or child, for the next generation.
Crossover fraction specifies the fraction of the next generation, other than elite individuals, that are produced by crossover.
Scattered Crossover: Scattered Crossover creates a random binary vector. It then selects the genes where the vector is a 1 from the first parent, and the genes where the vector is a 0 from the second parent, and combines the genes to form the child.
Mutation: Mutation makes small random changes in the individuals in the population, which provide genetic diversity and enable the GA to search a broader space. Gaussian Mutation: We call that the Mutation is Gaussian if the Mutation adds a random number to each vector entry of an individual. This random number is taken from a Gaussian distribution centered on zero. The variance of this distribution can be controlled with two parameters. The Scale parameter determines the variance at the first generation. The Shrink parameter controls how variance shrinks as generations go by. If the Shrink parameter is 0, the variance is constant. If the Shrink parameter is 1, the variance shrinks to 0 linearly as the last generation is reached.
Migration is the movement of individuals between subpopulations (the best individuals from one subpopulation replace the worst individuals in another subpopulation). We can control how migration occurs by the following three parameters.
Direction of Migration: Migration can take place in one direction or two. In the so-called "Forward migration" the nth subpopulation migrates into the (n+1)'th subpopulation. while in the so-called "Both directions Migration", the nth subpopulation migrates into both the (n-1)th and the (n+1)th subpopulation. Migration wraps at the ends of the subpopulations. That is, the last subpopulation migrates into the first, and the first may migrate into the last. To prevent wrapping, specify a subpopulation of size zero.
Fraction of Migration is the number of the individuals that we move between the subpopulations. So, Fraction of Migration is the fraction of the smaller of the two subpopulations that moves. If individuals migrate from a subpopulation of 50 individuals into a population of 100 individuals and Fraction is 0.1, 5 individuals (0.1 * 50) migrate. Individuals that migrate from one subpopulation to another are copied. They are not removed from the source subpopulation.
Interval of Migration counts how many generations pass between migrations.

The Nelder-Mead simplex algorithm appeared in 1965 and is now one of the most widely used methods for nonlinear unconstrained optimization [33]÷[35]. The Nelder-Mead method attempts to minimize a scalar-valued nonlinear function of n real variables using only function values, without any derivative information (explicit or implicit).

The Nelder-Mead method thus falls in the general class of direct search methods. The method is described as follows: Let $f(x)$ be the function for minimization.
x is a vector in n real variables. We select $n+1$ initial points for x and we follow the steps:

Step 1. *Order*. Order the $n+1$ vertices to satisfy $f(x_1) \le f(x_2) \le \ldots \le f(x_{n+1})$, using the tie-breaking rules given below.
Step 2. *Reflect*. Compute the *reflection point* x_r from $x_r = \bar{x} + \rho(\bar{x} - x_{n+1}) = (1+\rho)\bar{x} - \rho x_{n+1}$, where $\bar{x} = \sum_{i=1}^{n} x_i / n$ is the centroid of the n best points (all vertices except for x_{n+1}). Evaluate

$f_r=f(x_r)$. If $f_1 \le f_r < f_n$, accept the reflected point x_r and terminate the iteration.

Step 3. *Expand*. If $f_r < f_1$, calculate the *expansion point* x_e,

$$x_e = \bar{x} + \chi(x_r - \bar{x}) = \bar{x} + \rho\chi(\bar{x} - x_{n+1}) = (1+\rho\chi)\bar{x} - \rho\chi x_{n+1}$$

and evaluate $f_e=f(x_e)$. If $f_e < f_r$, accept x_e and terminate the iteration; otherwise (if $f_e \ge f_r$), accept x_r and terminate the iteration.

Step 4. *Contract*. If $f_r \ge f_n$, perform a *contraction* between $\bar{x}$ and the better of x_{n+1} and x_r.

Outside. If $f_n \le f_r < f_{n+1}$ (i.e. x_r is strictly better than x_{n+1}), perform an *outside contraction*: calculate

$$x_c = \bar{x} + \gamma(x_r - \bar{x}) = \bar{x} + \gamma\rho(\bar{x} - x_{n+1}) = (1+\rho\gamma)\bar{x} - \rho\gamma x_{n+1}$$

and evaluate $f_c = f(x_c)$. If $f_c \le f_r$, accept x_c and terminate the iteration; otherwise, go to step 5 (perform a shrink).

b. *Inside*. If $f_r \ge f_{n+1}$, perform an *inside contraction*: calculate

$x_{cc} = \bar{x} - \gamma(\bar{x} - x_{n+1}) = (1-\gamma)\bar{x} + \gamma x_{n+1}$, and evaluate $f_{cc} = f(x_{cc})$. If $f_{cc} < f_{n+1}$, accept x_{cc} and terminate the iteration; otherwise, go to step 5 (perform a shrink).

Step 5. *Perform a shrink step*. Evaluate f at the n points $v_i = x_1 + \sigma (x_i - x_1), i = 2, \ldots , n+1$. The (unordered) vertices of the simplex at the next iteration consist of $x_1, v_2, \ldots , v_{n+1}$.

After this preparation, we are ready to solve the $\min \int |\phi(u_n)|^p \, dv$ of (9) as minimization problem.

The minimization is achieved by using Genetic Algorithms (GA) and the method of Nelder-Mead exactly as we described previously. We can use the MATLB software package (MATLAB, Version 7.0.0, by Math Works).

In the next numerical example (Section 3) our GA has the following Parameters

Population type:
Double Vector Population size: 30

Creation function: Uniform

Fitness scaling: Rank

Selection function: roulette

Reproduction: 6 – Crossover fraction 0.8

Mutation: Gaussian – Scale 1.0,
Shrink 1.0

Crossover: Scattered

Migration: Both – fraction 0.2, interval: 20

Stopping criteria: 50 generations

EXAMPLES

For numerical examples the reader can see the paper: “Genetic Algorithms with Nelder-Mead Optimization for the Finite Elements Methods applied on Non-linear Problems in Fluid Mechanics” in the Proceedings of the 2nd WSEAS International Conference on FINITE DIFFERENCES - FINITE ELEMENTS - FINITE VOLUMES - BOUNDARY ELEMENTS (F-and-B'09) Tbilisi, Georgia, June 26-28, 2009. See [30].

3 Conclusion

In [29], the existence of a nontrivial solution to the nonlinear Schrodinger-Maxwell equations in R3, assuming on the nonlinearity the general hypotheses introduced by Berestycki & Lions has been proved. In this paper the Numerical Solution of the system of PDEs of Schrodinger-Maxwell equations (with a general nonlinear term) via Finite Elements and Genetic Algorithms with Nelder-Mead is proposed. The method of Finite Elements and Genetic Algorithms with Nelder-Mead that has been proposed by the author recently is also used.

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