A General Approach to the Formulae Used in the Conjugate Directions Method for Solving Linear Systems of Algebraic Equations

Andrei Nicolaide, *Member, IAENG*

Abstract—**A proof of the formulae used in the conjugate directions method for solving linear algebraic systems of equations is presented. The proof is based on the minimization of a functional connected with a change of variables, and differs from the proofs presented by other authors. It permits an accessible but deep understanding of the procedure removing some confusions of literature, and allowing new remarks. Some results may be easily verified by using Maple-soft programs.**

Index Terms—**Linear algebraic systems of equations; conjugate directions method; conjugate gradient method.**

I. Introduction

Among the methods for solving linear algebraic systems of equations, one of the best is the conjugate gradient method (for which we shall also use the denomination of conjugate directions method that seems more adequate), a good example being its use in the finite element method [1-3], where large systems of equations occur. The formulae used for applying this method have been derived in literature in various ways. We should add that there are various sets of formulae proposed by different authors. We shall shortly recall the typical variants for establishing the used formulae.

In a first variant [4, Part 2, p.167, 171], the formulae have been obtained by a congruent transformation containing a dyadic decomposition and an endogenous transformation, in fact by multiplying the matrix of coefficients with a normalization matrix and the transpose of the matrix of coefficients. Hence a normalization of the system is performed. Then, the obtained quadratic matrix is transformed into a diagonal one.

In a second variant, a set of formulae [5, p. 243] has been established by utilizing the iterative method with common steps and convergence acceleration coefficient, i.e., the method of Richardson, and putting the condition that the rests (residuals) of the system of equations be conjugate versus a certain symmetric matrix.

In a third variant [3], we have considered that for establishing the set of formulae it would be convenient to utilize the minimization of a functional. We have chosen for applying this procedure, the set of formulae of [5] (for which we prepared a computer program), which we found very efficient in many numerical experiments concerning practical applications in calculation of electromagnetic devices [2].

The procedure of [3] was criticised in Zentralblatt für Mathematik and the main argument has been that "The recursion relation for the conjugate gradient method is derived from a local optimization property. Optimality in the entire Krylov subspace is claimed in an indirect way, but it is not proved". We consider that this argument contains two inaccuracies as follows: 1° The minimization of a functional (there has been no optimization in general) or of a function of several variables is a problem of mathematical analysis and has nothing to do with Krylov subspace; 2° In several cases, the local minimum coincides with the global minimum. In fact, in the known papers in literature, many manners of presenting the method do not show a consistent procedure. Some of them start with the statement that the formulae would be based on a minimization procedure, and the necessary functional is written in the known form. However, further the derivation of many formulae is carried out by resorting to linear algebra including eigenvectors and assuming that rounding errors do not exist. Also, the finite number of necessary iterations is establishes by the same way. For this reason, since the conclusions are obtained for the case in which rounding errors do not exist, a supplementary proof should be included for to prove that the minimization of the functional takes place even in the case when rounding errors exist. Moreover, several questions remain unproved, for instance in the case of a symmetric positive definite matrix of coefficients, the pre-conditioning matrix should also be positive definite. Therefore, the usual manner of studying the method could be estimated as eclectic.

We consider that a consistent manner for deducing the formulae and studying the method should be based on the same principle for each property.

Having in view the mentions above, we consider that it would be useful to present a derivation of the concerned set of formulae, based consequently on a minimization procedure connected with a change of

Manuscript received November 29, 2010. Andrei Nicolaide is with the "Transilvania" University of Brasov, Romania. Address: "Transilvania" University of Brasov, Bd. Eroilor Nr. 29, Brasov, Cod 500036, Romania (e-mail: andrei.nicolaide@gmail.com).

variables, which is a general one, without resorting to proper values or to Krylov subspace, and proving that it leads to the global minimum, hence removing the mentioned doubts. The used procedure also allows for several analyses.

II. Principle for Establishing the Computation Formulae

Further on, we shall denote the square matrices by capital bold upright letters and the column matrices (vectors) by small bold upright letters. Let:

$$\mathbf{A}\,\mathbf{x} = \mathbf{b}, \tag{1}$$

be a system of linear equations, where **A** is a symmetric positive definite matrix with n rows and n columns. The solution of the system of equations (1) minimizes the functional:

$$F(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\,\mathbf{x} - \mathbf{x}^T \mathbf{b}, \quad \mathbf{A} = [a_{ij}]. \tag{2}$$

In all formulae, the product of two vector matrices is performed via transposition.

As known, F being a function of several variables, the values of these which rend the minimum must satisfy several conditions, the first being the following:

$$\frac{\partial F}{\partial x_i} = 0, \quad \forall i \in [1, n]. \tag{3}$$

From relations (2) and (3) there follows:

$$\sum_{j=1}^{j=n} a_{ij}\, x_j = b_i, \quad \forall i \in [1, n]. \tag{4}$$

Therefore the values of x_i which could minimize the function F represent just the solution of (1). In the considered case, the solution is unique, and the minimum should be a global one.

There remains to establish a procedure for to minimize the concerned function. For this purpose, an iterative procedure has been chosen. Let us use for the first step (iteration) the formula:

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)}, \tag{5}$$

where $x^{(0)}$ represents the starting (initial) value attributed to the vector (column matrix) of the unknowns to be determined. Also, a_0 and further a_m are coefficients to be determined for the functional (2) to be minimized, whereas $\mathbf{p}^{(0)}$ is a starting vector. Any further iteration of order $m+1$ will be:

$$\mathbf{x}^{(m+1)} = \mathbf{x}^{(m)} + a_m\,\mathbf{p}^{(m)}, \tag{6}$$

and the expression of the rest (residual) of iteration m will be:

$$\mathbf{r}^{(m+1)} = \mathbf{b} - \mathbf{A}\,\mathbf{x}^{(m+1)} = \mathbf{b} - \mathbf{A}\,\mathbf{x}^{(m)} - a_m\,\mathbf{A}\,\mathbf{p}^{(m)}, \tag{7}$$

therefore:

$$\mathbf{r}^{(m+1)} = \mathbf{r}^{(m)} - a_m\,\mathbf{A}\,\mathbf{p}^{(m)}, \tag{8}$$

where the following symbols have been used:

a_m – coefficient at iteration m;
m – iteration ordinal number;
n – number of equations;
$\mathbf{p}^{(m)}$ – column matrix (vector) at iteration m;
$\mathbf{r}^{(m)}$ – column matrix (vector) of the rest (residual) at iteration m.

For any iteration of order $m+1$, we may write:

$$F\left(\mathbf{x}^{(m+1)}\right) = \frac{1}{2}\left(\mathbf{x}^{(m)} + a_m\mathbf{p}^{(m)}\right)^T \mathbf{A}\left(\mathbf{x}^{(m)} + a_m\mathbf{p}^{(m)}\right) - \left(\mathbf{x}^{(m)} + a_m\mathbf{p}^{(m)}\right)^T \mathbf{b}. \tag{9}$$

III. The Change of Variables

In order to fix the ideas, and facilitate some remarks, without losing the generality, we shall consider the case $n = 3$. We shall take $\mathbf{x}^{(0)}$ as starting value and we shall write the first three iterations:

$$\begin{aligned}
\mathbf{x}^{(1)} &= \mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)};\\
\mathbf{x}^{(2)} &= \mathbf{x}^{(1)} + a_1\,\mathbf{p}^{(1)} = \mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)};\\
\mathbf{x}^{(3)} &= \mathbf{x}^{(2)} + a_2\,\mathbf{p}^{(2)} = \mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)} + a_2\,\mathbf{p}^{(2)}.
\end{aligned} \tag{10 a, b, c}$$

Correspondingly, the rests of the form

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\,\mathbf{x} \tag{11}$$

are:

$$\begin{aligned}
\mathbf{r}^{(1)} &= \mathbf{r}^{(0)} - a_0\,\mathbf{A}\mathbf{p}^{(0)};\\
\mathbf{r}^{(2)} &= \mathbf{r}^{(1)} - a_1\,\mathbf{A}\mathbf{p}^{(1)} = \mathbf{r}^{(0)} - a_0\,\mathbf{A}\mathbf{p}^{(0)} - a_1\,\mathbf{A}\mathbf{p}^{(1)};\\
\mathbf{r}^{(3)} &= \mathbf{r}^{(2)} - a_2\,\mathbf{A}\mathbf{p}^{(2)} = \mathbf{r}^{(0)} - a_0\,\mathbf{A}\mathbf{p}^{(0)} - a_1\,\mathbf{A}\mathbf{p}^{(1)} - a_2\,\mathbf{A}\mathbf{p}^{(2)};
\end{aligned} \tag{12 a, b, c}$$

and in general, the last equation above becomes:

$$\begin{aligned}
\mathbf{r}^{(n)} &= \mathbf{r}^{(n-1)} - a_{n-1}\,\mathbf{A}\mathbf{p}^{(n-1)}\\
&= \mathbf{r}^{(0)} - a_0\,\mathbf{A}\mathbf{p}^{(0)} - a_1\,\mathbf{A}\mathbf{p}^{(1)} - \ldots\\
&\ldots - a_{n-1}\,\mathbf{A}\mathbf{p}^{(n-1)}.
\end{aligned} \tag{13}$$

We may remark that for to minimize (2), in the case in which $n = 3$, we need to know the values of three quantities x_1, x_2, x_3 that constitute vector **x**. The vector **x** of (1) that is constituted by those three quantities can be expressed in function of the other three quantities of the set a_0, a_1, a_2 considered as exogenous variables.

For this purpose, we shall use relation (10 c). From formulae (10 a, b, c), it results that the solution represented by vector sets **x** is expressed in a vector basis formed by the set of three vectors $\mathbf{p}^{(0)}, \mathbf{p}^{(1)}, \mathbf{p}^{(2)}$ assumed, firstly, as exogenous variables. If the quantities of the two sets are related to each other, we can consider the quantities a_i exogenous, while the quantities $\mathbf{p}^{(i)}$ as endogenous. Therefore the variables $x_i \ \forall i \in [1, 3]$ will be changed (replaced) by the variables $a_i \ \forall i \in [0, 2]$, in expression (9).

The function to be minimized $F(x_1, x_2, x_3)$ becomes $F(a_0, a_1, a_2)$:

$$\begin{aligned} F(a_0, a_1, a_2) &= \\ &= \frac{1}{2}\left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)} + a_2\,\mathbf{p}^{(2)}\right)^T \mathbf{A} \\ &\times \left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)} + a_2\,\mathbf{p}^{(2)}\right) \\ &- \left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)} + a_2\,\mathbf{p}^{(2)}\right)^T \mathbf{b}, \end{aligned} \tag{14}$$

or in general, for the case of a system with *n* equations:

$$\begin{aligned} F(a_0, a_1, a_2, \ldots, a_{n-1}) &= \\ &= \frac{1}{2}\left[\mathbf{x}^{(0)} + \sum_{i=0}^{i=n-1} a_i\,\mathbf{p}^{(i)}\right]^T \mathbf{A}\left[\mathbf{x}^{(0)} + \sum_{i=0}^{i=n-1} a_i\,\mathbf{p}^{(i)}\right] \\ &- \left[\mathbf{x}^{(0)} + \sum_{i=0}^{i=n-1} a_i\,\mathbf{p}^{(i)}\right]^T \mathbf{b}. \end{aligned} \tag{15}$$

By replacing expression (12) into (3), and a_i instead of x_i we obtain:

$$\begin{aligned} \frac{\partial F}{\partial a_0} &= \left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)}\right) \\ &\quad - \left(\mathbf{p}^{(0)}\right)^T \mathbf{b} = 0; \\ \frac{\partial F}{\partial a_1} &= \left(\mathbf{p}^{(1)}\right)^T \mathbf{A}\left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)}\right) \\ &\quad - \left(\mathbf{p}^{(1)}\right)^T \mathbf{b} = 0; \\ \frac{\partial F}{\partial a_2} &= \left(\mathbf{p}^{(2)}\right)^T \mathbf{A}\left(\mathbf{x}^{(0)} + a_0\,\mathbf{p}^{(0)} + a_1\,\mathbf{p}^{(1)} + a_2\,\mathbf{p}^{(2)}\right) \\ &\quad - \left(\mathbf{p}^{(2)}\right)^T \mathbf{b} = 0, \end{aligned}$$

(16 a, b, c)

where we have had in view the symmetry of matrix **A**, and relation (7).

There follows:

$$\begin{aligned} \frac{\partial F}{\partial a_0} &= \left(\mathbf{p}^{(0)}\right)^T\left(-\mathbf{r}^{(0)} + a_0\,\mathbf{A}\,\mathbf{p}^{(0)}\right) \\ &= -\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(1)} = 0; \\ \frac{\partial F}{\partial a_1} &= \left(\mathbf{p}^{(1)}\right)^T\left(-\mathbf{r}^{(1)} + a_1\,\mathbf{A}\,\mathbf{p}^{(1)}\right) = 0; \\ \frac{\partial F}{\partial a_2} &= \left(\mathbf{p}^{(2)}\right)^T\left(-\mathbf{r}^{(2)} + a_2\,\mathbf{A}\,\mathbf{p}^{(2)}\right) = 0. \end{aligned} \tag{17 a, b, c}$$

IV. The Computing Formulae

A. Particular Case

From relations (17 a, b, c), we can determine the values of a_0, a_1, a_2 so that, every other quantity being supposed with fixed value, the relations will be fulfilled. We shall obtain:

$$a_0 = \frac{\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(0)}}{\left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\mathbf{p}^{(0)}}; \quad a_1 = \frac{\left(\mathbf{p}^{(1)}\right)^T \mathbf{r}^{(1)}}{\left(\mathbf{p}^{(1)}\right)^T \mathbf{A}\mathbf{p}^{(1)}}; \quad a_2 = \frac{\left(\mathbf{p}^{(2)}\right)^T \mathbf{r}^{(2)}}{\left(\mathbf{p}^{(2)}\right)^T \mathbf{A}\mathbf{p}^{(2)}}. \tag{18 a, b, c}$$

According to the structure of matrix **A**, it may be possible that $\mathbf{p}^{(2)}$ of (17 a, b, c) be equal to zero. Then, the solution will be given by relation (17 b). This circumstance means that the solution represented by vector **x** is obtained in a vector basis formed by the two vectors $\mathbf{p}^{(0)}, \mathbf{p}^{(1)}$.

B. General Case

Further on, we shall consider the case of a system with *n* equations. For more precision, a supplementary unknown coefficient c_m and a vector $\mathbf{z}^{(m)}$ will be introduced by the following relation set:

$$\begin{aligned} \mathbf{r}^{(m)} &= \mathbf{M}\,\mathbf{z}^{(m)}; \\ \mathbf{p}^{(m)} &= \mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}; \\ \mathbf{p}^{(0)} &= \mathbf{M}^{-1}\,\mathbf{r}^{(0)}, \end{aligned} \tag{19 a, b, c}$$

where **M** has been chosen as an invertible symmetric matrix of the same order as **A**, in particular it might be $\mathbf{M} = \mathbf{A}$. But, this case is not interesting because if we knew $\mathbf{M}^{-1}$, the solution would be immediate. For reasons further shown, after formula (25), **M** should be positive definite. By this formula, each iteration includes the results of the previous two. Also, we should add that in accordance with relations (19 a, b, c) the vectors of the form $\mathbf{p}^{(i)}$ will be partially exogenous variables, if $\mathbf{p}^{(0)}$ has to be introduced. With the above described relations, the expression of the functional can be written as follows:

$$F = \frac{1}{2}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right]^T \times \mathbf{A}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right] - \left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right]^T \mathbf{b}. \tag{20}$$

The first condition of minimum requires that the derivatives of the first order of the functional with respect to the unknown coefficients a_m and c_m are equal to zero. Therefore we shall obtain the condition for the derivatives of the first order:

$$\begin{aligned}\frac{\partial F}{\partial a_m} &= \left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)^T \times \mathbf{A}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right] - \left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)^T \mathbf{b} \\ &= \left(\mathbf{p}^{(m)}\right)^T\left(\mathbf{A}\,\mathbf{x}^{(m+1)} - \mathbf{b}\right) = -\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m+1)} = 0,\end{aligned} \tag{21a-d}$$

and

$$\begin{aligned}\frac{\partial F}{\partial c_m} &= a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right] - a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{b} \\ &= a_m\left(\mathbf{p}^{(m-1)}\right)^T\left(\mathbf{A}\mathbf{x}^{(m+1)} - \mathbf{b}\right) = -a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m+1)} = 0,\end{aligned} \tag{22 a-d}$$

be zero. Multiplying relation (8) by $\mathbf{p}^{(m-1)}$, we get:

$$\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m+1)} = \left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m)} - a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)}. \tag{23}$$

Taking into account expressions (21 d) and (22 d), relation (23) yields:

$$\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)} = 0. \tag{24}$$

The other conditions require the calculation of the derivatives of the second order of the functional. Taking into account relations (8), (19 b) and (21), we shall obtain:

$$\begin{aligned}\frac{\partial^2 F}{\partial a_m^2} &= \left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right) \\ &= \left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\mathbf{p}^{(m)} > 0; \\ \mathbf{A}\mathbf{p}^{(m)} &= \frac{1}{a_m}\left(\mathbf{r}^{(m)} - \mathbf{r}^{(m+1)}\right); \quad \left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\mathbf{p}^{(m)} \\ &= \frac{1}{a_m}\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m)} \\ &= \left(\mathbf{z}^{(m)} + c_{m-1}\,\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m)} = \left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m)} \\ &= \left(\mathbf{z}^{(m)}\right)^T \mathbf{M}\mathbf{z}^{(m)} > 0,\end{aligned} \tag{25 a-i}$$

and since (25 b) is positive because the matrix **A** has been chosen positive definite, the expression (25 i) must also be positive, hence matrix **M** *should be positive definite.*

Similarly, we shall obtain:

$$\frac{\partial^2 F}{\partial c_m^2} = a_m\,a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\left(\mathbf{p}^{(m-1)}\right). \tag{26}$$

Taking in view relations (21), (6), (19 b), (7), (22 d) and (24), we shall obtain:

$$\begin{aligned}\frac{\partial^2 F}{\partial a_m\,\partial c_m} &= \left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right] \\ &\quad + \left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,a_m\,\mathbf{p}^{(m-1)} - \left(\mathbf{p}^{(m-1)}\right)^T \mathbf{b} \\ &= \left(\mathbf{p}^{(m-1)}\right)^T\left(\mathbf{A}\,\mathbf{x}^{(m+1)} - \mathbf{b}\right) + a_m\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m-1)} \\ &= -\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m+1)} + a_m\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m-1)} = 0.\end{aligned} \tag{27 a-d}$$

From the three relations above, there follows that the conditions of minimum are fulfilled as below:

$$\frac{\partial^2 F}{\partial a_m^2} > 0; \quad \frac{\partial^2 F}{\partial c_m^2} > 0; \quad \frac{\partial^2 F}{\partial a_m^2}\cdot\frac{\partial^2 F}{\partial c_m^2} - \left(\frac{\partial^2 F}{\partial a_m\,\partial c_m}\right)^2 > 0. \tag{28 a, b, c}$$

From relation (21 a) and (19 b), there follows:

$$\begin{aligned}&\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\left[\mathbf{x}^{(m)} + a_m\left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)\right] - \left(\mathbf{z}^{(m)} + c_m\,\mathbf{p}^{(m-1)}\right)^T \mathbf{b} \\ &= \left(\mathbf{p}^{(m)}\right)^T\left(\mathbf{A}\,\mathbf{x}^{(m)} - \mathbf{b}\right) + a_m\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)} \\ &= -\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m)} + a_m\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)} = 0,\end{aligned} \tag{29 a, b, c}$$

wherefrom:

$$a_m = \frac{\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m)}}{\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)}}. \tag{30}$$

From relation (22 d), there follows:

$$\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m+1)} = 0. \tag{31}$$

From relations (27 a), (7), (19 b), (21 d) and (24), there follows:

$$\begin{aligned}&a_m\left(\mathbf{p}^{(m-1)}\right)^T\left(-\mathbf{r}^{(m)}\right) + a_m\,c_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\mathbf{p}^{(m-1)} \\ &= a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,\mathbf{z}^{(m)} + a_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,c_m\,\mathbf{p}^{(m-1)} = 0,\end{aligned} \tag{32 a, b}$$

wherefrom:

$$c_m = -\frac{\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,\mathbf{z}^{(m)}}{\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\,\mathbf{p}^{(m-1)}}. \tag{33}$$

Multiplying relation (19 b) by $\mathbf{r}^{(m+1)}$, we have:

$$\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m+1)} = \left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m+1)} + c_m\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{r}^{(m+1)} = 0, \tag{34}$$

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

and considering relations (21 d) and (22 d), we find:

$$\left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m+1)} = 0; \left(\mathbf{z}^{(m)}\right)^T \mathbf{M}\,\mathbf{z}^{(m+1)} = 0 \qquad \text{(35 a, b)}$$

Multiplying relation (19 b) by $\mathbf{r}^{(m)}$, and taking into account (21 d), there follows:

$$\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m)} = \left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m)}. \qquad (36)$$

We shall now use relation (36) for obtaining other expressions for a_m and c_m emphasising the matrix **M**. If we replace expression (36) into (30), we shall get:

$$a_m = \frac{\left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m)}}{\left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)}}. \qquad (37)$$

Multiplying both sides of (8) by $\mathbf{p}^{(m)}$ and considering expression (21 d), we get:

$$\left(\mathbf{p}^{(m)}\right)^T \mathbf{r}^{(m)} = a_m \left(\mathbf{p}^{(m)}\right)^T \mathbf{A}\,\mathbf{p}^{(m)}. \qquad (38)$$

The expression (33) can also be modified like (30). We shall start from relation (8) in the form:

$$a_m\,\mathbf{A}\,\mathbf{p}^{(m)} = \mathbf{r}^{(m)} - \mathbf{r}^{(m+1)}, \qquad (39)$$

where the index *m* has to be changed into (*m*-1). We can write:

$$\mathbf{A}\,\mathbf{p}^{(m-1)} = \frac{1}{a_{m-1}}\left(\mathbf{r}^{(m-1)} - \mathbf{r}^{(m)}\right). \qquad (40)$$

We shall multiply both sides of (40) by $\mathbf{z}^{(m)}$, use expression (37) for replacing a_{m-1} and remark that according to relation (39), because **M** is symmetric, the first term in parenthesis vanishes. Replacing the result into (33), we shall get:

$$c_m = -\frac{\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\mathbf{p}^{(m-1)}}{\left(\mathbf{z}^{(m-1)}\right)^T \mathbf{r}^{(m-1)}}\left[-\left(\mathbf{z}^{(m)}\right)^T \mathbf{r}^{(m)}\right]\frac{1}{\left(\mathbf{p}^{(m-1)}\right)^T \mathbf{A}\mathbf{p}^{(m-1)}}, \qquad (43)$$

and finally:

$$c_m = \frac{\left(\mathbf{z}^{m}\right)^T \mathbf{r}^{(m)}}{\left(\mathbf{z}^{(m-1)}\right)^T \mathbf{M}\,\mathbf{z}^{(m-1)}}. \qquad (44)$$

By minimizing the system of equations (1) with respect to the quantities a_0, a_1, a_2, the minimum, i.e., $-\frac{1}{2}\mathbf{x}^T\mathbf{b}$, will be the same as minimizing with respect to the quantities x_1, x_2, x_3, because we performed only a change of variables.

Using the formulae (6), (17 a, b, c) and (18 a, b, c) for the case with three variables, it follows that we achieved the minimization along three directions $\mathbf{p}^{(0)}, \mathbf{p}^{(1)}, \mathbf{p}^{(2)}$.

Therefore, we may expect that after the third direction we reached the solution of minimum. It results that we have used a procedure with a finite number of arithmetic operations. The number of iterations, except the introduction of starting quantities will be $n-1$, in the examined case, namely 2.

The final value, in the general case, after $n-1$ iterations, will be:

$$x^{(n)} = x^{(0)} + \sum_{i=0}^{i=n-1} a_i\,\mathbf{A}\,\mathbf{p}^{(i)}. \qquad (45)$$

However, it remains to prove that the obtained solution after $n-1$ iterations corresponds just to the minimum, as explained in the next section.

If the precision is not satisfactory, the precision could be improved by continuing the iterations. No other proofs are necessary for these conclusions unlike the case in which the proof of formulae had been established using the properties of conjugation with respect to a symmetric positive definite matrix.

V. Verifying the Solution Conditions

For the expression (45), together with (19 a, b, c), (37), (44), to represent the solution of (1), it suffices that the conditions:

$$\left(\mathbf{p}^{(i)}\right)^T \mathbf{r}^{(j)} = 0; \quad \left(\mathbf{p}^{(i)}\right)^T \mathbf{A}\,\mathbf{p}^{(j)} = 0; \forall\, i, j \in [0, n], i \neq j \qquad (46)$$

are satisfied, as clearly specified, further, after formula (54).

For to verify it, there is necessary to establish the general relations between the pairs of quantities $\mathbf{r}^{(i)}, \mathbf{r}^{(j)}$, and $\mathbf{p}^{(i)}, \mathbf{p}^{(j)}$, and also between the quantities of both pairs. For this purpose, we shall start from relations (21) and (22).

By using those relations, we can obtain the results that we can put into two sets, according their form, related to (21 d), (22 d), or (24) respectively. The first example: From relation (21), putting $m = 0$, there follows:

$$\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(1)} = 0, \qquad (47)$$

and we put the result of (47) into the first set. From relation (22), putting $m = 1$, there follows:

$$\left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\,\mathbf{p}^{(1)} = 0, \qquad (48)$$

and we put the result of (48) into the second set.
Now, we shall consider relations (8), (21 d) and (22 d), and look for

$$\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(2)} = \left(\mathbf{p}^{(0)}\right)^T \left(\mathbf{r}^{(1)} - a_1\,\mathbf{A}\,\mathbf{p}^{(1)}\right)$$
$$= a_1 \left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\,\mathbf{p}^{(1)} = 0, \qquad \text{(49 a-d)}$$
$$\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(2)} = 0,$$

and we put the result of (49 d) into the first set.

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

Similarly, considering the relations (8), (21), (19), (48) and (49), we have:

$$\begin{aligned}\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(3)} &= \left(\mathbf{p}^{(0)}\right)^T \left(\mathbf{r}^{(2)} - a_2\, \mathbf{A}\,\mathbf{p}^{(2)}\right)\\ &= -a_2 \left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\,\mathbf{p}^{(2)}\\ &= -a_2 \left(\mathbf{p}^{(0)}\right)^T \mathbf{A} \left(\mathbf{M}^{-1}\mathbf{r}^{(2)} + c_2\,\mathbf{p}^{(1)}\right)\\ &= -a_2 \left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\,\mathbf{M}^{-1}\mathbf{r}^{(2)}\\ &= -a_2 \left(\mathbf{A}\,\mathbf{p}^{(0)}\right)^T \mathbf{M}^{-1}\mathbf{r}^{(2)}\\ &= -a_2 \frac{1}{a_0}\left(\mathbf{r}^{(0)} - \mathbf{r}^{(1)}\right)^T \mathbf{M}^{-1}\mathbf{r}^{(2)},\end{aligned} \qquad \text{(50 a-f)}$$

but according to (19 a-c), and taking in view that matrix $\mathbf{M}$ is symmetric, we obtain:

$$\begin{aligned}&\mathbf{p}^{(0)} = \mathbf{z}^{(0)}; \quad \mathbf{p}^{(1)} = \mathbf{z}^{(1)} + c_1\,\mathbf{p}^{(0)};\\ &\mathbf{z}^{(0)} - \mathbf{z}^{(1)} = (1 + c_1)\mathbf{p}^{(0)} - \mathbf{p}^{(1)};\\ &\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(3)} = -a_2 \frac{1}{a_0}\left(\mathbf{r}^{(0)} - \mathbf{r}^{(1)}\right)^T \mathbf{z}^{(2)}\\ &\qquad = -a_2 \frac{1}{a_0}\left(\mathbf{z}^{(0)} - \mathbf{z}^{(1)}\right)^T \mathbf{r}^{(2)};\\ &\left(\mathbf{z}^{(0)} - \mathbf{z}^{(1)}\right)^T \mathbf{r}^{(2)} = \frac{1}{a_0}\left[(1 + c_1)\mathbf{p}^{(0)} - \mathbf{p}^{(1)}\right]^T \mathbf{r}^{(2)}\\ &\qquad = \frac{1}{a_0}(1 + c_1)\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(2)} - \frac{1}{a_0}\left(\mathbf{p}^{(1)}\right)^T \mathbf{r}^{(2)};\\ &\left(\mathbf{p}^{(1)}\right)^T \mathbf{r}^{(2)} = 0; \quad \left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(2)} = 0; \quad \left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(3)} = 0;\end{aligned} \qquad \text{(51 a-j)}$$

and we put the result of (51 j) into the first set.

Taking into account (50 a), (8), (49 d), we shall obtain:

$$\begin{aligned}&\left(\mathbf{p}^{(0)}\right)^T \mathbf{r}^{(3)} = \left(\mathbf{p}^{(0)}\right)^T \left(\mathbf{r}^{(2)} - a_2\,\mathbf{A}\,\mathbf{p}^{(2)}\right) = 0,\\ &\left(\mathbf{p}^{(0)}\right)^T \mathbf{A}\,\mathbf{p}^{(2)} = 0,\end{aligned} \qquad \text{(52 a, b)}$$

and we put the result of (52 b) into the second set.

Afterwards, we can repeat the calculations starting with the factor $\mathbf{p}^{(1)}$, and so on.

Finally, we can write, for the first set, the general relations:

$$\left(\mathbf{p}^{(i)}\right)^T \mathbf{r}^{(j)} = 0; \quad \forall i \in [0, n-1]; \quad j \in [1, n]; \quad i < j, \qquad (53)$$

and

$$\left(\mathbf{p}^{(i)}\right)^T \mathbf{A}\,\mathbf{p}^{(j)} = 0; \quad \forall i \in [0, n-1]; \quad j \in [1, n]; \quad i < j. \qquad (54)$$

The relation (54) remains valid even if the order of superscripts indices is taken conversely.

Multiplying both sites of relation (13) with $\mathbf{p}^{(i)}, \forall i \in [0, n-1]$, taking into account relations (53) and (54), it results that the right-hand side is zero, and if the projections of a vector with n components on n independent directions is zero, it means that the considered vector, i.e., $\mathbf{r}^{(n)}$ is zero. Therefore the global minimum has been reached.

All relations from this section can be easily verified by using Maple-soft programs, [6], prepared by the author for systems of linear equations. For instance, in the case of a linear system of algebraic equation with all coefficients rational numbers, the relations of type (54) are exactly fulfilled being an obvious confirmation of the deduction carried out.

References

[1] A. Nicolaide, Calcul des champs électromagnétiques par la méthode des éléments finis. In: Revue Générale de l'Électricité, No. 9, pp. 3-9, 1991, Paris, France.

[2] A. Nicolaide, The Application of the Pre-Conditioned Conjugate Gradient Methods for Computer Aided Solving Large Systems of Linear Equations in Electrical Engineering. In: Proceedings of the 5th International Conference on Optimization of Electric and Electronic Equipments. Brasov, May 15-27, 1996, pp. 3-22.

[3] A. Nicolaide, New Proof of the Formulae Used in the Conjugate Gradient Method with Pre-conditioning for Solving Large Systems of Linear Equations. Demonstratio Mathematica, vol. XXX, No. 4, 1997, pp. 761-774, Warsaw, Poland.

[4] R. Zurmühl, S. Falk, Matrizen und ihre Anwendungen. (Matrices and their Applications, Part 2, Numerical methods), Springer Verlag, Berlin, Heidelberg, New York, Tokio, 1986.

[5] G.H. Golub, G.A. Meurant, Résolution numérique des grands systèmes linéaires (Numerical Solution of Large Systems of Linear Equations), Editions Eyrolles, Paris, 1983.

[6] A. Nicolaide, Maple computer program for solving systems of linear algebraic equations, Maple-Solving-1, for proving the case of formulae without rounding errors. Research and Modelling Electrotechnical Laboratory, *Transilvania* University of Brasov, 2010.

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)