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A Finite Difference Numerical Scheme Formulation (Based On Poisson's Equation) For Piezoelectric Application

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***Abstract*—A finite difference numerical scheme has been presented for piezoelectric application, the intended finite grid solver is presented and a succinct discussion of relevant concepts has been presented.**

Keywords—Finite difference, Piezoelectric, Poisson's equation, Cgs (Conjugate gradient square).

1. Introduction

The Poisson's equation suffices, given the dielectric constants, and the volume charge distribution density, the potential of an arbitrary medium can be determined.

In mathematics, Poisson's equation is a partial differential equation of elliptic type [1, 2, 3, 4, 5] with broad utility in electrostatics, mechanical engineering and theoretical physics. It is used, for instance, to describe the potential energy field caused by a given charge or mass density distribution. The equation is named after the French mathematician, geometer, and physicist Siméon Denis Poisson [6].

A. Electrostatics

One of the cornerstones of electrostatics is setting up and solving problems described by the Poisson equation, this could be extended to piezoelectricity. Solving the Poisson equation amounts to finding the electric potential φ for a given charge distribution ρ_f.

The mathematical details behind Poisson's equation in electrostatics are as follows (SI units are used rather than Gaussian units which are also frequently used in electromagnetism).

Starting with Gauss's law for electricity (also one of Maxwell's equations)[7] in differential form, we have:

$$\nabla \cdot \mathbf{D} = \rho_f \quad \text{.....(1)}$$

where $\nabla \cdot$ is the divergence operator, **D** =electric displacement field, and ρ_f = free charge density (describing charges brought from outside). Assuming the medium is linear, isotropic, and homogeneous (see polarization density), we have the constitutive equation:

$$\mathbf{D} = \varepsilon \mathbf{E} \quad \text{.....(2)}$$

where ε = permittivity of the medium and **E** = electric field. Substituting this into Gauss's law and assuming ε is spatially constant in the region of interest obtains:

$$\nabla \cdot \mathbf{E} = \frac{\rho_f}{\varepsilon} \quad \text{.....(3)}$$

In the absence of a changing magnetic field, **B**, Faraday's law of induction gives:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = 0 \quad \text{.....(4)}$$

where × is the curl operator and *t* is time. Since the curl of the electric field is zero, it is defined by a scalar electric potential field, φ (see Helmholtz decomposition).

$$\mathbf{E} = -\nabla \varphi \quad \text{.....(5)}$$

The derivation of Poisson's equation under these circumstances is straightforward. Substituting the potential gradient for the electric field

$$\nabla \cdot \mathbf{E} = \nabla \cdot (-\nabla \varphi) = -\nabla^2 \varphi = \frac{\rho_f}{\varepsilon}, \quad \text{(6)}$$

directly obtains **Poisson's equation** for electrostatics, which is:

$$\nabla^2 \varphi = -\frac{\rho_f}{\varepsilon}. \quad \text{.....(7)}$$

Solving Poisson's equation for the potential requires knowing the charge density distribution. If the charge density is zero, then Laplace's equation results. If the charge density follows a Boltzmann distribution, then the Poisson-Boltzmann equation results. The Poisson–Boltzmann equation plays a role in the development of the Debye-huckel theory of dilute electrolyte solutions .

The above discussion assumes that the magnetic field is not varying in time. The same Poisson equation arises even if it does vary in time, as long as the Coulomb gauge is used. In this more general context, computing φ is no longer sufficient to calculate **E**, since **E** also depends on the magnetic vector potential **A**, which must be independently

computed. See 'Maxwell's equation' in potential formulation [7] for more on φ and **A** in Maxwell's equations and how Poisson's equation is obtained in this case.

2. Discussion

A. Poisson's equation

Statement of the equation

Poisson's equation is

$$\Delta\varphi = f \quad \text{.....(8)}$$

where Δ is the Laplace operator, and f and φ are real or complex-valued functions on a manifold. Usually, f is given and φ is sought. When the manifold is Euclidean space, the Laplace operator is often denoted as ∇^2 and so Poisson's equation is frequently written as

$$\nabla^2\varphi = f, \quad \text{.....(9)}$$

In three-dimensional Cartesian coordinates, it takes the form

n

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z) = f(x,y,$$

..(10)

When $f = 0$ we retrieve Laplace's equation. Poisson's equation may be solved using a Green's function; a general exposition of the Green's function for Poisson's equation is given in the article on the screened Poisson equation. There are various methods for numerical solution. The relaxation method, an iterative algorithm, is one example.

B. Green's functions for the Laplacian

Green's functions for linear differential operators involving the Laplacian may be readily put to use using the second of Green's identities.

To derive Green's theorem, begin with the divergence theorem (otherwise known as Gauss's theorem):

$$\int_V \nabla\cdot\vec{A}\,dV = \int_S \vec{A}\cdot d\hat{\sigma}. \quad \text{.....(11)}$$

Let $\vec{A} = \phi\nabla\psi - \psi\nabla\phi$ and substitute into Gauss' law. Compute $\nabla\cdot\vec{A}$ and apply the product rule for the ∇ operator:

$$\begin{aligned}\nabla\cdot\vec{A} &= \nabla\cdot(\phi\nabla\psi - \psi\nabla\phi)\\ &= (\nabla\phi)\cdot(\nabla\psi) + \phi\nabla^2\psi - (\nabla\phi)\cdot(\nabla\psi) - \psi\nabla^2\phi\\ &= \phi\nabla^2\psi - \psi\nabla^2\phi.\end{aligned}$$

.(12)

Plugging this into the divergence theorem produces Green's theorem:

$$\int_V(\phi\nabla^2\psi - \psi\nabla^2\phi)dV = \int_S(\phi\nabla\psi - \psi\nabla\phi)\cdot d\hat{\sigma}.$$

.(13)

Suppose that the linear differential operator L is the Laplacian, ∇^2, and that there is a Green's function G for the Laplacian. The defining property of the Green's function still holds:

$$LG(x,x') = \nabla^2 G(x,x') = \delta(x-x').$$

,.(14)

Let $\psi = G$ in Green's theorem. Then:

$$\int_V\left[\phi(x')\delta(x-x') - G(x,x')\nabla^2\phi(x')\right]d^3x' = \int_S[\phi(x')\nabla'G(x,x') - G(x,x')\nabla'\phi(x')]\cdot d\hat{\sigma}'.$$

,.(15)

Using this expression, it is possible to solve Laplace's equation $\nabla^2\phi(x) = 0$ or Poisson's equation $\nabla^2\phi(x) = -\rho(x)$, subject to either Neumann or Dirichlet boundary conditions. In other words, we can solve for $\phi(x)$ everywhere inside a volume where either (1) the value of $\phi(x)$ is specified on the bounding surface of the volume (Dirichlet boundary conditions), or (2) the normal derivative of $\phi(x)$ is specified on the bounding surface (Neumann boundary conditions).

Suppose the problem is to solve for $\phi(x)$ inside the region. Then the integral

$$\int_V \phi(x')\delta(x-x')\,d^3x' \quad \text{.....(16)}$$

reduces to simply $\phi(x)$ due to the defining property of the Dirac delta function and we have:

$$\phi(x) = \int_V G(x,x')\rho(x')\,d^3x' + \int_S[\phi(x')\nabla'G(x,x') - G(x,x')\nabla'\phi(x')]\cdot d\hat{\sigma}'.$$

,.(17)

This form expresses the well-known property of harmonic functions that if the value or normal derivative is known on a bounding surface, then the value of the function inside the volume is known everywhere.

In electrostatics, $\phi(x)$ is interpreted as the electric potential, $\rho(x)$ as electric density, and the normal derivative $\nabla\phi(x')\cdot d\hat{\sigma}'$ as the normal component of the electric field.

If the problem is to solve a Dirichlet boundary value problem, the Green's function should be chosen such that $G(x,x')$ vanishes when either x or x' is on the bounding surface. Thus only one of the two terms in the surface integral remains. If the problem is to solve a Neumann boundary value problem, the Green's function is chosen such that its normal derivative

vanishes on the bounding surface, as it would seem to be the most logical choice. (See Jackson J.D. classical electrodynamics, page 39) [8]. However, application of Gauss's theorem to the differential equation defining the Green's function yields

$$\int_S \nabla' G(x,x') \cdot d\hat{\sigma}' = \int_V \nabla'^2 G(x,x') d^3x' = \int_V \delta(x-x') d^3x' = 1$$,..(18)

meaning the normal derivative of $G(x,x')$ cannot vanish on the surface, because it must integrate to 1 on the surface. (Again, see Jackson J.D. classical electrodynamics, page 39 for this and the following argument) [8]. The simplest form the normal derivative can take is that of a constant, namely $1/S$, where *S* is the surface area of the surface. The surface term in the solution becomes

$$\int_S \phi(x') \nabla' G(x,x') \cdot d\hat{\sigma}' = \langle \phi \rangle_S$$,..(19)

where $\langle \phi \rangle_S$ is the average value of the potential on the surface. This number is not known in general, but is often unimportant, as the goal is often to obtain the electric field given by the gradient of the potential, rather than the potential itself.

With no boundary conditions, the Green's function for the Laplacian (Green's function for the three-variable Laplace equation) is:

$$G(x,x') = \frac{1}{|x-x'|}.$$ .....(20)

Supposing that the bounding surface goes out to infinity, and plugging in this expression for the Green's function, this gives the familiar expression for electric potential in terms of electric charge density as

$$\emptyset(x) = \int_V \frac{\rho(x)}{|x-x'|} d^3x'$$,.....(21)

C. Poisson's equation

We have seen that the electric field generated by a set of stationary charges can be written as the gradient of a scalar potential, so that

$$\mathbf{E} = -\nabla \phi.$$ (22)

This equation can be combined with the field equation (3), previously done in (6) to give a partial differential equation for the scalar potential:

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}.$$ (23)

This is an example of a very famous type of partial differential equation known as *Poisson's equation [9]*.

In its most general form, Poisson's equation is written

$$\nabla^2 u = v,$$ (24)

where $u(r)$ is some scalar potential which is to be determined, and $v(r)$ is a known ``source function.'' The most common boundary condition applied to this equation is that the potential u is zero at infinity. The solutions to Poisson's equation are completely superposable. Thus, if u_1 is the potential generated by the source function v_1, and u_2 is the potential generated by the source function v_2, so that

$$\nabla^2 u_1 = v_1, \qquad \nabla^2 u_2 = v_2,$$ (25)

then the potential generated by $v_1 + v_2$ is $u_1 + u_2$, since

$$\nabla^2 (u_1 + u_2) = \nabla^2 u_1 + \nabla^2 u_2 = v_1 + v_2.$$ (26)

Poisson's equation has this property because it is *linear* in both the potential and the source term.

The fact that the solutions to Poisson's equation are superposable suggests a general method for solving this equation. Suppose that we could construct all of the solutions generated by point sources. Of course, these solutions must satisfy the appropriate boundary conditions. Any general source function can be built up out of a set of suitably weighted point sources, so the general solution of Poisson's equation must be expressible as a weighted sum over the point source solutions. Thus, once we know all of the point source solutions we can construct any other solution. In mathematical terminology, we require the solution to

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$ (27)

which goes to zero as $|r| \to \infty$ [10,11]. The function $G(r,r')$ is the solution generated by a unit point source located at position $\mathbf{r}'$. This function is known to mathematicians as a *Green's function*. The solution generated by a general source function $v(r)$ is simply the appropriately weighted sum of all of the Green's function solutions:

$$u(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}')\, v(\mathbf{r}')\, d^3\mathbf{r}'.$$ (28)

We can easily demonstrate that this is the correct solution:

$$\nabla^2 u(\mathbf{r}) = \int \left[\nabla^2 G(\mathbf{r}, \mathbf{r}')\right] v(\mathbf{r}')\, d^3\mathbf{r}' = \int \delta(\mathbf{r} - \mathbf{r}')\, v(\mathbf{r}')\, d^3\mathbf{r}' = v(\mathbf{r}).$$ (29)

Let us return to Eq. (23):

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0}. \qquad (30)$$

The Green's function for this equation satisfies Eq. (27) with $|G| \to \infty$ as $|r| \to 0$. It follows from Eq. (20) that

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi}\frac{1}{|\mathbf{r} - \mathbf{r}'|}. \qquad (31)$$

Note, from Eq. (20), that the Green's function has the same form as the potential generated by a point charge. This is hardly surprising, given the definition of a Green's function. It follows from Eq. (21) and (28) that the general solution to Poisson's equation, (30), is written

$$\phi(\mathbf{r}) = \frac{1}{4\pi\,\epsilon_0}\int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}\, d^3\mathbf{r}'. \qquad (32)$$

3. Further discussion

A. Finite grid solver

The piezoelectric charge distribution density is given as,

$\rho_{piezo}(r) = \epsilon_0\, \nabla.\{\epsilon_s\,(r)\nabla V_{piezo}(r)\}$ .....(33)

The reduced proper piezoelectric tensor is,

$\vec{e}_{\mu j} = \frac{dP_\mu}{d\eta_j} = \vec{e}^{\,0}_{\mu j} + \sum_k \vec{B}_{\mu jk}\eta_k$ .....(34)

,where $\eta_j (j = 1,6)$ denotes strain in the Voigt notation.

Also, $\rho_{piezo}(r) = \frac{-e}{a_0^2}\nabla.P.$ .....(35)

Table 1. List of constants from DFT $(^{C}/_{m^2})$.

	e_{14}	B_{114}	B_{124}	B_{156}
InAs	−0.115	−0.531	−4.076	−0.120
GaAs	−0.230	−0.439	−3.765	−0.492

$\boldsymbol{A(r) = xA_{InAs} + (1 - x)A_{GaAs}(r)}$ .....(36)

, $A = \epsilon_s$, is position dependent dielectric constant, hence, $A = e_{\mu s}$ or $B_{\mu jk}$, x is the ion concentration.

B. Finite grid solver Scheme

$$\begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ u_{3,1} \\ u_{3,2} \\ u_{3,3} \end{bmatrix} = h^2 \begin{bmatrix} g_{1,1} \\ g_{1,2} \\ g_{1,3} \\ g_{2,1} \\ g_{2,2} \\ g_{2,3} \\ g_{3,1} \\ g_{3,2} \\ g_{3,3} \end{bmatrix} .(37)$$

$,(i, j = 1,2,3.)$.

The matrix is obtained viz the finite difference scheme treating the elliptic pde, Poisson's equation and the resulting linear system can be solved by a suitable available algorithm like the, '**Conjugate-gradient algorithm'** or its variant. The values of u which could be the desired potential sought can be obtained for a defined g, which is some volume distribution function, ∈ is the dielectric constant of the medium and h is the mesh size.

4. Conclusion

An explicit mathematical delineation of piezoelectric materials would give indepth insight into salient features, and physical attributes. Following, delineation of the Poisson's equation and salient constitutive equations, a finite difference numerical scheme has been formulated for an insightful and elaborate treatment and understanding of the behaviour and properties of piezoelectric materials and piezoelectric applications in turn.

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