Finite Element Method: Variational Method assuming a piece-wise linear function.

Introduction

COMSOL Multiphysics is a finite element package that can be used to solve a partial differential equation such as Poisson's equation. As discussed in lecture, Poisson's equation is:

$$\nabla^2 \psi = \vec{\nabla} \cdot \vec{\nabla} \psi = f(\vec{r}) \qquad [1]$$

where $\psi(\vec{r})$ is some scalar field and $f(\vec{r})$ is the density of field sources that depends on the position vector $\vec{r}$. Poisson's equation is a linear, second order, partial differential equation that can be solved for some geometries by analytical techniques. In your EMT and Classical Mechanics courses, you may have already studied solutions of Poisson's equation for various geometries that have a high degree of symmetry (i.e. spherical, cylindrical etc.). COMSOL's execution of the Finite Element Method allows it to solve more complex problems, efficiently and quickly. Note that the differential equation relates the 2nd derivative of the scalar field ψ to the source field *f*. For our discussion, the scalar field is the potential at any point in space, and the source field is the distribution of the charge density on whatever surface or volume we are considering. In Cartesian coordinates the one-dimensional Poisson equation becomes:

$$\frac{\partial^2 \psi(x)}{\partial x^2} = f(x) \qquad [2]$$

Note that the special case where f(x) is equal to zero turns equation (2) into Laplace's equation:

$$\frac{\partial^2 \psi(x)}{\partial x^2} = 0 \qquad [2b]$$

The two most frequently used numerical methods to solve Poisson's and Laplace's equations are:

1. The finite difference method
2. The finite element method

Comsol Multiphysics, uses the finite element method.

Minimum Energy Principles in Electrostatics

Jackson shows in section 1.12 that minimizing the functionals described by equations 1.63 and 1.67 is equivalent for solving the Poisson equation. You find a similar proof in math textbooks.

This equivalence is also valid for other differential equations. The figure below shows a table with different differential equations and the corresponding functional that needs to be minimized.

Name of equations	PDE	Variational principle
Homogeneous wave equation with sources	$\nabla^2\Phi + k^2\Phi = g$	$I(\Phi) = \frac{1}{2}\int_v \left[\lvert\nabla\Phi\rvert^2 - k^2\Phi^2 + 2g\Phi\right] dv$
Homogeneous wave equation without sources	$\nabla^2\Phi + k^2\Phi = 0$	$I(\Phi) = \frac{1}{2}\int_v \left[\lvert\nabla\Phi\rvert^2 - k^2\Phi^2\right] dv$
Diffusion equation	$\nabla^2\Phi - k\frac{\partial\Phi}{\partial t} = 0$	$I(\Phi) = \frac{1}{2}\int_t\int_v \left[\lvert\nabla\Phi\rvert^2 - k^2\Phi\frac{\partial\Phi}{\partial t}\right] dv\,dt$
Homogenous Poisson's equation	$\nabla^2\Phi = -g$	$I(\Phi) = \frac{1}{2}\int_v \left[\lvert\nabla\Phi\rvert^2 - 2g\Phi\right] dv$
Homogenous Laplace's equation	$\nabla^2\Phi = 0$	$I(\Phi) = \frac{1}{2}\int_v \left[\lvert\nabla\Phi\rvert^2\right] dv$

Note that the functional can be interpreted as some type of energy expressions. Consider for example a Dirichlet boundary value problem with no volume charge density. The functional to be minimized is given by Jackson equation 1.63, i.e.

$$I[\psi] = \frac{1}{2}\iiint_V \nabla\psi\cdot\nabla\psi d^3x - \iint_V g\psi d^3x$$

Which is minimum if ψ satisfies a Poisson-like equation within volume V and the departures $\delta\psi$ vanishes on the boundary; so for $\psi\rightarrow\Phi$ and $g\rightarrow \rho/\varepsilon_o$ the minimization yields the equation of motion. For a case where $\rho=0$ this expression changes to:

$$I[\psi] = \frac{1}{2}\iiint_V \nabla\psi\cdot\nabla\psi d^3x$$

So multiplying this with ε_o gives the total electrostatic energy of the system since the term under the integral is E^2.

Jackson outlines in section 1.12 how these functionals can be used to find an approximation for the electric potential of such boundary value problem. The first step is to determine a good guess solution for the electric potential that obeys the boundary conditions of the problem. This approximation of the electric potential contains parameters that still need to be determined. To determine those parameters one first finds an expression for the functional using the trial solution and the given volume charge density using the correct functional from the table above. After that

one minimizes the functional, and of course minimalization of a functional is done by setting the derivative of the functional towards those constants equal to zero and solving the set of linear equations. This process is also sketched in the figure below.

For Dirichlet problems: Functional to be minimized is $I(\Phi) = \frac{1}{2}\int_v \left[|\nabla\Phi|^2 - 2g\Phi\right] dv$

Choose suitable electric potential expression obeying the boundary conditions:
This is often a polynomial function that contains several constants that need to be determined, for example Φ(x)=a+ bx+cx^2+dx^3+ex^4

Use given volume charge density and Φ(x) to determine the functional. Note that this is a lot of work. The functional will depend on the constants, so
I(Φ)=f(a, b, c, d, e)

In addition to your Φ(x), you also need to use the volume charge density given by the problem description

Now determine the values for a, b, c, d, and e that will minimize the functional:
of course this is done by setting the partial derivatives of f towards those constants equal to zero and solving the linear equations.

The remaining part of this section proves in a different way that minimizing of the above given functional is the same as solving the differential equation. To avoid the Green's function and keep the math simple we will restrict ourselves here to the 1-dimensional case. For the 2-dimensional and the 3-dimensional case just double and triple the terms.

Proof for 1D Dirichlet problem with zero volume charge density: We first provide the proof for the case that no volume charge density is present, so Laplace's equation can be solved to find the potential. Furthermore, we assume that *u(x)* is an approximation for *ψ(x)*, the solution of Laplace's equation. Therefore, *u(x)* does not need to be an exact solution of Laplace's equation and differs from *ψ(x)* such that:

$$u(x) = \psi(x) + e(x) \qquad [3]$$

where *e(x)* is the error in the approximate solution *u(x)*. Furthermore, the approximation function *u(x)* is exact at the endpoints of each interval. Therefore, the error function *e(x)* is necessarily zero at the endpoints of each interval, $[x_1, x_2]$, i.e.

$$e(x_1) = e(x_2) = 0$$

$$\therefore u(x_1) = \psi(x_1) \; and \; u(x_2) = \psi(x_2) \qquad [4]$$

For Laplace's equation the proof is rather straight forward. In the absence of charge the energy of the system, *F*, is given by:

$$F = \frac{\varepsilon_0}{2}\int E^2 dx = \frac{\varepsilon_0}{2}\int\left(-\vec{\nabla}\psi\right)^2 dx = \frac{\varepsilon_0}{2}\int\left(\frac{\partial\psi}{\partial x}\right)^2 dx \quad [5]$$

Therefore, an approximation to the energy of the system using *u(x)* on the interval $[0,1]$ provides:

$$F \approx \frac{\varepsilon_0}{2}\int_0^1\left(\frac{\partial u}{\partial x}\right)^2 dx = \frac{\varepsilon_0}{2}\int_0^1\left(\frac{\partial\psi}{\partial x}+\frac{\partial e}{\partial x}\right)^2 dx$$

$$= \frac{\varepsilon_0}{2}\int_0^1\left\{\left(\frac{\partial\psi}{\partial x}\right)^2 + 2\frac{\partial\psi}{\partial x}\frac{\partial e}{\partial x}+\left(\frac{\partial e}{\partial x}\right)^2\right\}dx \quad [6]$$

The middle term of this last line can be cleverly rewritten using the product rule for differentiation. This rewrite (see below) breaks it into two terms, each of which are equal zero for independent reasons. The first term of equation [7] is zero because *e=0* at the boundaries since the boundary conditions provide the exact value of ψ at *x=0* and *x=1*. We see the second term is zero because of Laplace's equation, i.e. $\frac{d^2\psi}{dx^2} = 0$, hence:

$$\int_0^1\frac{\partial\psi}{\partial x}\frac{\partial e}{\partial x}dx = \int_0^1\left\{\frac{d}{dx}\left(\frac{\partial\psi}{\partial x}e\right) - e\frac{d^2\psi}{dx^2}\right\}dx$$

$$= \left[\frac{\partial\psi}{\partial x}e\right]_0^1 + \int_0^1 e\frac{d^2\psi}{dx^2}dx \;\; = \;0 + \int_0^1 e\cdot 0\,dx \;\; = 0 \quad [7]$$

With this simplification the electrostatic energy in one dimension becomes:

$$F \approx \frac{\varepsilon_0}{2}\int_0^1\left\{\left(\frac{\partial\psi}{\partial x}\right)^2 + \left(\frac{\partial e}{\partial x}\right)^2\right\}dx \quad [8]$$

Note that both terms are positive due to the squares. The first term represents the total energy of the system for $\psi(x)$, the solution to Laplace's equation. The 2nd term will be small if du/dx (the approximated electric field) is close to $d\psi/dx$ (the electric field that is a solution of Laplace's equation). So the total energy of *u(x)* is close to the total energy of $\psi(x)$ but always larger.

Proof for 1D Dirichlet problem with non-zero volume charge density: In the case where space charge is present, this statement is still true, but the expression is a little more complicated. The electrostatic energy is no longer given by equation (3). To find the total electrostatic energy it is now necessary to subtract the contributions of the fixed charges, $\rho_s\psi$, approximated with $\rho_s u$, from the approximated field energy density:

$$F = \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left(\frac{\partial \psi}{\partial x} \right)^2 - \rho_s \psi \right\} dx \approx \int_0^1 \frac{\varepsilon_0}{2} \left\{ \left(\frac{\partial u}{\partial x} \right)^2 - \rho_s u \right\} dx$$

$$= \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + 2 \frac{\partial \psi}{\partial x} \frac{\partial e}{\partial x} + \left(\frac{\partial e}{\partial x} \right)^2 \right] - \rho_s u \right\} dx \qquad [9]$$

As shown earlier, we can simplify by rewriting the second term in the integrand. However, we use Poisson's equation instead of Laplace's equation for the final substitution, and therefore is nonzero:

$$\int_0^1 \frac{\partial \psi}{\partial x} \frac{\partial e}{\partial x} dx = \int_0^1 \left\{ \frac{d}{dx} \left(\frac{\partial \psi}{\partial x} e \right) - e \frac{d^2 \psi}{dx^2} \right\} dx$$

$$= \left[\frac{\partial \psi}{\partial x} e \right]_0^1 + \int_0^1 e \frac{d^2 \psi}{dx^2} dx$$

$$= \int_0^1 e \cdot \frac{\rho_s}{\varepsilon_0} dx \qquad [11]$$

Using the simplification of equation [11] we can now write the total electrostatic energy F as:

$$F = \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial e}{\partial x} \right)^2 \right] + e \cdot \rho_s + \left(\frac{\partial e}{\partial x} \right)^2 - \rho_s u \right\} dx$$

$$= \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial e}{\partial x} \right)^2 \right] - \rho_s (u - e) \right\} dx \qquad [12]$$

This can be further simplified using $-e = \psi$:

$$F = \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left[\left(\frac{\partial \psi}{\partial x} \right)^2 + \left(\frac{\partial e}{\partial x} \right)^2 \right] - \rho_s \psi \right\} dx = \int_0^1 \left\{ \frac{\varepsilon_0}{2} \left(\frac{\partial \psi}{\partial x} \right)^2 - \rho_s \psi \right\} dx + \int_0^1 \frac{\varepsilon_0}{2} \left(\frac{\partial e}{\partial x} \right)^2 dx \qquad [13]$$

The first two terms on the right hand side give the electrostatic energy of the solution of Poisson's equation while the third term is clearly the error. Later, we will see how when minimizing F we arrive at differential equations involving $u(x)$ which makes $e(x)$ approach zero. This sort of minimization algorithm is shown in the next section, and is a method of the calculus of variations, as used in classical mechanics to find the equations of motion.

Finite Element Method.

The finite element method uses the same approach but the approximation for the electric potential is via a piece-wise linear function. So the total space is divided up in small intervals and for each interval the electric potential is approximated by a linear function. The parameters of the electric potential are the electric potential at the internal boundaries of the interval. Summaring:

1. u(x) will consist of a piece wise linear function defined over n intervals referred to by finite elements. We assume that u(x) is defined over the interval [0,L], so $u(x) \rightarrow u_1(x)$ *for* $0<x<x_1$, $u_2(x)$ *for* $x_1<x<x_2$, $\ldots u_n(x)$ *for* $x_{n-1}<x<L$.
2. Parameterize $u(x)$ by the electric potential at the internal boundaries, $u_1(x_1)$, $u_2(x_2)$, $\ldots u_{n-1}(x_{n-1})$
3. $u_1(0)$=*left boundary value*, $u_n(L)$=*right boundary value.*
4. We define the following short-hand: $u_1(x_1)=u_1$, $u_2(x_2)=u_2$, $\ldots u_{n-1}(x_{n-1})=u_{n-1}$.
5. Derive an expression for the functional of the system using the given volume charge density and u(x) in terms of parameters u_1, u_2, $\ldots u_{n-1}$. *Note that you have to sum over all intervals.*
6. Find values for the parameters that will minimize the functional given by equation 1.63 in Jackson.

Parameterize $u(x)$: To do so we divide the space up in small intervals (1D), surface areas (2D), or volumes (3D), called finite elements. For each element the solution of Poisson's equation is approximated by a polynomial function; for example for element i the function u is given by $u_i(x)$. For 1D-problems this polynomial function could be a simple straight line, a parabola, or a more complicated polynomial function. For 2D-problems this polynomial function could be a simple plane, a 2-dimensional parabola, or a more complicated curved surface, etc. To keep the math simple we will limit ourselves here to a 1D problem with the following boundary conditions, $\psi = 0$ at $x = 0$ and $\psi = Vo$ at $x = L$. Furthermore we will assume that the space charge is zero and we will approximate the solution of Laplace's equation in each element by a first order polynomial.

We divide the space between 0 and 1 up in N finite elements and approximate in each finite element ψ by a linear function u i.e.

$$u(x) = b_1 x + a_1 \; for \; 0 < x < x_1 \qquad [14]$$

$$u(x) = b_2 x + a_2 \; for \; x_1 < x < x_2 \qquad [15]$$

$$\vdots$$

$$u(x) = b_n x + a_n \; for \; x_{n-1} < x < x_n \qquad [16]$$

Note that $a_1, a_2, \ldots . a_n$, and $b_1, b_2, \ldots b_n$ are unknowns that depend on the internal estimates for the electric potential at the boundaries between the intervals. The objective is to determine values for

$a_1, a_2, \ldots . a_n$, and $b_1, b_2, \ldots b_n$ so the piece wise linear function u is as close as possible to the real solution of Poisson's equation. From the boundary condition at $x = 0$ we can conclude that $a_1 = 0$. Since ψ is continuous across the space, also *u* should be continuous. If we assume that u_1 is the approximation of ψ at the boundary between element 1 and 2 (i.e. at position x_1), and u_2 is the approximation of ψ at the boundary between element 2 and 3 (i.e at position x_2), etc., we can determine good estimates for a_1, a_2, ….a_n, and b_1, b_2, …b_n from good estimates of ψ at the boundaries between the elements, i.e. from u_1, u_2, … u_n. This leads to the following equations:

$$b_1 = \frac{u_1}{x_1}$$

$$a_2 = u_1 - \frac{u_2 - u_1}{x_2 - x_1} x_1 \qquad b_2 = \frac{u_2 - u_1}{x_2 - x_1}$$

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$$a_n = u_{n-1} - \frac{u_n - u_{n-1}}{x_n - x_{n-1}} x_{n-1} \qquad b_n = \frac{u_n - u_{n-1}}{x_n - x_{n-1}} = \frac{Vo - u_{n-1}}{L - x_{n-1}} \qquad [17]$$

Where in the last equation the boundary condition at $x=L$ is used and in the first expression the boundary condition at $x=0$ is applied. In addition to using the boundary conditions, we also divided the space up in small intervals (defined a mesh) and approximated $\psi(x)$ by a piece-wise linear function using the best estimations of $u(x)$ at the boundaries of each interval as parameters.

Find an expression for F: An expression for the functional provided above can be found from equation [5]. The integral in equation [5] can be split in n integrals, one for each finite element, and then be evaluated using the equations [17]. For this particular 1D case F is given by the following expression:

$$F = \int_0^{x_1} b_1^2 dx + \int_{x_1}^{x_2} b_2^2 dx + \ldots + \int_{x_{n-1}}^{1} b_n^2 dx = b_1^2 x_1 + b_2^2 (x_2 - x_1) + \ldots + b_n^2 (L - x_{n-1}) =$$

$$\frac{(u_1 - 0)^2}{x_1 - 0} + \frac{(u_2 - u_1)^2}{x_2 - x_1} + \ldots + \frac{(V_o - u_{n-1})^2}{L - x_{n-1}} \qquad [18]$$

Minimize *F*: The best estimate for $\psi(x)$ can be found by minimizing *F*, i.e. taking the partial derivatives towards $u_1, u_2, \ldots u_{n-1}$, setting them equal to zero, and solving for $u_1, u_2, \ldots u_{n-1}$. This gives the following set of linear equations:

$$\frac{\partial F}{\partial u_1} = 0 \Leftrightarrow 2\frac{u_1}{x_1} - 2\frac{u_2 - u_1}{x_2 - x_1} = 0$$

$$\frac{\partial F}{\partial u_2} = 0 \Leftrightarrow 2\frac{u_2 - u_1}{x_2 - x_1} - 2\frac{u_3 - u_2}{x_3 - x_2} = 0$$

..

$$\frac{\partial F}{\partial u_{n-1}} = 0 \Leftrightarrow 2\frac{u_{n-1} - u_{n-2}}{x_{n-1} - x_{n-2}} - 2\frac{V_o - u_{n-1}}{L - x_{n-1}} = 0 \qquad [19]$$

Here forth, the *n-1* linear equations can be solved using matrices. The above example assumes there is no space charge. If space charge is present equation [18] needs to be modified, but the algorithm is equivalent.

To solve these equations in the matrix, COMSOL adjusts the approximation functions $u_i(x)$ on each internal boundary until the error function $e(x)$ is below a predetermined tolerance and thus the solutions match at the boundaries. In the approximation to the solution, several iterations are needed to make solutions at the boundaries have a difference below the error tolerance. Incidentally, the solution of Poisson's equation has the lowest electrostatic energy, and therefore it is this solution that also satisfies the differential equations arrived at via variational calculus.