A Point Collocation Method for Meshless Analysis of Microelectronic and Microelectromechanical Devices

N. R. Aluru

3217 Beckman Institute, MC-251
Department of General Engineering
University of Illinois at Urbana-Champaign
Urbana, IL 61801
e-mail: aluru@uiuc.edu, http://www.staff.uiuc.edu/~aluru/

The present approach to modeling and design of microelectronic and microelectromechanical devices (MEMS) (hereafter simply referred to as a microdevice) involves the generation of a geometric model for the complicated two or three-dimensional microdevice, the generation of a mesh for the geometric model, a mesh based numerical analysis, and postprocessing steps such as visualization. The time consuming steps in such an approach are the generation of a mesh and mesh-based numerical analysis. Meshless methods, which do not require the generation of a mesh, are very attractive for numerical solution of partial differential equations. In this paper we introduce a new meshless technique, referred to as a point collocation method, for numerical solution of partial differential equations. The effectiveness of the point collocation method is demonstrated by solving one and two-dimensional Poisson equation, the solution of which is required in the analysis of both electronic and microelectromechanical devices.

1. Introduction

The idea of a meshless or a meshfree method for numerical analysis of partial differential equations is very appealing as a meshfree method does not require the generation of a mesh for complicated two and three dimensional structures. Meshfree methods are even more appealing for emerging technologies such as microelectromechanical systems (MEMS) ([1], [4]) because of the mixed-technology nature of microdevices. For example, if we consider electromechanical systems involving coupled elastic and electrostatic energy domains, one needs to generate a volume mesh for the electromechanical microdevice to perform finite-element based elastic analysis and a surface mesh for the same microdevice to perform exterior electrostatic analysis based on accelerated boundary-element methods [4]. A requirement is that the surface mesh has to be compatible with the volume mesh so one does not have to worry about interpolating solutions from one mesh to another mesh. When a microfluidic energy domain is also encountered, such as in the design of MEMS based accelerometers, three different types of meshes are required. The complexity of mesh generation grows significantly when more than one energy domain is involved and microelectromechanical system designs often involve at least two energy domains.

In this paper we describe a new meshless technique referred to as a point collocation method based on reproducing kernel approximations. Using this technique, the numerical solution of partial differential equations can be performed by simply sprinkling points. This paper is organized as follows: The reproducing kernel technique is introduced in Section 2. The point collocation method based on reproducing kernel approximations is described in Section 3 and numerical results are shown in Section 4.

2. Reproducing Kernel Technique

The key idea in a reproducing kernel method is to construct an approximation $u^a(x, y)$ to $u(x, y)$ by employing a corrected kernel ([2]). In two-dimensions, a corrected kernel approximation can be written as

$$u^a(x, y) = \int_{\Omega} \bar{w}_d(x-s, y-s)u(s)\ ds \tag{1}$$

where $\bar{w}_d(x-s, y-s)$ is the corrected kernel function which is given by

$$\bar{w}_d(x-s, y-s) = C(x, y, s)w_d(x-s, y-s) \tag{2}$$

where $C(x, y, s)$ is a correction function and $w_d(x-s, y-s)$ is the kernel function. If the correction function is taken to be unity i.e. $C(x, y, s) = 1$, then the approximation reduces to the classical smooth particle hydrodynamics technique ([3]). The smooth particle hydrodynamics approach is, however, not a stable method for numerical solution of partial differential equations posed on finite domains.

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The correction function is typically expressed as a linear combination of polynomial basis functions. The highest order polynomial terms to be included in the correction function definition depends on the highest order derivative terms contained in the governing partial differential equations. For second order partial differential equations, a correction function that can exactly reproduce up to second derivatives is

$$C(x, y, s) = c_0 + c_1(x-s) + c_2(y-s) + c_3(x-s)^2 + c_4(y-s)^2 + c_5(x-s)(y-s) \tag{3}$$

where $c_0, c_1, \ldots, c_5$ are the unknown correction function coefficients. Note that if only the first derivative calculation is required, then only the first three coefficients need to be considered in the correction function definition. The correction function coefficients can be determined by establishing the reproducing conditions. To obtain the reproducing conditions, consider a Taylor series expansion for $u(s)$ in two-dimensions

$$u(s) = u(x, y) - (x-s)\frac{\partial u}{\partial x} - (y-s)\frac{\partial u}{\partial y} + \frac{(x-s)^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{(y-s)^2}{2!}\frac{\partial^2 u}{\partial y^2} + (x-s)(y-s)\frac{\partial^2 u}{\partial x \partial y} + \ldots \tag{4}$$

Substituting the expansion for $u(s)$ and the definition of the corrected kernel function given in equation (2) into equation (1), one obtains

$$u^a(x, y) = u(x, y)\overline{m}_0 - \frac{\partial u}{\partial x}\overline{m}_1 - \frac{\partial u}{\partial y}\overline{m}_2 + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\overline{m}_3 + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}\overline{m}_4 + \frac{\partial^2}{\partial x \partial y}(u)\overline{m}_5 \tag{5}$$

where

$$\overline{m}_0 = c_0 m_{00} + c_1 m_{10} + c_2 m_{01} + c_3 m_{20} + c_4 m_{02} + c_5 m_{11} \tag{6}$$

$$\overline{m}_1 = c_0 m_{10} + c_1 m_{20} + c_2 m_{11} + c_3 m_{30} + c_4 m_{12} + c_5 m_{21} \tag{7}$$

$$\overline{m}_2 = c_0 m_{01} + c_1 m_{11} + c_2 m_{02} + c_3 m_{21} + c_4 m_{03} + c_5 m_{12} \tag{8}$$

$$\overline{m}_3 = c_0 m_{20} + c_1 m_{30} + c_2 m_{21} + c_3 m_{40} + c_4 m_{22} + c_5 m_{31} \tag{9}$$

$$\overline{m}_4 = c_0 m_{02} + c_1 m_{12} + c_2 m_{03} + c_3 m_{22} + c_4 m_{04} + c_5 m_{13} \tag{10}$$

$$\overline{m}_5 = c_0 m_{11} + c_1 m_{21} + c_2 m_{12} + c_3 m_{31} + c_4 m_{13} + c_5 m_{22} \tag{11}$$

and

$$m_{ij}(x, y) = \int_{\Omega} (x-s)^i (y-s)^j w_d(x-s, y-s) ds \tag{12}$$

To exactly reproduce the function, we enforce $u^a(x, y) = u(x, y)$. From equation (5), the reproducing conditions for the function can be obtained as

$$\begin{aligned} \overline{m}_0(x, y) &= 1 \\ \overline{m}_k(x, y) &= 0 \qquad k = 1, 2, \ldots, 5 \end{aligned} \tag{13}$$

The unknown correction function coefficients can be determined by satisfying the above moment conditions. Using the definitions given in equations (6) - (11), equation (13) can be written in a matrix form to obtain the correction function coefficients.

$$M\overline{C} = \overline{M} \tag{14}$$

where M is the 6×6 moment coefficient matrix, $\overline{C}$ is the 6×1 unknown coefficient vector and $\overline{M}$ is the known 6×1 right-hand side vector. In a similar manner, the first and the second derivatives of the correction function coefficients can be computed by deriving the reproducing conditions for the first and second derivatives of the function, respectively.

Assuming that the domain Ω is represented by NP distinct points or particles, a discrete approximation for equation (1) can be written as

$$u^a(x, y) = \sum_{I=1}^{NP} \overline{w}_d(x-x_I, y-y_I) u(x_I, y_I) \Delta V_I \tag{15}$$

where x_I, y_I are the x- and y-coordinates of point I, $u(x_I, y_I)$ is a nodal value associated with point I, and ΔV_I is a volume (or area in 2-D) associated with node I. Note that, in general, the value of the unknown function at node I is given by $u^a(x_I, y_I)$ and not $u(x_I, y_I)$. The discrete form of a corrected kernel function is given as

$$\overline{w}_d(x-x_I, y-y_I) = C(x-x_I, y-y_I) w_d(x-x_I, y-y_I) \tag{16}$$

The multidimensional kernel function is constructed as products of one-dimensional kernel functions. In two dimensions

$$w_d(x-x_I, y-y_I) = \frac{1}{d_x} w\left(\frac{x-x_I}{d_x}\right) \frac{1}{d_y} w\left(\frac{y-y_I}{d_y}\right) \tag{17}$$

where d_x, d_y are the dilational parameters along the x and y directions, respectively, and the kernel function is taken as the cubic spline function i.e.

$$w(z_I) = \begin{cases} 0 & z_I < -2 \\ \frac{1}{6}(z_I + 2)^3 & -2 \le z_I \le -1 \\ \frac{2}{3} - z_I^2\left(1 + \frac{z_I}{2}\right) & -1 \le z_I \le 0 \\ \frac{2}{3} - z_I^2\left(1 - \frac{z_I}{2}\right) & 0 \le z_I \le 1 \\ -\frac{1}{6}(z_I - 2)^3 & 1 \le z_I \le 2 \\ 0 & z_I > 2 \end{cases} \tag{18}$$

where $z_I = (x - x_I)/d_x$ for the x-dimensional kernel function and $z_I = (y - y_I)/d_y$ for the y-dimensional kernel function.

3. Point Collocation Method

The key idea in a point collocation approach is to satisfy the governing partial differential equation at each of the points covering the domain of interest. If a Dirichlet or a Neumann boundary condition is imposed on a node that is on the boundary, then an equation that satisfies the boundary condition is developed for the boundary node instead of satisfying the governing partial differential equation.

Let us denote N_d to be the number of points carrying a Dirichlet boundary condition, N_n to be the number of points carrying a Neumann boundary condition and N_r to be the remaining nodes with no boundary conditions. The total number of points covering the domain equals $N_d + N_n + N_r$. To illustrate the point collocation approach, consider the following model problem

$$\begin{aligned} \mathcal{L}u &= f \quad in\ \Omega \\ u &= g \quad on\ \Gamma_g \\ \frac{\partial u}{\partial n} &= h \quad on\ \Gamma_h \end{aligned} \tag{19}$$

where $\mathcal{L}$ is the differential operator, u is the unknown, f is the forcing term, Γ_g is the portion of the boundary where Dirichlet boundary conditions are specified and Γ_h is the portion of the boundary where Neumann boundary conditions are specified. In a point collocation method, the idea is to find an approximate solution $u^a(x, y)$ that approaches the exact solution $u(x, y)$ as the number of points NP increases. $u^a(x, y)$ then satisfies the governing equations in (19)

$$\begin{aligned} \mathcal{L}u^a &= f \quad in\ \Omega \\ u^a &= g \quad on\ \Gamma_g \\ \frac{\partial u^a}{\partial n} &= h \quad on\ \Gamma_h \end{aligned} \tag{20}$$

In a point collocation approach, equation (20) is satisfied at every point or a node. For a node that is in the interior and is not constrained, the collocation approach satisfies the equation

$$\mathcal{L}u^a(x_i, y_i) = f(x_i, y_i) \qquad i = 1, 2, \ldots, N_r \tag{21}$$

For points that are constrained by a Dirichlet boundary condition, the point collocation technique satisfies

$$u^a(x_i, y_i) = g(x_i, y_i) \qquad i = 1, 2, \ldots, N_d \tag{22}$$

and for points with Neumann boundary conditions, the following equation is satisfied

$$\frac{\partial u^a}{\partial n}(x_i, y_i) = h(x_i, y_i) \qquad i = 1, 2, \ldots, N_n \tag{23}$$

Employing a discrete approximation for u^a as given in equation (15), the point collocation approach gives rise to a matrix problem

$$Ku = b \tag{24}$$

where $K \in \Re^{NP \times NP}$ is the coefficient matrix, $u \in \Re^{NP \times 1}$ is the unknown vector and $b \in \Re^{NP \times 1}$ is the known right-hand side vector.

4. Results

The first example we will consider is a one dimensional problem with a known exact solution. The governing equation is

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= 2 \qquad 0 < x < 2 \\ u(0) &= 0 \\ u(8) &= 64 \end{aligned} \tag{25}$$

The exact solution is given by

$$u(x) = x^2 \tag{26}$$

The point collocation method for this problem gives nodally exact results. A random distribution of 11 points is considered and the distribution of the points is as shown in Figure 1. Note that some points are very close to each other

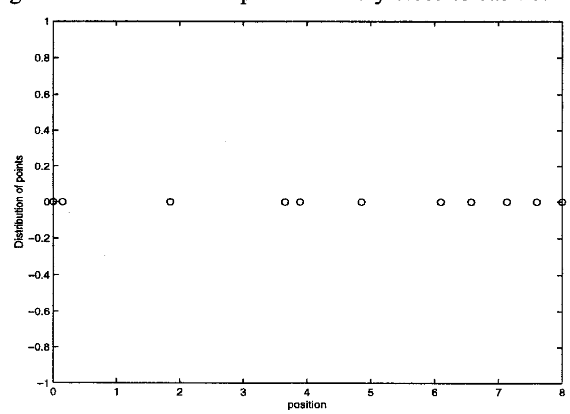

Figure 1 Random point distribution for one-dimensional analysis of the Poisson equation

and this does not pose any problem to the point collocation method. The computed solution is shown in Figure 2. The numerical solution and its derivative match exactly with the exact solutions.

The next example is a two-dimensional Poisson problem with a constant forcing term. The governing equation is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 4 \qquad 0 < x < 2 \qquad 0 < y < 2 \tag{27}$$

and Dirichlet boundary conditions are applied along the four edges

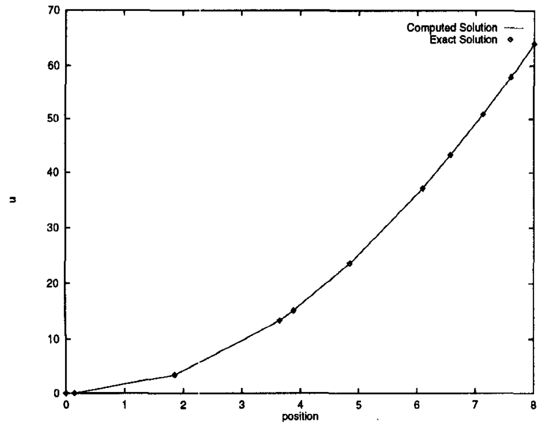

Figure 2 Numerical solution, u, matches the exact solution

$$\begin{aligned} u(x=0) &= y^2 \\ u(x=2) &= 4+y^2 \\ u(y=0) &= x^2 \\ u(y=2) &= 4+x^2 \end{aligned} \tag{28}$$

The exact solution for this Dirichlet Poisson problem is given by

$$u(x,y) = x^2+y^2 \tag{29}$$

The point collocation method, for all discretizations, produces the exact solution. We show results again for a random distribution of points, which is shown in Figure 3. The

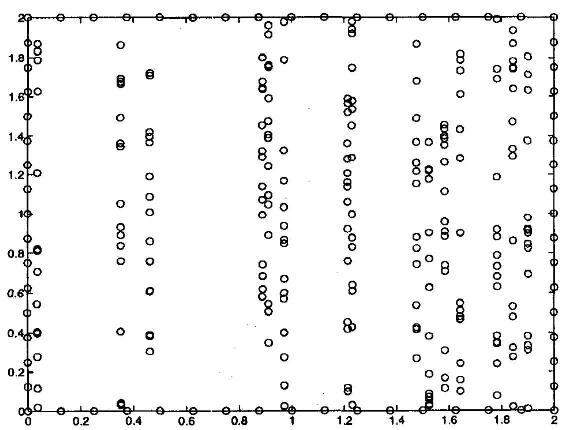

Figure 3 A random point distributions considered for the solution of the two-dimensional Poisson equation

solution, u, obtained with the random discretizations is shown in Figure 4. The computed solution matches with the exact solution. The computed derivatives also match with the exact derivatives. From this example we can conclude that the point collocation method exactly reproduces a quadratic solution for a Dirichlet Poisson problem. Even though we do not show the results here, a point collocation method can also exactly reproduce a linear solution for a Dirichlet Poisson

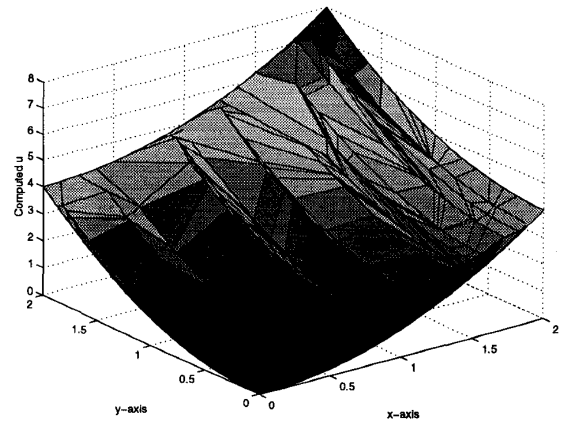

Figure 4 Computed solution obtained with a random distribution of points.

problem. A closer look at the random distribution of points in Figure 3 shows that some points are positioned very close to each other. The point collocation method is not sensitive to such point distributions and exact solutions are obtained for all point distributions for this Dirichlet Poisson problem

5. Conclusion

A point collocation method is described in this paper for analysis of one and two-dimensional partial differential equations. Numerical results are shown for a Poisson equation and the accuracy of the point collocation method is established. The results indicate that the point collocation method is a promising technique for meshless analysis of electronic and microelectromechanical devices.

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