A Finite Point Method Based on Directional Derivatives for Diffusion Equation

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Abstract—This paper presents a finite point method based on directional derivatives for diffusion equation on 2D scattered points. To discretize the diffusion operator at a given point, a six-point stencil is derived by employing explicit numerical formulae of directional derivatives, namely, for the point under consideration, only five neighbor points are involved, the number of which is the smallest for discretizing diffusion operator with first-order accuracy. A method for selecting neighbor point set is proposed, which satisfies the solvability condition of numerical derivatives. Some numerical examples are performed to show the good performance of the proposed method.

Keywords—Finite point method, directional derivatives, diffusion equation, method for selecting neighbor point set.

I. INTRODUCTION

In recent years, the meshless methods have become an alternative to the classical mesh methods and made great progress in scientific and engineering computational problems. In this field, the strong-form meshless methods have attracted much attention, since they are inherent meshless, simple and straightforward. The finite point method (FPM) [1]-[5] employed in the present paper falls into this category.

In essence, the FPM can be viewed as the finite difference method (FDM) to solving partial differential equations (PDEs) on scattered points. Compared with the classical finite difference method on the uniform point distribution, the FPM is more difficult to perform due to disorders of scattered points. The first difficulty lies in the approximation to the derivatives of a smooth function by using the information of a given point and its neighbor points. In Taylor expansion framework, there are always two approaches to approximate derivatives. One [7], [8] is employing just adequate points to solve for derivatives in Taylor series. This approach is always encountered the problem of singularity. The other [3]-[6] is employing much more points than unknowns to ensure the existence of inverse matrix and the matrix being well-conditioned, such as in the classical least squares (LSQ) method, the weighting least squares (WLS) method and the moving least squares (MLS) method. In this procedure, it seems that singularity issue seldom emerges, however, too much points lead to a large stencil which seriously affects the computational efficiency. Besides this, the number of points employed has not an optimal value in theory, hence is always determined by numerical experiments.

In [1], by using the information of the master point and only five proper neighbor points, L. Shen et al. derive the explicit formulae for approximating the first-order and second-order directional derivatives with second-order and first-order accuracy, respectively. Above all, solvability conditions of numerical derivatives are explicitly given and discussed in detail, which give a general guiding principle for selecting five neighbors. In [2], based on the method employed in [1], new formulae for the second-order mixed directional derivatives are presented.

This paper will apply the methods employed in [1] and [2] to numerically solving diffusion equations. Also, we will present a method for selecting neighbor points.

In later discussion, we consider the diffusion equation in the form

$$\nabla \cdot (\kappa(x,y)\nabla u) = f(x,y), \quad (x,y) \in \Omega$$

(1)

with Dirichlet boundary condition

$$u(x,y) = g(x,y), \quad (x,y) \in \partial \Omega,$$

(2)

where $\Omega$ is the computational domain with boundary $\partial \Omega$, $\kappa(x,y)$ is the diffusion coefficient which may be discontinuous, and $f, g$ are proper smooth functions given by relevant problems.

The rest of this paper is organized as follows: Section II recalls the methods in [1] and [2]; Section III presents a new method for numerically solving diffusion equations; Section IV designs a method for selecting neighbor point set; Section V performs numerical examples to show the good performance of the proposed method; conclusions are drawn in Section VI.

II. THE FPM BASED ON DIRECTIONAL DERIVATIVES

In this section, we briefly present the FPM Based on directional derivatives [1].

Let us introduce some denotations and definitions following [1]. Denote by $i$ the index of point $(x_i, y_i)$, $O$ a specific point, and $\Delta l_i$ the distance from "$i"$ to "$O$". We also have the following:

- $(i \ j \ k) := \sin(k \ i, k \ j)$, and $(i \ j \ k) := \cos(k \ i, k \ j)$. Specially, $(i \ j) := (i \ O)$, and $(i \ j) := (i \ O)$.

- $(i \ j) = \frac{1}{2} (i \ j \ k) \Delta l_i \Delta l_j$. Specially, $(i \ j) := (i \ j \ O)$.
Definition 1 (Algorithm (1)) Given $i, j, k$ ($k \geq 3$) positive integers, an addition of $i$ and $j$ with period of $k$ is defined by

$$i \oplus j = i + j - sk,$$

where $s$ is a positive integer satisfying inequality $sk < i + j \leq (s + 1)k$.

Let $I = \{1, 2, 3, 4, 5\}$, for $i \in I$, denote

- $(i^+) = \{i_1, i_2, i_3, i_4, i_5\}$
- $(i^-) = \{i_1, i_4, i_3, i_2, i_5\}$

Define two functions of indices

$$\xi(i_1, i_2, i_3, i_4, i_5) = \xi(i_1, i_2, i_4, i_3, i_5),$$
$$\eta(i, j) = \text{sgn}(i - j)(-1)^{i+j}(i - j)(i_1, i_2, i_3, i_4, i_5),$$

where $i_1, i_2, i_3, i_4, i_5 \in I$, $i, j \in I$, and $k_1 < k_2 < k_3$.

Suppose that for point $O$ and its five neighbor points $1, \ldots, 5$ numbered freely (see Fig. 1), the differences $\Delta \xi(i = 1, \ldots, 5)$ of the smooth function $u(x, y)$ are available. Then numerical formulae termed five-point formulae for the first- and second-order directional derivatives of the smooth function $u(x, y)$ at point $O$ are derived.

Theorem 1 (five-point formulae of the first-order directional derivatives) Given point $O$ and its five neighbor points numbered $1, \ldots, 5$, if the condition of uniform steplengths as

(C1) For $\Delta \xi(i = 1, 2, \ldots, 5) \rightarrow 0$, there exists a constant $\alpha$, $0 < \alpha < 1$, that always satisfies

$$\alpha \max_{1 \leq i \leq 5} \Delta \xi_i \leq \min_{1 \leq i \leq 5} \Delta \xi_i,$$

and the solvability condition as

$$M \neq 0$$

are satisfied, then the first-order derivatives of the smooth function $u(x, y)$ can be approximated with the second-order truncation error as

$$\frac{\partial u}{\partial l_i} = \frac{1}{M \Delta l_i} \sum_{j=1}^{5} a_{ij} \Delta u_j + O(\Delta l^2), \quad i = 1, \ldots, 5,$$

where

$$a_{ij} = \left\{ \begin{array}{ll} \xi(i^+) + \xi(i^-), & i = 1, \ldots, 5, \ j = i, \\ \eta(i, j), & i = 1, \ldots, 5, \ j \in I \setminus \{i\}, \end{array} \right.$$ 

and

$$M = (23)\langle 41 \rangle\langle 125 \rangle\langle 345 \rangle - (12)\langle 34 \rangle\langle 235 \rangle\langle 415 \rangle.$$ 

Theorem 2 (five-point formulae of the second-order directional derivatives) Under the same conditions as Theorem 1, the second-order derivatives of the smooth function $u(x, y)$ can be approximated with the first-order truncation error as

$$\frac{\partial^2 u}{\partial l_i^2} = \frac{2}{M \Delta l_i^2} \sum_{j=1}^{5} b_{ij} \Delta u_j + O(\Delta l), \quad i = 1, \ldots, 5,$$

where

$$b_{ij} = \left\{ \begin{array}{ll} M - a_{ij}, & i = 1, \ldots, 5, \ j = i, \\ -a_{ij}, & i = 1, \ldots, 5, \ j \in I \setminus \{i\}, \end{array} \right.$$ 

and the expressions of $a_{ij}$ and $M$ are as given in (5) and (6), respectively.

In [1], the authors express the Laplace operator by three second-order derivatives in three nonparallel directions, i.e.

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = - \left( \left( \begin{array}{cc} 2 & 3 \\ 1 & 2 \end{array} \right) \frac{\partial^2 u}{\partial l_1^2} + \left( \begin{array}{cc} 3 & 1 \\ 1 & 2 \end{array} \right) \frac{\partial^2 u}{\partial l_2^2} \right)
\left( \begin{array}{cc} (2 & 3) \\ (2 & 3) \end{array} \right) \frac{\partial^2 u}{\partial l_3^2} ,$$

and then employ the aforementioned formulae to derive the discrete scheme for the Laplace operator.

In the present paper, we will employ two nonparallel directions to express a general diffusion operator, and design a method for selecting neighbor point set other than the one in [1]. To this end, we need the following Lemma [1].

Lemma 1 Suppose that two directions $\overrightarrow{l_1}, \overrightarrow{l_2}$ are non-parallel. If $\overrightarrow{l_3}$ is another direction, then for $(x, y) \in \Omega$ the following relation is established:

$$\frac{\partial^m u(x, y)}{\partial l_3^m} = \left(12\right)^{-m} \sum_{k=0}^{m} C_{m}^{k} \frac{\partial^m u(x, y)}{\partial l_1^{m-k} \partial l_2^k} ,$$

where $C_{m}^{k} = \frac{m(m-1)\cdots(m-k+1)}{k!}$. By employing (10), we have

$$(12)^2\frac{\partial^2 u}{\partial x^2} = (2x)^2\frac{\partial^2 u}{\partial l_1^2} + 2(2x)(x) \frac{\partial^2 u}{\partial l_1 \partial l_2} + (x)^2\frac{\partial^2 u}{\partial l_2^2} ,$$

and

$$(12)^2\frac{\partial^2 u}{\partial y^2} = (2y)^2\frac{\partial^2 u}{\partial l_1^2} + 2(2y)(y) \frac{\partial^2 u}{\partial l_1 \partial l_2} + (y)^2\frac{\partial^2 u}{\partial l_2^2} .$$
hence by simple operation, we have
\[
\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \left(1 - \frac{1}{2^2}\right) \left(\frac{\partial^2 u}{\partial l_1^2} - 2\left(1 - \frac{1}{2^2}\right) \frac{\partial^2 u}{\partial l_1 \partial l_2} + \frac{\partial^2 u}{\partial l_2^2}\right),
\]
(11)
where \((1 2) \neq 0\).

To discretize the diffusion operator, the approximation of the second order mixed derivatives \([2]\) is required.

Suppose that \(l_1, l_2, l_3\) are three nonparallel directions, then by (10), \(\frac{\partial^2 u}{\partial l_1 \partial l_2}\) is expressed by
\[
2(3)(3 1) \frac{\partial^2 u}{\partial l_1 \partial l_2} \Delta l_1 \Delta l_2 = -(2 3)^2 \frac{\partial^2 u}{\Delta l_1^2} - (3 1)^2 \frac{\partial^2 u}{\Delta l_2^2} + (1 2)^2 \frac{\partial^2 u}{\Delta l_3^2}.
\]
Consequently, using (7) gives the approximation of \(\frac{\partial^2 u}{\partial l_1 \partial l_2}\) immediately, i.e.,
\[
\frac{\partial^2 u}{\partial l_1 \partial l_2} = \frac{1}{M \Delta l_1 \Delta l_2} \sum_{j=1}^{5} c_j \Delta u_j + O(\Delta l),
\]
(12)
where \(M\) is as given in (6), and the detailed expressions of \(c_j (j = 1, \ldots, 5)\) can be found in [2].

III. DISCRETIZATION METHOD

Suppose that \(\kappa(x, y)\) is sufficiently smooth, rewrite the diffusion operator in (1) as
\[
\nabla \cdot (\kappa(x, y) \nabla u) = \frac{\partial u}{\partial x} \left(\kappa(x, y) \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \kappa(x, y) \frac{\partial u}{\partial y}\right)
\]
(13)
By using (10), \(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\) can be expressed by two nonparallel directional derivatives \(\frac{\partial u}{\partial l_1}\) and \(\frac{\partial u}{\partial l_2}\)
\[
\frac{\partial u}{\partial x} = \left(1 - \frac{1}{2^2}\right) \left(2 \frac{\partial u}{\partial l_1} + (1 \times 2) \frac{\partial u}{\partial l_2}\right),
\]
\[
\frac{\partial u}{\partial y} = \left(1 - \frac{1}{2^2}\right) \left(2 \frac{\partial u}{\partial l_1} + (1 \times y) \frac{\partial u}{\partial l_2}\right).
\]
(14)
Therefore, by using (11) and (14), (13) is reformed as
\[
\nabla \cdot (\kappa(x, y) \nabla u) = \frac{1}{M \Delta l_1 \Delta l_2} \sum_{j=1}^{5} c_j \Delta u_j + \frac{\partial u}{\partial x} \kappa(x, y) \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \kappa(x, y) \frac{\partial u}{\partial y} + O(\Delta l),
\]
(15)
Note that \(\kappa(x, y)\) is a known function, so \(\frac{\partial \kappa(x, y)}{\partial x}, \frac{\partial \kappa(x, y)}{\partial y}\) can be analytically expressed.

Hence, at a given point \(O\) with five proper neighbors indexed by \(1, 2, 3, 4, 5\), using (4), (7) and (12) leads to the discrete scheme to the diffusion operator as
\[
\left(\nabla \cdot (\kappa(x, y) \nabla u)\right)_O = \frac{1}{M \Delta l_1 \Delta l_2} \sum_{j=1}^{5} \Delta u_j \left\{ \frac{2 \kappa(x, y)}{(1 2) \Delta l_1} \frac{b_{1j}}{\Delta l_1} + \frac{\kappa(x, y)}{(1 2) \Delta l_1} \left(-\frac{1}{2} c_j\right) \right\} + \left(\begin{array}{c}
(x 2) \frac{\partial \kappa(x, y)}{\partial x} + (y 2) \frac{\partial \kappa(x, y)}{\partial y}
\end{array}\right) \left(\begin{array}{c}
a_{11} \frac{\partial u}{\partial l_1}
\end{array}\right) + \left(\begin{array}{c}
(x 1) \frac{\partial \kappa(x, y)}{\partial x} + (y 1) \frac{\partial \kappa(x, y)}{\partial y}
\end{array}\right) \left(\begin{array}{c}
a_{22} \frac{\partial u}{\partial l_2}
\end{array}\right).
\]
(16)
where \(\kappa(x, y), \frac{\partial \kappa(x, y)}{\partial x}, \frac{\partial \kappa(x, y)}{\partial y}\) are defined at point \(O\).

Obviously, (16) gives a stencil just involving six points, and it is interesting that (16) degenerates into the classical FD scheme on the uniform distributed points.

If \(\kappa(x, y)\) is discontinuous, (1) is no longer satisfied at the multimedia interface, while interface joint condition holds, i.e. \(\kappa^+ \frac{\partial u}{\partial x} = -\kappa^- \frac{\partial u}{\partial x}\) - here, superscripts ‘+’ and ‘-’ refer to quantities on two sides of interface, and \(\kappa\) is a vector normal to the interface. Our strategy is to place points on the interface, and at every point on the interface, discretize \(\frac{\partial u}{\partial l_1}\) and \(\frac{\partial u}{\partial l_2}\) by selecting neighbor points (e.g., selecting five neighbor points) at single side of the interface, respectively, and then discretize the interface joint condition. Detailed discussion will be presented elsewhere.

The discretized interface joint condition and (16) build up a global linear system, which can be solved by some classical linear solvers (e.g., GMRES, BiCGSTAB).

IV. SELECTING NEIGHBOR POINTS

In above discussion, the solvability condition \(M \neq 0\) is always supposed true. In practical computation, to keep the numerical process stable, \(|M| \geq C > 0 (C\) is a positive constant) should be satisfied for every point. In a method for selecting neighbor point set, both distances and angles should be taken into consideration and be well balanced. Therefore, rewrite \(M\) as
\[
M = M^* \Delta l_1 \Delta l_2 \Delta l_3 \Delta l_4 \Delta l_{15} \Delta l_{25} \Delta l_{35} \Delta l_{45},
\]
where
\[
M^* = (2 3)(4 1)(1 2 5)(3 4 5) - (1 2)(3 4)(2 3 5)(4 1 5).
\]
Obviously, the size of \(M^*\) mirrors angle measure. Now, we can design a method for selecting neighbor point set. First of all, for any point \(i\), prepare a point set denoted by \(G_i\) including point \(i\) and its neighbor points about 20. In computation procedure of diffusion problems, as scattered points are fixed, background grids can be introduced to quickly define \(G_i\). For point \(i\), select its neighbor points in \(G_i\) as follows:

**Step 1:** select a nearest point to “1” in \(G_i\), as "1."
Step 2: select a nearest point to "i" in $G_i$ as "2" which satisfies $(1\ 2) \geq \sin \alpha_0$, where $\alpha_0$ is a parametric angle.

Step 3: select a nearest point to "i" in $G_i$ as "3" which satisfies $(2\ 3) \geq \sin \alpha_0$.

Step 4: select a nearest point to "i" in $G_i$ other than "1", "2" and "3" as "4", and if $(1\ 3) = 0$ then $(3\ 4) \geq \sin \alpha_0$ should be satisfied.

Step 5: select a nearest point to "i" in $G_i$ other than "1", "2", "3" and "4" as "5" which satisfies $|M^*| \geq C_0$, where $C_0$ is a positive constant always given by $C_0 = 0.1$ in practical application.

Note that, for a multimedia diffusion problem, five neighbors of point $i$ should be limited in a single media.

V. NUMERICAL RESULTS

Suppose that $\Omega$ is discretized by scattered points $\{(x_i, y_i), i = 1, 2, \ldots, N\}$, and $N$ is the total number of discrete points. Define the discrete norm error by

$$E_N^2 = \left\{ \sum_{i=1}^{N} (U_i - u(x_i, y_i))^2/N \right\}^{1/2},$$

$$E_N^\infty = \max_{1 \leq i \leq N} |U_i - u(x_i, y_i)|,$$

where $U_i$ and $u(x_i, y_i)$ are the numerical solution and the exact solution, respectively.

To investigate the convergence, we first define an average distance

$$h = \sqrt{S/N},$$

where $S$ is the area of $\Omega$.

The convergence rate of the method is given by

$$\text{Rate} = \frac{\log E_{N_1}^N - \log E_{N^2}^N}{\log h_1 - \log h_2},$$

where $h_1$ and $h_2$ are corresponding to $N_1$ and $N_2$, respectively.

The following test example is rebuilt from [9].

Example 1. Solve the equation

$$\begin{cases} \Delta u = f, & (x, y) \in \Omega, \\ u(x, y) = g, & (x, y) \in \partial\Omega, \end{cases}$$

where $\Omega = \{(x, y)|\ 0 \leq x^2 + y^2 \leq 1\}$, and $f$, $g$ are given by the exact solution $u(x, y) = \frac{25}{25(x-0.2)^2+y^2}$. The point distribution in $\Omega$ is shown in Fig. 2.

The corresponding convergence results are presented in Tables I-III.

<table>
<thead>
<tr>
<th>Table I</th>
<th>Errors for solution $u$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$E_N^2$</td>
</tr>
<tr>
<td>221</td>
<td>1.8234E-005</td>
</tr>
<tr>
<td>841</td>
<td>5.0510E-006</td>
</tr>
<tr>
<td>1861</td>
<td>2.4716E-006</td>
</tr>
<tr>
<td>3281</td>
<td>1.4697E-006</td>
</tr>
<tr>
<td>7321</td>
<td>6.4173E-007</td>
</tr>
<tr>
<td>Rate</td>
<td>1.91</td>
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<table>
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<tr>
<th>Table II</th>
<th>Errors for $\partial u/\partial x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$E_N^2$</td>
</tr>
<tr>
<td>221</td>
<td>2.6275E-005</td>
</tr>
<tr>
<td>841</td>
<td>7.4451E-006</td>
</tr>
<tr>
<td>1861</td>
<td>3.4563E-006</td>
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<tr>
<td>Rate</td>
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<table>
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<th>Table III</th>
<th>Errors for $\partial u/\partial y$</th>
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<tr>
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<td>2.9898E-006</td>
</tr>
<tr>
<td>Rate</td>
<td>2.01</td>
</tr>
</tbody>
</table>

In Tables I-III, it is shown that the approximation to the solution is almost second-order accuracy, and to the first-order directional derivatives of the solution is more than first-order accuracy.
Example 2. Solve the equation (from [10])
\[
\begin{align*}
-\Delta u &= (6 + 4x^2 + 16y^2)e^{(x^2+2y^2)}, \quad (x, y) \in \Omega, \\
u(x, y) &= -e^{(x^2+2y^2)}, \quad (x, y) \in \partial \Omega,
\end{align*}
\]
where \( \Omega = [0, 1] \times [0, 1] \) and the exact solution is \( u = -e^{(x^2+2y^2)} \).

The point distribution is shown in Fig. 3.

The purpose of this example is to compare the FPM with the classical Least Square method (LSQ). In LSQ, neighbor points are the nearest ones, the number of which is about 10.

The convergence rates are graphically depicted in Fig. 4.

In Fig. 4, it appears that the FPM has almost the same convergence rate as that of the LSQ, and the FPM is with higher accuracy. Besides, more neighbor points selected in LSQ lead to a large discrete stencil which consequently results in low computational efficiency.

Example 3. Solve the equation with discontinuous diffusion coefficient (from [10])
\[
\begin{align*}
-\nabla \cdot (\kappa(x,y) \nabla u) &= f, \quad (x, y) \in \Omega, \\
u(x, y) &= g, \quad (x, y) \in \partial \Omega,
\end{align*}
\]
where \( \kappa(x,y) = \begin{cases} 1, & 0 < x \leq 0.5, \\ \kappa, & 0.5 < x < 1, \end{cases} \)
and \( f, g \) are computed from the known solution \( u = 1 + x + y + (x - 0.5)e^{x+y} \) for \( 0 < x \leq 0.5 \), \( u = 3\kappa - 1 + \frac{x}{2\kappa} + \kappa + y + (x - 0.5)^2e^{x+y} \) for \( 0.5 < x < 1 \).

The point distribution is almost the same as that of Example 2, but at \( x = 0.5 \) uniformly distributed points are placed to coincide with the multimedia interface (shown in Fig. 5).

In Fig. 5, it appears that the FPM has almost the same convergence rate as that of the LSQ, and the FPM is with high accuracy. Besides, more neighbor points selected in LSQ lead to a large discrete stencil which consequently results in low computational efficiency.

Tables IV, V show that the solutions to the diffusion equation with discontinuous coefficient are second-order accurate, which verify the good performance of the proposed method.
VI. CONCLUSION

This paper presents a method to numerically solving diffusion equation by the FPM, which results in a six-point stencil to discretize diffusion operator. Numerical experiments demonstrate that the proposed method is second-order accurate and is better than the LSQ method. The method can be generalized to a general elliptic equation. The method for selecting neighbor point set is an interesting and important topic which is in our ongoing work.

ACKNOWLEDGMENT

The authors would like to thank the support by the National Natural Science Foundation of China(10871029, 11071025), the Foundation of CAEP(2010A0202010) and the Foundation of LCP.

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