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A NODAL METHOD FOR ABSORPTION - DIFFUSION PROBLEMS

M. ASADZADEH[*] AND A. SOPASAKIS[†]

Abstract. We construct a nodal method for a two dimensional absorption–diffusion problem. The method gives rise to a seven point stencil for which the truncation error analysis shows an accuracy of at least $O(\Delta^2)$. We devise a numerical method which constructs a matrix whose entries are amplified according to contributions from each of the nodes in a rectangular domain. Numerical implementations are provided for selected examples where the exact solutions are known for comparison purposes.

Key words. Nodal method, diffusion, absorption, consistency, truncation error

AMS subject classifications. 65N22, 65N99

1. Introduction . The purpose of this paper is to construct and implement a nodal diffusion method for an absorption-diffusion problem in a two-dimensional convex polygonal domain Ω associated with some boundary conditions:

$$\begin{cases} -\mathrm{div}(D \cdot \nabla\phi) + \sigma_a \phi = 0, & \text{in} \quad \Omega, \\ \alpha\phi + \beta(n \cdot \nabla\phi) = S, & \text{on} \quad \partial\Omega, \end{cases} \tag{1.1}$$

where $D = D(x, y)$ is a piecewise smooth coefficient, σ_a is an absorption coefficient, α and β are certain parameters to determine the character of the boundary condition. Finally $S = S(x, y)$ is a smooth source function and $n = n(x, y)$ is the outward unit normal to the boundary at the point $(x, y) \in \partial\Omega$. Problem (1.1) arise, e.g. as a diffusion approximation of a particle transport equation governed by absorption, scattering and fission events. Nodal methods are often applied in discretizing particle transport equations and are studied in various settings, e.g. a self-consistent nodal method is considered in [1] and variational nodal methods are studied in [2]–[4]. Numerical analysis of the nodal methods are, mostly, due to the works by Hennart and his group where they analyze also different hybrids with both finite element and finite difference schemes, see ,e.g. [5], [6] and [7]. Other related studies can be found, e.g. in [8]–[11]. Our goal in this work is to derive a consistent second order nodal diffusion scheme approximating an absorption-diffusion problem with piecewise smooth diffusion coefficient. We implement the problem in two settings; in an absorption-free and also full absorption-diffusion case. The absorption-free assumption is for simplicity reasons. Otherwise the absorption term is regularizing and the results of absorption-free case would obviously be valid for the full absorption-diffusion problem.

An outline of this paper is as follows: we start in Section 2 by presenting a nodal method for a general absorption–diffusion problem in two dimensions. We construct a seven point scheme which will be used in the numerical implementations. We analyze the consistency of the scheme in Section 3. Subsequently, in Section 4 we consider the absorption-free case and we present a succinct truncation analysis of it in Section 5. In Section 6 we introduce the idea of implementing a solution to the nodal method which is suitable for seven point stencils in general and is therefore not restricted to just this nodal method in particular. Two examples are subsequently presented which

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are chosen specifically for benchmark and comparison purposes since their solutions are known. In the first example, in Subsection 6.1 we solve a very simple constant coefficients Laplacian. Then in Subsection 6.2 the full example of an absorption - diffusion problem with variable coefficients is presented and solved. Some concluding comments are presented in Section 7.

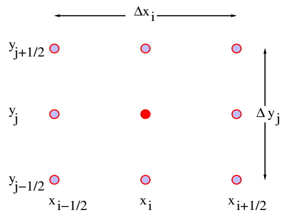
2. The Problem and the Method. We consider a general two–dimensional absorption–diffusion problem,

$$\frac{\partial}{\partial x}\left(D_1(x,y)\frac{\partial\phi(x,y)}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_2(x,y)\frac{\partial\phi(x,y)}{\partial y}\right) - \sigma_a(x,y)\phi(x,y) = 0, \tag{2.1}$$

on a rectangular domain $\Omega := \{(x, y) : 0 < x < X, 0 < y < Y\}$, with a non-negative absorption coefficient ($\sigma_a \geq 0$) associated with a Robin type boundary condition:

$$\alpha\phi + \beta\underline{n} \cdot \underline{\nabla} = S. \tag{2.2}$$

We develop a nodal method for this problem which will be based on the usual current unknowns. To begin with, we impose a grid. The unknowns are the scalar fluxes and currents on the cell edges. The configuration and definition of the unknowns is provided below.



where

$$x_i = \frac{1}{2}(x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}})$$
$$y_j = \frac{1}{2}(y_{j+\frac{1}{2}} + y_{j-\frac{1}{2}})$$
$$\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$$
$$\Delta y_j = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$$

$$\phi_{i+\frac{1}{2},j} = \lim_{x \to x_{i+\frac{1}{2}}} \frac{1}{\Delta y_j}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \phi(x,y)dy, \tag{2.3}$$

$$J_{i+\frac{1}{2},j} = -\lim_{x \to x_i+\frac{1}{2}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} D_1(x,y)\frac{\partial\phi}{\partial x}(x,y)dy, \tag{2.4}$$

$$\phi_{i,j+\frac{1}{2}} = \lim_{y \to y_{j+\frac{1}{2}}} \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \phi(x,y)dx, \tag{2.5}$$

$$J_{i,j+\frac{1}{2}} = -\lim_{y \to y_{j+\frac{1}{2}}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} D_2(x,y)\frac{\partial\phi}{\partial y}(x,y)dx. \tag{2.6}$$

Note that the underlying mesh is a uniform rectangular grid with the element size $\Delta x \times \Delta y$ and with a hexagonally coupled mesh of seven point stencil (6 vertices plus the center). We also note that the integrals on the right side of (2.3) and (2.4) are continuous functions of x, while the integrals on the right side of (2.5) and (2.6) are continuous functions of y.

Operating on (2.1) by $\frac{1}{\Delta y_j}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}(\cdot)dy$, we obtain,

$$\frac{d}{dx}\left(D_{1,ij}\frac{d}{dx}\phi_j(x)\right)-\sigma_{a,ij}\phi_j(x)=-\frac{1}{\Delta y_j}D_{2,ij}\left[\frac{\partial\phi}{\partial y}(x,y_{j+\frac{1}{2}})-\frac{\partial\phi}{\partial y}(x,y_{j-\frac{1}{2}})\right]. \quad (2.7)$$

We assumed that D_1, D_2 and σ_a are constant for sufficiently small $\Delta x\times\Delta y$. We also define $D_{n,ij}$ and ϕ_j viz:

$$D_{n,ij}=D_n(x,y),\ \text{for}\quad x_{i-\frac{1}{2}}<x<x_{i+\frac{1}{2}},\ y_{j-\frac{1}{2}}<y<y_{j+\frac{1}{2}},\quad n=1,2. \quad (2.8)$$

$$\phi_j(x)=\frac{1}{\Delta y_j}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}\phi(x,y)dy,\ \text{for}\ x_{i-\frac{1}{2}}<x<x_{i+\frac{1}{2}}. \quad (2.9)$$

Note that, due to assumptions on D and σ_a (2.7) is exact. Now, using (2.6), we approximate the right hand side of (2.7) by replacing it by its average value over x and taking a limit in y. We therefore obtain for $x_{i-\frac{1}{2}}<x<x_{i+\frac{1}{2}}$,

$$\begin{aligned} D_{1,ij}\frac{d^2}{dx^2}\phi_j(x)-\sigma_{a,ij}\phi_j(x) &\approx \frac{1}{\Delta y_j}\left[\frac{1}{\Delta x_i}J_{i,j+\frac{1}{2}}-\frac{1}{\Delta x_i}J_{i,j-\frac{1}{2}}\right] \quad (2.10)\\ &= \frac{1}{\Delta x_i\Delta y_j}(J_{i,j+\frac{1}{2}}-J_{i,j-\frac{1}{2}}). \end{aligned}$$

Applying the boundary condition, $\phi_j(x_{i\pm\frac{1}{2}})=\phi_{i\pm\frac{1}{2},j}$ (see Eqs. (2.3) and (2.9)) and defining $l_{1,ij}=\sqrt{\frac{\sigma_{a,ij}}{D_{1,ij}}}$ we write the solution for (2.10) as follows,

$$\phi_j(x)=-\frac{J_{i,j+\frac{1}{2}}-J_{i,j-\frac{1}{2}}}{D_{1,ij}\Delta x_i\Delta y_j}+C_1e^{l_{1,ij}x}+C_2e^{-l_{1,ij}x}. \quad (2.11)$$

with $C_1\equiv C_1(J_{i,j-\frac{1}{2}},J_{i,j+\frac{1}{2}})$ and $C_2\equiv C_2(J_{i,j-\frac{1}{2}},J_{i,j+\frac{1}{2}})$ are provided in detail in the Appendix.

Our main objective will be to establish equations in the unknown J. To this end we operate on (2.11) obtaining,

$$\frac{d}{dx}\phi_j(x)=C_1l_{1,ij}e^{l_{1,ij}x}-C_2l_{1,ij}e^{-l_{1,ij}x}.$$

Evaluating the above at $x=x_{i\pm\frac{1}{2}}$ and applying (2.4) we get,

$$-J_{i+\frac{1}{2},j}=a_1\phi_{i-\frac{1}{2},j}+b_1\phi_{i+\frac{1}{2},j}+c_1J_{i,j+\frac{1}{2}}-c_1J_{i,j-\frac{1}{2}}, \quad (2.12)$$

$$-J_{i-\frac{1}{2},j}=-b_1\phi_{i-\frac{1}{2},j}-a_1\phi_{i+\frac{1}{2},j}-c_1J_{i,j+\frac{1}{2}}+c_1J_{i,j-\frac{1}{2}}, \quad (2.13)$$

Note: all coefficients for these equations and those that will follow are provided in the Appendix unless otherwise specified.

Now, going through exactly the same procedure, except transverse – integrating in the y-direction rather than the x-direction, we obtain the following "rotated" version of (2.12) and (2.13),

$$-J_{i,j+\frac{1}{2}}=c_2J_{i+\frac{1}{2},j}-c_2J_{i-\frac{1}{2},j}+b_2\phi_{i,j+\frac{1}{2}}+a_2\phi_{i,j-\frac{1}{2}}, \quad (2.14)$$

$$-J_{i,j-\frac{1}{2}}=-c_2J_{i+\frac{1}{2},j}+c_2J_{i-\frac{1}{2},j}-a_2\phi_{i,j+\frac{1}{2}}-b_2\phi_{i,j-\frac{1}{2}}, \quad (2.15)$$

It is now possible to solve for the J's in equations (2.12-2.15). Thus obtaining,

$$J_{i+\frac{1}{2},j}=E_1\phi_{i-\frac{1}{2},j}+E_2\phi_{i+\frac{1}{2},j}+E_3\phi_{i,j+\frac{1}{2}}+E_3\phi_{i,j-\frac{1}{2}} \quad (2.16)$$

$$J_{i-\frac{1}{2},j}=E_4\phi_{i-\frac{1}{2},j}-E_4\phi_{i+\frac{1}{2},j}-E_3\phi_{i,j+\frac{1}{2}}-E_3\phi_{i,j-\frac{1}{2}} \quad (2.17)$$

where, to avoid notational complexity, once again we display all coefficients in the Appendix. Replacing "i" by "$i+1$" in (2.17) we obtain an alternatine equation for $J_{i+\frac{1}{2},j}$ which we use in order to design our numerical scheme by setting $J_{i+\frac{1}{2},j}\equiv J_{i-\frac{1}{2},j}|_{i:\to i+1}$:

$$\begin{aligned} 0 = {} & E_1\phi_{i-\frac{1}{2},j}+E_3\phi_{i,j+\frac{1}{2}}+E_3\phi_{i,j-\frac{1}{2}}+(E_2-E_4)\phi_{i+\frac{1}{2},j} \quad (2.18)\\ &+-E_3\phi_{i+1,j+\frac{1}{2}}-E_3\phi_{i+1,j-\frac{1}{2}}-E_4\phi_{i+3/2,j}, \end{aligned}$$

This seven point stencil is centered at $(i+1/2,j)$ around the (i,j) and $(i+1,j)$ cells, as can be seen in Figure 2.1.

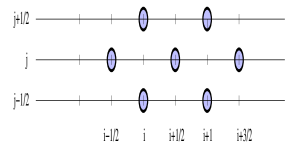


FIG. 2.1. *The stencil*

An analogous equation holds in the y direction for the (i,j) and $(i,j+1)$ cells. Boundary conditions involving $\phi(x,y)$ can be obtained using (2.2), (2.16) and (2.17).

3. Consistency Analysis. Here we will use a truncation analysis to argue that (2.18) and its rotated analog, in the y direction, limit to the continuous equation (2.1) as Δx and $\Delta y\to 0$. We do this by expanding (2.18) about the center point $(x_{i+\frac{1}{2}},y_j)$. In an effort to make the analysis more readable we distinguish between the unknowns $\phi_{i+\frac{1}{2},j}$ that line on the horizontal cell edges, and the unknowns $\phi_{i,j+\frac{1}{2}}$ that line on the vertical cell edges by using the following notation,

$$f_{i+\frac{1}{2},j}=\phi_{i+\frac{1}{2},j}\qquad g_{i,j+\frac{1}{2}}=\phi_{i,j+\frac{1}{2}}. \quad (3.1)$$

For simplicity we assume a quasi-uniform mesh (uniform in each direction) with $\Delta x\approx\Delta x_i$ and $\Delta y\approx\Delta y_j$, but the procedure can be similarly implemented for variable mesh sizes. Recall that f and g are cell-average unknowns from (2.3) and (2.5) respectively; hence by Taylor expansion

$$\begin{aligned} f_{i+\frac{1}{2},j} &= \frac{1}{\Delta y}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}f(x_{i+\frac{1}{2}},y)dy \quad (3.2)\\ &= \frac{1}{\Delta y}\int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}}[f(x_{i+1/2},y_j)+(y-y_j)f_y(x_{i+1/2},y_j)\\ &\qquad +\frac{1}{2}(y-y_j)^2f_{yy}(x_{i+1/2},y_j)+\ldots]dy\\ &= f(x_{i+\frac{1}{2}},y_j)+\frac{\Delta y^2}{24}f_{yy}(x_{i+\frac{1}{2}},y_j)+O(\Delta^4). \end{aligned}$$

Note that $f_{i+1/2,j}$ is not the same as $f(x_{i+1/2}, y_j)$. We now set

$$F_{i+\frac{1}{2},j} = f(x_{i+\frac{1}{2}}, y_j),\ F_{yy,i+\frac{1}{2},j} = f_{yy}(x_{i+\frac{1}{2}}, y_j),$$

etc. Then,

$$f_{i+\frac{1}{2},j} = F_{i+\frac{1}{2},j} + \frac{\Delta y^2}{24}F_{yy,i+\frac{1}{2},j} + \frac{\Delta y^4}{1920}F_{yyyy,i+\frac{1}{2},j} + O(\Delta y^6), \tag{3.3}$$

$$g_{i,j+\frac{1}{2}} = G_{i,j+\frac{1}{2}} + \frac{\Delta x^2}{24}G_{xx,i,j+\frac{1}{2}} + \frac{\Delta x^4}{1920}G_{xxxx,i,j+\frac{1}{2}} + O(\Delta x^6). \tag{3.4}$$

Note that similar expansions are carried out about $(x_{i+1/2}, y_j)$ for the remaining nodes appearing in our stencil (2.18). To further simplify the resulting expression we apply the same procedure as in (3.2), and expand as follows

$$\begin{aligned}
F_{i-1/2,j} &= F - \Delta x F_x + \Delta x^2 \frac{F_{xx}}{2} - \Delta x^3 \frac{F_{xxx}}{6} + \Delta x^4 \frac{F_{xxxx}}{24} + O(\Delta x^6),\\
F_{yy,i-1/2,j} &= F_{yy} - F_{yyx}\Delta x + \Delta x^2 \frac{F_{yyxx}}{2} - \Delta x^3 \frac{F_{yyxxx}}{6} + O(\Delta x^4),\\
F_{yyyy,i-1/2,j} &= F_{yyyy} - \Delta x F_{yyyyx} + \cdots + O(\Delta x^4),\\
&\vdots \quad \text{etc.}
\end{aligned}$$

for both F and G components. We therefore substitute (3.3), (3.4) and the expansions above in (2.18) thus obtaining, for piecewise constant D and a quasi-uniform mesh, that the truncation error is no more than $O(\Delta x^2 + \Delta y^2)$. The calculation is extensive due to the large number of parameters involved but quite routine and as such we do not include it here (however a similar such calculation is undertaken in detail in Section 5).

4. The Nodal Method for Problems with $\sigma_a = 0$. In this section we establish a nodal scheme for the special case of $\sigma = 0$. We therefore consider the following problem,

$$\frac{\partial}{\partial x}\left(D_1(x,y)\frac{\partial \phi}{\partial x}(x,y)\right) + \frac{\partial}{\partial y}\left(D_2(x,y)\frac{\partial \phi}{\partial y}(x,y)\right) = 0, \tag{4.1}$$

with the same boundary condition, (2.2). This problem, and the nodal method we will develop here, are unusual in that there is no absorption, whereas conventional nodal methods require $\sigma_a \neq 0$. The procedure just outlined in Section 2 is no longer applicable since among other things the form of the solution (2.11) changes radically for $\sigma_a = 0$. Instead the method which we develop below relies on scalar flux unknowns, rather than the usual current unknowns. We will use the same grid as before and the same configuration and definitions for our unknowns (2.3-2.6). Working in exactly the same way as in (2.7) - (2.10) we now obtain the analog of (2.11) which is now valid for $\sigma = 0$:

$$\begin{aligned}
\phi_j(x) = &\frac{J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}}}{2D_{ij}\Delta x_i \Delta y_j}(x - x_{i+\frac{1}{2}})(x - x_{i-\frac{1}{2}})\\
&+ (x_{i+\frac{1}{2}} - x)\frac{\phi_{i-\frac{1}{2},j}}{\Delta x_i} + (x - x_{i-\frac{1}{2}})\frac{\phi_{i+\frac{1}{2},j}}{\Delta x_i}.
\end{aligned} \tag{4.2}$$

Thus, we now have

$$D_{ij}\frac{d}{dx}\phi_j(x) = \frac{J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}}}{\Delta x_i \Delta y_j}(x - x_i) + \frac{D_{ij}}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}).$$

Evaluating this at $x = x_{i\pm\frac{1}{2}}$ and using (2.4), we get

$$-J_{i\pm\frac{1}{2},j} = \pm\frac{1}{2}(J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}}) + D_{ij}\frac{\Delta y_j}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}).$$

Subtracting and adding these two equations we get,

$$J_{i+\frac{1}{2},j} + J_{i,j+\frac{1}{2}} = J_{i-\frac{1}{2},j} + J_{i,j-\frac{1}{2}} \tag{4.3}$$

$$J_{i+\frac{1}{2},j} + J_{i-\frac{1}{2},j} = -2D_{ij}\frac{\Delta y_j}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}), \tag{4.4}$$

respectively. Note that (4.3) is just the balance equation.

Now, going through exactly the same procedure, except transverse – integrating in the y-direction rather than the x-direction, we again obtain (4.3), and the following "rotated" version of (4.4):

$$J_{i,j+\frac{1}{2}} + J_{i,j-\frac{1}{2}} = -2D_{ij}\frac{\Delta x_i}{\Delta y_j}(\phi_{i,j+\frac{1}{2}} - \phi_{i,j-\frac{1}{2}}) \quad . \tag{4.5}$$

For system (4.3)-(4.4) to be solvable we need a fourth equation. To get this, we operate on (4.2) by $\frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}(\cdot)dx$ to obtain,

$$\phi_{ij} \equiv \frac{1}{\Delta x_i}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\phi_j(x)dx = -\frac{1}{12}\frac{\Delta x_i}{D_{ij}\Delta y_j}(J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}}) + \frac{1}{2}(\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j}). \tag{4.6}$$

We also get the analogous equation,

$$\phi_{ij} = -\frac{1}{12}\frac{\Delta y_j}{D_{ij}\Delta x_i}(J_{i+\frac{1}{2},j} - J_{i-\frac{1}{2},j}) + \frac{1}{2}(\phi_{i,j+\frac{1}{2}} + \phi_{i,j-\frac{1}{2}}). \tag{4.7}$$

Eliminating ϕ_{ij} between (4.6) and (4.7), we obtain:

$$\begin{aligned}
&-\frac{1}{12}\frac{\Delta x_i}{D_{ij}\Delta y_j}(J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}}) + \frac{1}{2}(\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j})\\
&= -\frac{1}{12}\frac{\Delta y_j}{D_{ij}\Delta x_i}(J_{i+\frac{1}{2},j} - J_{i-\frac{1}{2},j}) + \frac{1}{2}(\phi_{i,j+\frac{1}{2}} + \phi_{i,j-\frac{1}{2}}) \quad .
\end{aligned} \tag{4.8}$$

This condition makes $\phi_j(x)$ (defined by (4.2)) and $\phi_i(y)$ to have the same average value in the (i,j)-cell. Note that(4.3)-(4.5) and (4.8) give us 4 equations per cell. Thus, there are a total of 4 IJ such equations. In addition (see (2.2)) there is a boundary condition of the form,

$$(\text{constant})\ \phi + (\text{constant})\ J = \text{Source},$$

at each edge on the outer boundary. There are a total of $2I + 2J$ such conditions. Hence,

$$\begin{aligned}
\#\text{ of equations} &= 4IJ + 2I + 2J = 2(2IJ + I + J)\\
&= 2[I(J+1) + (I+1)J] = 2[\#\text{ of all edges}]
\end{aligned}$$

Since there are exactly two unknowns per cell edge, then we have the same number of equation as unknowns.

Now we shall show that it is possible to eliminate the J's from these equations, thereby reducing the number of unknowns by a factor of two. From (4.3) we get,

$$J_{i,j+\frac{1}{2}} - J_{i,j-\frac{1}{2}} = -(J_{i+\frac{1}{2},j} - J_{i-\frac{1}{2},j}).$$

Hence, (4.8) can be written as

$$-\frac{12D_{ij}}{\left(\frac{\Delta y_j}{\Delta x_i} + \frac{\Delta x_i}{\Delta y_j}\right)}\frac{1}{2}\left[\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j} - \phi_{i,j+\frac{1}{2}} - \phi_{i,j-\frac{1}{2}}\right] = J_{i+\frac{1}{2},j} - J_{i-\frac{1}{2},j}. \tag{4.9}$$

Adding (4.4) and (4.9), we get

$$J_{i+\frac{1}{2},j} = -D_{ij}\frac{\Delta y_j}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}) - \frac{3D_{ij}(\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j} - \phi_{i,j+\frac{1}{2}} - \phi_{i,j-\frac{1}{2}})}{\left(\frac{\Delta y_j}{\Delta x_i} + \frac{\Delta x_i}{\Delta y_j}\right)}. \tag{4.10}$$

Subtracting (4.4) from (4.9), we get

$$J_{i-\frac{1}{2},j} = -D_{ij}\frac{\Delta y_j}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}) + \frac{3D_{ij}(\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j} - \phi_{i,j+\frac{1}{2}} - \phi_{i,j-\frac{1}{2}})}{\left(\frac{\Delta y_j}{\Delta x_i} + \frac{\Delta x_i}{\Delta y_j}\right)}. \tag{4.11}$$

Replacing "i" by "$i+1$" in (4.11) we find

$$\begin{aligned} J_{i+\frac{1}{2},j} = & -D_{i+1,j}\frac{\Delta y_j}{\Delta x_{i+1}}(\phi_{i+\frac{3}{2},j} - \phi_{i+\frac{1}{2},j}) \\ & + \frac{3D_{i+1,j}}{\left(\frac{\Delta y_j}{\Delta x_{i+1}} + \frac{\Delta x_{i+1}}{\Delta y_j}\right)}(\phi_{i+\frac{3}{2},j} + \phi_{i+\frac{1}{2},j} - \phi_{i+1,j+\frac{1}{2}} - \phi_{i+1,j-\frac{1}{2}}) \end{aligned} \tag{4.12}$$

Finally, eliminating $J_{i+\frac{1}{2},j}$ between (4.10) and (4.12), we obtain the following equation for the ϕ's:

$$\begin{aligned} 0 = & -\frac{D_{i+1,j}}{\Delta x_{i+1}}(\phi_{i+\frac{3}{2},j} - \phi_{i+\frac{1}{2},j}) + \frac{D_{ij}}{\Delta x_i}(\phi_{i+\frac{1}{2},j} - \phi_{i-\frac{1}{2},j}) \\ & + \left(\frac{3D_{ij}\Delta x_i}{\Delta x_i^2 + \Delta y_j^2}\right)(\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j} - \phi_{i,j+\frac{1}{2}} - \phi_{i,j-\frac{1}{2}}) \\ & + \left(\frac{3D_{i+1,j}\Delta x_{i+1}}{\Delta x_{i+1}^2 + \Delta y_j^2}\right)(\phi_{i+\frac{3}{2},j} + \phi_{i+\frac{1}{2},j} - \phi_{i+1,j+\frac{1}{2}} - \phi_{i+1,j-\frac{1}{2}}) \\ & := L_1 + L_2 + L_3, \end{aligned} \tag{4.13}$$

where by L_1, L_2 and L_3 we denote the first, second and third lines of (4.13) respectively. This equation spans the (i,j) and $(i+1,j)$ cells. An analogous equation holds for the (i,j) and $(i,j+1)$ cells. Boundary conditions involving only ϕ can be obtained using (2.2), (4.10) and (4.11).

5. Truncation Analysis . Once again we will show that (4.13) is consistent with (4.1) by expanding (4.13) about the point $(x_{i+\frac{1}{2}}, y_j)$. We use the same notation as in (3.1). For this section we will assume a uniform mesh and let $D = 1$. Then using the same expansion (3.3,3.4,etc) the first line of (4.13) becomes,

$$\begin{aligned} L_1 = & -\frac{1}{\Delta x}(\phi_{i+\frac{3}{2},j} - 2\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j}) \\ = & -\frac{1}{\Delta x}\Big[F_{i+\frac{3}{2},j} + \frac{\Delta y_j^2}{24}F_{yy,i+\frac{3}{2},j} - 2\Big(F_{i+\frac{1}{2},j} + \frac{\Delta y_j^2}{24}F_{yy,i+\frac{1}{2},j}\Big) \\ & + \Big(F_{i-\frac{1}{2},j} + \frac{\Delta y_j^2}{24}F_{yy,i-\frac{1}{2},j}\Big) + O(\Delta^4)\Big] \\ = & -\frac{1}{\Delta x}\Big[F_{i+\frac{1}{2},j} + \Delta x F_{x,i+\frac{1}{2},j} + \frac{\Delta x^2}{2}F_{xx,i+\frac{1}{2},j} + \frac{\Delta y^2}{24}F_{yy,i+\frac{1}{2},j} \\ & - 2\Big(F_{i+\frac{1}{2},j} + \frac{\Delta y^2}{24}F_{yy,i+\frac{1}{2},j}\Big) \\ & + F_{i+\frac{1}{2},j} - \Delta x F_{x,i+\frac{1}{2},j} + \frac{\Delta x^2}{2}F_{xx,i+\frac{1}{2},j} + \frac{\Delta y^2}{24}F_{yy,i+\frac{1}{2},j} + O(\Delta^4)\Big] \end{aligned}$$

Thus,

$$L_1 = -\frac{1}{\Delta x}(\phi_{i+\frac{3}{2},j} - 2\phi_{i+\frac{1}{2},j} + \phi_{i-\frac{1}{2},j}) = -\Delta x F_{xx,i+\frac{1}{2},j} + O(\Delta^3). \tag{5.1}$$

Similarly, the second and third lines of (4.13) can be written as:

$$\begin{aligned} L_2 + L_3 = & \frac{3\Delta x}{\Delta x^2 + \Delta y^2}\Big[(4F_{i+\frac{1}{2},j} + \Delta x^2 F_{xx,i+\frac{1}{2},j} + \frac{\Delta y^2}{6}F_{yy,i+\frac{1}{2},j}) \\ & - \Big(G_{i,j+\frac{1}{2}} + \frac{\Delta x^2}{24}G_{xx,i,j+\frac{1}{2}} + G_{i,j-\frac{1}{2}} + \frac{\Delta x^2}{24}G_{xx,i,j-\frac{1}{2}} \\ & + G_{i+1,j+\frac{1}{2}} + \frac{\Delta x^2}{24}G_{xx,i+1,j+\frac{1}{2}} + G_{i+1,j-\frac{1}{2}} + \frac{\Delta x^2}{24}G_{xx,i+1,j-\frac{1}{2}}\Big) + O(\Delta^4)\Big]. \end{aligned} \tag{5.2}$$

Therefore,

$$\begin{aligned} L_2 + L_3 = & \frac{3\Delta x}{\Delta x^2 + \Delta y^2}\Big[\Big(4F + \Delta x^2 F_{xx} + \frac{\Delta y^2}{6}F_{yy}\Big) \\ & - \Big(4G + \frac{2}{3}\Delta x^2 G_{xx} + \frac{1}{2}\Delta y^2 G_{yy}\Big) + O(\Delta^4)\Big]. \end{aligned} \tag{5.3}$$

Using (5.1) and (5.3), we may write (4.13) as,

$$-F_{xx} + \frac{3[(4F + \Delta x^2 F_{xx} + \frac{\Delta y^2}{6}F_{yy}) - (4G + \frac{2}{3}\Delta x^2 G_{xx} + \frac{1}{2}\Delta y^2 G_{yy})]}{\Delta x^2 + \Delta y^2} = O(\Delta^2). \tag{5.4}$$

The corresponding equation is obtained by interchanging x and y, and F and G:

$$-G_{yy} + \frac{3\left[(4G + \Delta y^2 G_{yy} + \frac{\Delta x^2}{6}G_{xx}) - (4F + \frac{2}{3}\Delta y^2 F_{yy} + \frac{1}{2}\Delta x^2 F_{xx})\right]}{\Delta y^2 + \Delta x^2} = O(\Delta^2). \tag{5.5}$$

We now add (5.4) and (5.5), to get

$$-(F_{xx} + G_{yy}) + \frac{3}{2(\Delta x^2 + \Delta y^2)}[\Delta x^2\partial_{xx} - \Delta y^2\partial_{yy}](F - G) = O(\Delta^2). \tag{5.6}$$

We note that (5.4) and (5.5) implies $G = F + O(\Delta^2)$. Using this, (5.6) immediately becomes,

$$-(F_{xx} + G_{yy}) = O(\Delta^2).$$

This shows, at least for D = constant and a uniform mesh, that the truncation error is no more than $O(\Delta^2)$.

6. Numerical Implementations and Examples. We provide numerical implementations which validate our approximations. We display in particular two examples. First, and as a basic benchmark, we solve a Laplacian equation in two dimensions with constant coefficients corresponding to a less regular absorption-free case. Then we move into our more elaborate example which is a full two dimensional absorption diffusion equation with ***variable coefficients*** for which the exact solution is also known.

We implement the seven point nodal scheme using an idea similar to that of constructing a mass matrix from contributions of each element of our domain much in the same way done in the finite element procedure. We start by establishing "center" points in our domain. A "center" is any point corresponding to $(x_{i+1/2}, y_j)$ in Figure 2.1 around which we have nodes in the same positions as our seven point stencil in that figure requires. Once those "centers" are found we write an algorithm which will run through them building a system of equations (one equation per "center" point). Each equation will of course be just copies of our seven point nodal scheme. Note that the coefficients of our nodal schemes are well established in Sections 2 and 4 leaving the corresponding ϕ values as unknowns. As we move through the "centers" establishing our equations some of the ϕ values corresponding to boundary points are known. Otherwise they are unknown. In that respect each of those equations will be placed in a row of its own while building our "load" matrix A. In other words we establish a system of equations which in matrix form can be written as, $AX = B$. If for instance we are at equation i, which would correspond to center i, the coefficients of the unknown ϕ's are placed in row i of matrix A while the ϕ's which are on the boundary, if any for that particular equation, will be placed into matrix B in row, i. The placement of the coefficients of each of the stencil points in matrix A is based on the position of the nodes in that stencil. In that respect the size of A is, [# of centers, # number of nodes] while that of B is, [# of centers, 1]. The solution is established by solving the system $AX = B$. Note that the number of equations is bigger than the number of unknowns once the number of nodes becomes higher than 20. In general we solve this system as a least squares problem.

6.1. Example 1. Nodal method for a simple Laplacian. The following simple example equation is solved here,

$$\frac{\partial}{\partial x} D(x,y) \frac{\partial \phi}{\partial x}(x,y) + \frac{\partial}{\partial y} D(x,y) \frac{\partial \phi}{\partial y}(x,y) = 0, \qquad (6.1)$$

where $D(x,y)$ is taken to be 1. We specify the following exact solution for (6.1),

$$\phi(x,y) = e^y(\cos(x) + \sin(x)),$$

which also provides the boundary conditions used for any domain size we choose. A variety of different domains are used which are made specific in the corresponding figures and tables. The nodal scheme (4.13) from Section 4 is implemented in a matlab code and the exact solution superimposed together with the approximate can

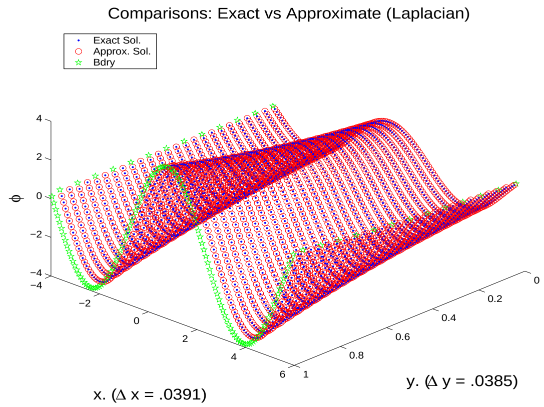


FIG. 6.1. *Example 1. Location: [x]×[y] = [-4 6]×[0 1]. The exact and approximate solutions for the Laplacian equation. We obtain* 3187 *nodes in our domain by setting* $\Delta x \approx .03$ *and* $\Delta y \approx .03$ *in this particular example.*

be seen in Figure 6.1. Our algorithm automatically creates 3187 total nodes (using only the information from the boundary) to produce the solution in the figure for the section $-4 < x < 6$ and $0 < y < 1$. In Figure 6.2 we display a different section of the solution ($20 < x < 25$ and $20 < y < 28$) as it increases exponentially. We carry out a comparison of errors in the following table. The domains for carrying out our error estimates are randomly chosen.

Absolute and relative errors per step size

Location [x] x [y]	Δx	Δy	Max. Abs. err.	(Rel. Err.)	# nodes
[1, 2]x[1, 2]	.16	.5	.026	(.131)	7
	.1	.25	.004	(.05)	31
	.05	.125	.0067	(.036)	127
	.029	.0625	.000097	(.020)	511
	.015	.031	.000015	(.011)	2047
[-1, 4]x[4, 5]	.16	1	14.4	(1.17)	22
	.16	.5	1.16	(.22)	47
	.1	.25	.11	(.07)	175
	.05	.125	.01	(.029)	671
	.029	.0625	.002	(.018)	2063
[-10, -9]x[10, 11]	.16	.5	184	(.13)	7
	.1	.25	31.09	(.05)	31
	.05	.125	4.8	(.03)	127
	.03	.06	.7	(.02)	511
	.015	.03	.10	(.01)	2047

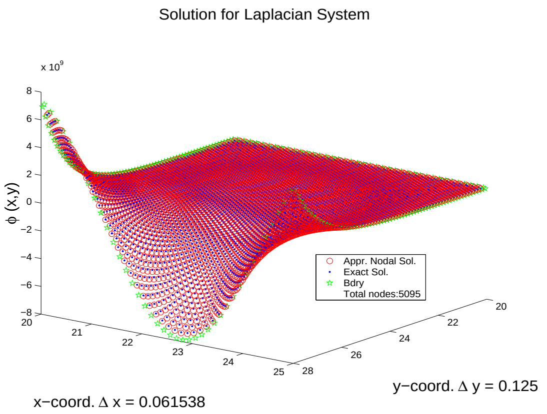


FIG. 6.2. *Example 1. A different location: [x]×[y] = [20 25]×[20 28]. The exact and approximate solutions for the Laplacian equation. The solution is exploding exponentially. Total nodes:* 5095, $\Delta x \approx .0615$ *and* $\Delta y \approx .125$.

6.2. Example 2. A diffusion problem with variable coefficients. A more elaborate example problem is solved here for the following variable coefficients diffusion problem,

$$\frac{\partial}{\partial x} x \frac{\partial \phi}{\partial x}(x,y) + \frac{\partial}{\partial y}\frac{1}{x}\frac{\partial \phi}{\partial y}(x,y) - xb^2\phi(x,y) = 0, \tag{6.2}$$

which has the following analytic solution,

$$\phi(x,y) = ae^{-xb}\sqrt{\frac{2}{x}}\cos\left(\frac{y}{2}\right), \tag{6.3}$$

where $a = 100$ and $b = .0999$. The solution is presented, for the domain $\Omega_1 = (4,5)\times(0,10)$ in Figure 6.3 as well as, for a larger domain Ω_2 containing Ω_1 in Figure 6.4. We let $\Omega_2 = (2,10)\times(-10,10)$. The actual errors are once again presented at the following table,

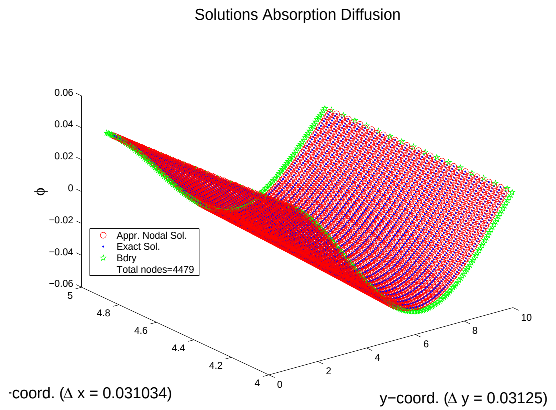


FIG. 6.3. *Example 2. The exact and approximate solutions for the full absorption diffusion equation. Location: [x]×[y] = [4 5]×[0 10]. Here we allow* 4409 *nodes by setting* $\Delta x \approx .03$ *and* $\Delta y \approx .03$.

Absolute and relative errors per step size

Location [x] x [y]	Δx	Δy	max Abs. err.	(Rel. Err.)	# nodes
[1, 2]x[1, 2]	.32	.5	.11	(.030)	7
	.16	.25	.00625	(.0050)	31
	.1	.125	.0039	(.015)	127
	.05	.0625	.0015	(.023)	511
	.029	.03125	.00047	(.027)	2047
[5, 6]x[7, 8]	.33	.5	.003	(.002)	7
	.14	.2	.001	(.005)	58
	.09	.1	.001	(.016)	199
	.04	.05	.00032	(.019)	799
	.024	.025	.00009	(.02)	3199
[5, 6]x[23, 24]	.14	.2	.0005	(.003)	58
	.09	.1	.00034	(.0057)	199
	.04	.05	.00011	(.0076)	799
	.024	.025	.00003	(.0087)	3199

7. Conclusions. We have shown that the nodal-diffusion method applied for the absorption-diffusion problems is at lease second order accurate. We investigate the consistency of our discrete scheme which corresponds to a seven-point finite difference or a finite volume scheme. For simplicity our truncation error analysis is performed for the absorption-free problems. However, theoretically in the presence of absorption term this accuracy may be further improved. This is due to the fact that positive absorption in, e.g. particle transport problems, adding to the loss term, would increase the regularity of the exact solution. The absorption term is reconsidered in the

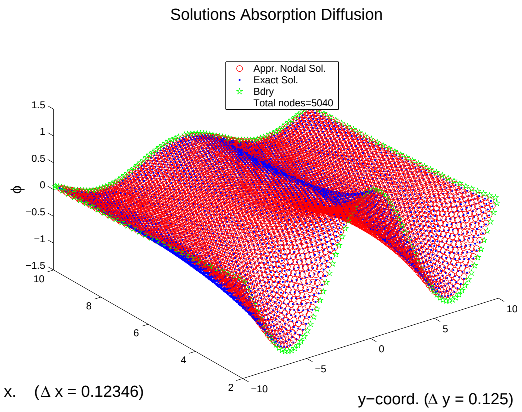


FIG. 6.4. *Example 2. The exact and approximate solutions for the full absorption diffusion equation. Location: [x]×[y] = [2 10]×[-10 10]. Here we allow* 5040 *nodes by setting* $\Delta x \approx .123$ *and* $\Delta y \approx .125$.

implementations through concrete examples. Both analysis and implementations can be extended to the cases of analytical as well as variational nodal-diffusion methods.

8. Appendix. Note: $D_{1,ij}, D_{2,ij}$ and S_{ij} denote the value of $D_1(x,y), D_2(x,y)$ and $S(x,y)$ at $x_{i-1/2} < x < x_{i+1/2}$ and $y_{j-1/2} < y < y_{j+1/2}$.

$$\begin{aligned} C_1 =& e^{-l_{1,ij}x_{i+\frac{1}{2}}} \Big(-J_{i,j+\frac{1}{2}} + J_{i,j+\frac{1}{2}} e^{-l_{1,ij}\Delta x_i} + J_{i,j-\frac{1}{2}} - J_{i,j-\frac{1}{2}} e^{-l_{1,ij}\Delta x_i} \\ &+ \phi_{i-\frac{1}{2},j} S_{ij} \Delta x_i \Delta y_j e^{-l_{1,ij}\Delta x_i} - \phi_{i+\frac{1}{2},j} S_{ij}\Delta x_i \Delta y_j \Big) / (S_{ij}\Delta x_i \Delta y_j (e^{-2l_{1,ij}\Delta x_i} - 1)) \\ C_2 =& e^{l_{1,ij}x_{i-\frac{1}{2}}} \Big(-J_{i,j+\frac{1}{2}} + J_{i,j+\frac{1}{2}} e^{-l_{1,ij}\Delta x_i} + J_{i,j-\frac{1}{2}} - J_{i,j-\frac{1}{2}} e^{-l_{1,ij}\Delta x_i} \\ &+ \phi_{i+\frac{1}{2},j} S_{ij} \Delta x_i \Delta y_j e^{-l_{1,ij}\Delta x_i} - \phi_{i-\frac{1}{2},j} S_{ij}\Delta x_i \Delta y_j \Big) / (S_{ij}\Delta x_i \Delta y_j (e^{-2l_{1,ij}\Delta x_i} - 1)) \end{aligned}$$

We also define:

$$\begin{aligned} &E_1 = -(a_1 + 2c_1c_2(a_1 - b_1))/d, \quad E_2 = (b_1 + 2c_2c_1(b_1 - a_1))/d, \\ &E_3 = c_1(b_2 + a_2)/d \qquad E_4 = 2c_2c_1(a_1 - b_1)/d, \qquad d = -4c_2c_1 - 1 \end{aligned}$$

where the a_k, b_k and c_k are defined as follows for $k = 1, 2$:

$$a_k = \frac{2D_{k,ij}l_{k,ij}e^{-l_{k,ij}\Delta x_k}}{(e^{-2l_{k,ij}\Delta x_k} - 1)} \qquad b_k = \frac{-D_{k,ij}l_{k,ij}(e^{-2l_{k,ij}\Delta x_k} + 1)}{(e^{-2l_{k,ij}\Delta x_k} - 1)}$$

$$c_k = -\frac{(-1 + e^{-l_{k,ij}\Delta x_k})l_{k,ij}D_{k,ij}}{(1 + e^{-l_{k,ij}\Delta x_k})\Delta y_j \Delta x_i S_{ij}} \qquad \text{for } \Delta x_1 = \Delta x_i, \quad \Delta x_2 = \Delta y_j$$

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