Numerical approximation of linear two-dimensional advection–diffusion processes in rectangular spatial domains

T. V. HROMADKA II and G. L. GUYMON
Department of Civil Engineering, School of Engineering, University of California, Irvine, Calif 92717, USA

INTRODUCTION

Numerical solutions of two-dimensional linear and nonlinear partial differential equations such as occur in the theory of advection–diffusion processes are generally limited to solution by the finite difference or Galerkin finite element methods. Finite difference approximations, such as described by Spalding, can be derived for regular and irregular rectangular two-dimensional subdomains. The Galerkin finite element approach can also be applied to irregular rectangular domains. Both numerical methods are often compared to each other for numerical "efficiency" or other descriptions of superiority.

Recently, Hromadka and Guymon have developed a new numerical approach called the nodal domain integration method which has been applied to one-dimensional linear and nonlinear problems. From this numerical model, the finite difference, subdomain, and Galerkin finite element methods are included in a single numerical statement.

In this note, the nodal domain integration method is applied to a two-dimensional irregular rectangular element domain. As special cases, the Galerkin finite element, subdomain, and finite difference numerical models are determined by the appropriate specification of a single parameter in the resulting nodal domain integration numerical statement.

The first objective of this note is to present a basic description of the nodal domain integration procedure as applied to the class of partial differential equations generally encountered in the theory of advection–diffusion processes. Detailed mathematical derivations and applications of this numerical approach for a one-dimensional problem are contained in other papers. The theoretical foundations of this numerical method are based on the well-known subdomain technique of the finite element weighted residuals approach.

The second objective is to develop a simple numerical statement which can represent the finite element Galerkin statement, subdomain numerical statement, finite difference integration control volume statement, and the nodal domain integration numerical statement, by the specification of a single parameter in the resulting nodal domain integration numerical approximation.

Hromadka and Guymon used the nodal domain integration approach to numerically approximate the one-dimensional advection–diffusion process:

\[
\frac{\partial}{\partial t} \left[ D \frac{\partial U}{\partial x} \right] = \frac{\partial}{\partial x} \left( \frac{\partial U}{\partial x} \right) \quad \text{in} \Omega
\]

where \(D\) and \(U\) are the diffusion and advection parameters respectively; \(\theta\) is the state variable; \(x, t\) are spatial and temporal coordinates; and \(\Omega\) is the spatial domain of definition. For constant parameters, equation (1) can be rewritten into the linear form:

\[
D \frac{\partial^2 \theta}{\partial x^2} + U \frac{\partial \theta}{\partial x} = \frac{\partial \theta}{\partial t} \quad \text{x} \in \Omega
\]

Discretizing the spatial domain \(\Omega\) by \(m\) nodal points into \(m\) subdomains, \(R_x\), Hromadka and Guymon use the subdomain version of the weighted residuals method to develop a one-dimensional numerical statement for each nodal point value:

\[
\frac{D}{2} \left[ \theta_j^{(i+1)} - 2\theta_j^{(i)} + \theta_{j-1}^{(i)} + \theta_{j+1}^{(i)} - 2\theta_j^{(i)} \right] -
\]

\[
U \theta_j^{(i)} \left[ \theta_j^{(i+1)} - \theta_{j-1}^{(i)} \right] / 2 + \left( \theta_{j+1}^{(i)} - \theta_{j-1}^{(i)} \right) / 2
\]

where nodal value \(\theta_j^{(i)} = \theta(x = x_j, t = k\Delta t)\). It was shown that the \(\eta\) term in equation (3) can vary between \(R_x\) with respect to time in order to approximate a higher order or more complex trial function for the state variable \(\theta\). It was also shown that for a linear polynomial trial function for \(\theta\) and a Crank–Nicolson time advancement approximation, equation (3) represents the Galerkin finite element, subdomain integration, and finite difference numerical approximations for constant \(\eta\) values of (2,3,\(x\)) respectively.

In the following, the one-dimensional numerical statement of equation (3) will be extended to the case of a two-dimensional irregular rectangular subdomain. The problem domain, \(\Omega\), is discretized into a set of nodal domains, \(\Omega_j\), defined by the intersection of a finite element cover, \(\Omega_k\), and subdomain cover, \(\Omega_j\), of \(\Omega\). Integrating the governing partial differential equations with respect to both space and time on each nodal domain results in a numerical contribution which can be combined with other nodal domain contributions to form a finite difference statement or a finite element matrix system. Similar to the one-dimensional case, the resulting nodal domain integration numerical statement will be shown to also represent the Galerkin finite element, subdomain integration, and finite difference numerical statements by the appropriate specification of a single parameter.
NODAL DOMAIN DISCRETIZATION OF SOLUTION DOMAIN

Consider the partial differential operation:

\[ A(\varphi) = f: (x,y) \in \Omega, \Omega = \Omega \cup \Gamma \]  \hspace{1cm} (4)

with boundary condition types of Dirichlet or Neumann specified on boundary \( \Gamma \). A n-nodal point distribution can be defined in \( \Omega \) with arbitrary density (Fig. 1) such that an approximation \( \hat{\varphi} \) for \( \varphi \) is defined in \( \Omega \) by:

\[ \hat{\varphi} = \sum_{j=1}^{n} N_j(x,y) \varphi_j; (x,y) \in \Omega \]  \hspace{1cm} (5)

where \( N_j(x,y) \) are linearly independent global shape functions and \( \varphi_j \) are assumed values of the state variable, \( \varphi \), at nodal point \( j \). In equation (5) it is assumed that:

\[ \lim_{n \to \infty} \hat{\varphi} = \lim_{n \to \infty} \hat{\varphi}_{\text{max},(x,y)\in \Omega} = \varphi; (x,y) \in \Omega \]  \hspace{1cm} (6)

A closed connected spatial subset \( R_j \) is defined for each nodal point \( j \) such that:

\[ \Omega = \bigcup_{j=1}^{n} R_j \]  \hspace{1cm} (7)

with supplementary conditions of:

\[ (x,y) \in R_j; (x,y) \in R_k, j \neq k \]  \hspace{1cm} (8)

and

\[ R_j = R_j \cup B_j \]  \hspace{1cm} (9)

where \( (x,y) \) are the spatial coordinates of node \( j \) and \( B_j \) is the boundary of \( R_j \). It is assumed that every subdomain is disjoint except along shared boundaries, i.e.

\[ R_j \cap R_k = B_j \cap B_k \]  \hspace{1cm} (10)

The subdomain method of the finite element weighted residuals approach approximates equation (4) by solving the \( m \) equations:

\[ \int_{\Omega} (A(\varphi) - f) w_j \ dA = 0 \]  \hspace{1cm} (11)

where

\[ w_j = \begin{cases} 1, & (x,y) \in R_j \\ 0, & (x,y) \in \Omega \setminus R_j \end{cases} \]  \hspace{1cm} (12)

A second cover of \( \Omega \) is defined by the finite element method with:

\[ \Omega = \bigcup \hat{\Omega}_c \]  \hspace{1cm} (13)

where \( \hat{\Omega}_c \) is the closure of finite element domain \( \Omega_c \) and its boundary \( \hat{\Gamma}_c \).

Let \( S_c \) be the set of nodal points defined by:

\[ S_c = \{ j | \hat{\Omega}_c \cap R_j \neq \emptyset \} \]  \hspace{1cm} (14)

Then a set of nodal domains \( \Omega_j \) is defined for each finite element domain \( \Omega_c \) by:

\[ \Omega_j = \hat{\Omega}_c \cap R_j; j \in S_c \]  \hspace{1cm} (15)

The subdomain method of weighted residuals as expressed by equation (11) can be rewritten in terms of the subdomain cover of \( \Omega \) by:

\[ \int_{\Omega} (A(\varphi) - f) w_j \ dA = \int_{\Omega} (A(\varphi) - f) dA \]  \hspace{1cm} (16)

With respect to the finite element discretization of \( \Omega_c \):

\[ \int_{\Omega_c} (A(\varphi) - f) dA = \int_{\Omega_c} (A(\varphi) - f) dA \]  \hspace{1cm} (17)

where for each finite element domain \( \hat{\Omega}_c \):

\[ \int_{\Omega_c \setminus \hat{\Omega}_c} (A(\varphi) - f) dA = \int_{\Omega_c \setminus \hat{\Omega}_c} (A(\varphi) - f) dA \]  \hspace{1cm} (18)

From the above subset definitions and set covers of \( \Omega_c \), application of the usual subdomain method to the governing partial differential operation of equation (4) is accomplished by an integration of the governing equations over the nodal domains interior of each finite element, resulting in a finite element matrix system similar to that determined by the Galerkin finite element method. The spatial definition of each nodal domain \( \hat{\Omega}_c \) depends on the definition of both the finite element and subdomain covers of \( \Omega_c \), and is therefore somewhat arbitrary. A convenient criterion is to define the nodal domains such that the resulting finite element matrix system is symmetric. This symmetry property is used for the definition of finite element nodal domains in the following model development of a two-dimensional advection-diffusion process.
NODAL DOMAIN INTEGRATION PROCEDURE

A two-dimensional advection-diffusion process similar to equation (1) is given by:

$$\frac{\partial}{\partial x}\left[D \frac{\partial \theta}{\partial x} - DX \theta\right] + \frac{\partial}{\partial z} \left[D \frac{\partial \theta}{\partial z} - DW \theta\right] = \frac{\partial \theta}{\partial t} \text{ (x,z) } \in \Omega \quad (19)$$

where $\Omega$ is a two-dimensional rectangular spatial domain of definition; $(U, W)$ are advection parameters in the $(x,z)$ directions respectively; and $D = D(x,z)$.

An operator relationship for the two-dimensional advection-diffusion process of equation (19) is defined by:

$$A(\phi) \cdot j = \frac{\partial}{\partial x} \left[D \frac{\partial \theta}{\partial x} - DX \theta\right] + \frac{\partial}{\partial z} \left[D \frac{\partial \theta}{\partial z} - DW \theta\right] - \frac{\partial \theta}{\partial t} \left(19\right)$$

Substituting equation (20) into equation (18) gives the finite element matrix system for $\Omega_e$ (Fig. 3).

$$\left\{ \int_{\Gamma_e} \left[ \frac{\partial}{\partial x} \left(D \frac{\partial \theta}{\partial x} - DX \theta\right) \right] ds + \int_{\Gamma_e} \left[ \frac{\partial}{\partial z} \left(D \frac{\partial \theta}{\partial z} - DW \theta\right) \right] ds \right\} \left[ \begin{array}{c} \theta_0 \end{array} \right] = \left( \begin{array}{c} \phi \end{array} \right) \text{ (j) }$$

(21)

Expanding equation (21) gives:

$$\left\{ \int_{\Gamma_e} \left[ \frac{\partial}{\partial x} \left(D \frac{\partial \theta}{\partial x} - DX \theta\right) \right] ds + \int_{\Gamma_e} \left[ \frac{\partial}{\partial z} \left(D \frac{\partial \theta}{\partial z} - DW \theta\right) \right] ds \right\} \left[ \begin{array}{c} \theta_0 \end{array} \right] = \left( \begin{array}{c} \phi \end{array} \right) \text{ (j) }$$

where the first term of equation (22) cancels due to flux contributions from neighbouring finite elements (Fig. 4) or satisfies zero-flux natural boundary conditions on $\Gamma_e$.

The finite element discretization of $\Omega$ is assumed to be composed of rectangles with vertex-located nodal points associated to each finite element domain $\Omega_e$ (Fig. 2).

Figure 2. Finite element $\Omega_e$ with vertex located nodal points

$$\begin{array}{c}
\text{Figure 3. Nodal domain cover of finite element } \Omega_e.
\end{array}$$

$$\begin{array}{c}
\text{Figure 4. Subdomain } R, \text{ as the union of all nodal domains associated to nodal point } j.
\end{array}$$

Integration of the governing flow equation on each $\Omega_e$ involves the definition and integration of non-linear parameters $\bar{D}$ and $\bar{U}$. Hromada and Guymon expand the non-linear parameters by Taylor series and integrate the expanded infinite series expression resulting in an equivalent numerical approximation as a function of the assumed trial function nodal point values. Another approach to handling the non-linearity problem is to approximately linearize the governing flow equation by assuming the non-linear parameters to be uniform in the finite element for small durations of time, $\Delta t$. Some methods of determining quasi-constant values for non-linear parameters are examined for a one-dimensional problem in Hromada and Guymon.

Using quasi-constant values of $\bar{D}^{\text{n0}}$ and $\bar{U}(t)$ for the non-linear parameters of the governing flow equation for a small time step $\Delta t$ simplifies the finite element system of equation (22) to:

$$\left\{ \int_{\Gamma_e} \left[ \frac{\partial}{\partial x} \left(D^{\text{n0}} \frac{\partial \theta}{\partial x} - \bar{D}(t) \theta\right) \right] ds + \int_{\Gamma_e} \left[ \frac{\partial}{\partial z} \left(D^{\text{n0}} \frac{\partial \theta}{\partial z} - \bar{D}(t) \theta\right) \right] ds \right\} \left[ \begin{array}{c} \theta_0 \end{array} \right] = \left( \begin{array}{c} \phi \end{array} \right) \text{ (j) } - \left( \begin{array}{c} \phi \end{array} \right)$$

(23)

The nodal domain integration method solves equation (23) for each $\Omega_e$ by defining functions for a $\Delta t$ timestep:

$$\int_{\Gamma_e} \frac{\partial \theta}{\partial x} ds = \int_{\Gamma_e} \frac{\partial \theta}{\partial t} ds \text{ (j) }$$

(24)

$$\int_{\Gamma_e} \frac{\partial \theta}{\partial z} ds = \int_{\Gamma_e} \frac{\partial \theta}{\partial t} ds \text{ (j) }$$

(25)

$$\int_{\Gamma_e} \frac{\partial \theta}{\partial x} ds = \int_{\Gamma_e} \frac{\partial \theta}{\partial t} ds \text{ (j) }$$

(26)
where \( f(\theta, u, t) \) is a function of time and finite element domain \( \Omega \), associated nodal points correction factor \( c(\theta, \Omega) \) is a function of time; and \( \theta \) is a linear trial function for \( \Omega \). The above function definitions are extensions of a similar set of function definitions determined for a one-dimensional flow problem. In the study of one-dimensional problems, it was concluded that the \( f(\theta, u, t) \) functions had a far greater effect on model accuracy than did the \( c(\theta, \Omega) \) functions and that the simplifying definition could be made:

\[
c(\theta, \Omega) = 1
given for many problems. This conclusion is valid for both first and second order polynomial trial functions where the finite element discretization is composed of nodal domains satisfying the matrix symmetry criterion.

For the assumed rectangular finite element discretization of \( \Omega \), a definition of nodal domains \( \Omega_i \) is required in order to evaluate the \( f(\theta, u, t) \) functions. Using matrix symmetry as a criterion, element nodal domains are defined by the intersection of perpendicular bisectors (Fig. 3) partitioning the rectangle into four equal areas. The definition of \( f(\theta, u, t) \) used for each nodal domain \( \Omega_i \) is given by extending the one-dimensional function definitions to obtain:

\[
f(\theta, u, t) = \left\{ \begin{array}{ll}
\sum_{k \in S_c} \eta_{ij}(\theta, u, t) / 4 & \text{if } (i, j) \in S_c \\
\sum_{k \in S_c} \eta_{ij}(\theta, u, t) / 4 & \text{if } (i, j) \notin S_c
\end{array} \right.
\]

where \( A(x) \) is the area of rectangle \( \Omega_i \). In order to provide element matrix symmetry,

\[
f(\theta, u, t) = f(\bar{\eta}(\theta, u, t), \theta_i) ; (i, j) \in S_c
\]

where \( \bar{\eta}(\theta, u, t) \) is the average of the \( \eta_{ij}(\theta, u, t) \) in finite element \( \Omega_i \) given by:

\[
\bar{\eta}(\theta, u, t) = \frac{1}{4} \sum_{k \in S_c} \eta_{ij}(\theta, u, t)
\]

**NODAL DOMAIN INTEGRATION NUMERICAL MODEL**

For constant advection–diffusion parameters, equation (19) reduces to the linear partial differential equation:

\[
\frac{\partial \theta}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial \theta}{\partial x} \right) - \frac{\partial}{\partial x} \left( \frac{\partial \theta}{\partial x} \right) = \frac{\partial}{\partial x} \left( \frac{\partial \theta}{\partial x} \right)
\]

where \( \alpha_x \) and \( \beta \) are constant throughout \( \Omega \). Pinder and Gray\(^8\) develop a Galerkin finite element analogue for equation (30). Also, equation (30) is readily approximated by the well known finite difference method, and the subdomain version of the weighted residuals method.

A comparison of the Galerkin finite element [linear trial function], finite difference, and subdomain integration numerical statements to the nodal domain integration numerical statement indicates that the nodal domain integration analogue can represent each of the above methods.

For the \( x \)-direction diffusion term \( D_x \frac{\partial^2 \theta}{\partial x^2} \), the Galerkin, subdomain integration, and finite difference modeling statement (for a linear polynomial trial function) are given by:

\[
D_x \frac{\partial^2 \theta}{\partial x^2} = \frac{1}{2} \left( \frac{\partial \theta}{\partial x} - \frac{\partial \theta}{\partial x} + \frac{\partial \theta}{\partial x} \right) - \frac{\partial}{\partial x} \left( \frac{\partial \theta}{\partial x} \right)
\]

and the nodal domain integration statement is:

\[
D_x \frac{\partial^2 \theta}{\partial x^2} = \frac{1}{2} \left( \frac{\partial \theta}{\partial x} - \frac{\partial \theta}{\partial x} + \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\partial \theta}{\partial x} \right)
\]

where equations (31), (32) and (33) are the numerical statements determined by the Galerkin finite element, subdomain integration, and finite difference methods, respectively. The nodal domain integration model of equation (34) is an equivalent statement for the three models considered for \( \eta = (2, 3, 4, \ldots) \) respectively.
where equations (35), (36) and (37) are determined from the Galerkin finite element, subdomain integration, and finite difference methods, respectively. The nodal domain integration model equation of (39) is an equivalent statement for equations (35), (36) and (37) for \( \eta = (2, 3, x) \).

Finally, the capacitance (time derivative) term \( \frac{\partial}{\partial t} \) \( \frac{\partial C}{\partial t} \) numerical statements are:

\[
\frac{\partial C}{\partial t} = \frac{\partial C}{\partial t} \frac{\partial C}{\partial t} = \frac{\partial C}{\partial t} \frac{\partial C}{\partial t} + \frac{\partial C}{\partial t} \frac{\partial C}{\partial t} + \frac{\partial C}{\partial t} \frac{\partial C}{\partial t} \]

where the Galerkin finite element, nodal domain integration, and finite difference methods are given by \( \eta = (2, 3, x) \) respectively. Equation (43) can be directly compared to the Galerkin finite element results in Pinder and Gray. (Table IV.2).

Other constant values of \( \eta \) in equation (43) represent other numerical approximations. For example, \( \eta = 11 \) represents an approximation based on the subdomain method of weighted residuals for a second order polynomial trial function. Additionally, by use of the function definitions of equations (24) and (25), a variable \( \eta \) between subdomains (or finite element matrices) and with respect to time can be obtained.

CONCLUSIONS
The nodal domain integration numerical approach has been used to determine a numerical analogue which incorporates the Galerkin finite element, subdomain, and integrated finite difference methods as special cases. The resulting numerical statement involves the same computational requirements as does the Galerkin finite element procedure. Thus, a computer program may be prepared based on the nodal domain integration numerical approximation which inherently contains the Galerkin finite element, subdomain integration, and finite difference numerical approximations for the considered class of partial differential equations.

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REFERENCES