COMPARISON OF THE NODAL INTEGRAL METHOD AND NONSTANDARD FINITE-DIFFERENCE SCHEMES FOR THE FISHER EQUATION*

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Abstract. The relationship between the so-called nonstandard finite-difference schemes and the nodal integral method (NIM) is investigated using the Fisher equation as a model problem. Exact and best finite-difference schemes are reviewed first. Next, the NIM for the Fisher equation is developed. It is shown that the NIM leads to a nonstandard evaluation of the derivatives. Moreover, the resulting scheme possesses the desirable characteristics of the nonstandard finite difference schemes, such as the nonlocal evaluation of the nonlinear terms. Thus, the NIM provides a systematic framework to obtain schemes similar to the best finite-difference schemes. Numerical results for a propagating front problem show that the NIM can capture the shape and speed of the front very accurately. Results also show that the best finite-difference scheme is stable for large grid sizes but only at the cost of inaccuracy in the front propagation speed. Additional results are obtained using the NIM for symmetric and asymmetric initial conditions. These describe the interaction of two fronts of advantageous genes that approach each other and merge. It is noted that the traveling fronts evolving from certain asymmetric initial conditions become indistinguishable from those that evolve from symmetric initial conditions.

Key words. nodal integral method, best finite-difference schemes, semianalytical numerical schemes, Fisher equation, wave propagation

AMS subject classifications. 65P99, 77A99

PII. S1064827597325463

1. Introduction. Several nodal methods have been developed over the last two decades to solve partial differential equations (PDEs) [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. A common feature among these is the analytical or semianalytical treatment of at least a part of the PDE(s). This is accomplished, for example, by introducing known solutions of one-dimensional, steady-state problems in multidimensional or time-dependent problems, or by reducing the PDEs to a set of ordinary differential equations (ODEs) via the transverse integration process, and then approximately solving the ODEs. Hence, a class of these methods is also known as analytical nodal methods [6, 8]. A major advantage of these methods is that they yield an accurate solution over large grid/step sizes. Consequently, these methods are especially suitable for problems with large spatial and/or time domains. The details of one particular kind of nodal method—the so-called nodal integral (or integration) method (NIM) [2, 5]—will be given in section 3 in the context of the Fisher equation (FE).

A different approach for the solution of PDEs (and ODEs) that also relies on analytical solutions or conservation laws leads to nonstandard finite-difference (NSFD) schemes such as the exact finite-difference (EFD) and/or the best finite-difference (BFD) schemes [12, 13, 14, 15, 16]. A finite-difference (FD) scheme is called an EFD scheme if the solution for all step sizes at all grid points is equal to the exact analytical solution of the differential equation at the corresponding grid points. It is intuitively expected that only those differential equations that have a closed form exact solution

*Received by the editors August 4, 1997; accepted for publication (in revised form) August 16, 2000; published electronically February 21, 2001.
http://www.siam.org/journals/sisc/22-6/32546.html
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1926
will lead to EFD schemes. Not surprisingly, the interest in the EFD schemes—which are available for a limited number of ODEs and even fewer PDEs—is in their utility in gaining numerical insight for the development of improved FD schemes for problems that do not admit EFD schemes. For differential equations that do not admit EFD schemes, the corresponding notion of BFD schemes is developed—as the next best thing to an EFD scheme. While the idea of the EFD scheme is fairly well defined, the notion of the BFD scheme is a little vague. An FD scheme is called a BFD scheme if the important properties of its solutions correspond exactly to the related properties of the solutions to the differential equation for all values of the step size [15]. Specific important properties may include conservation laws, special cases of known exact solutions, and stability properties of fixed points, etc. BFD schemes for complex problems are developed by taking advantage of the known EFD schemes for simpler problems—imparting an analytical component to the BFD schemes.

A word on terminology: a node in the NIM (which roughly corresponds to the grid point in the FD methods) refers to a finite region in the space of independent variables. The discrete unknowns in the NIM are the phase variables averaged over \((n - 1)\) dimensional surfaces of these nodes, where \(n\) is the number of independent variables in the problem.

Given the properties of the BFD schemes and the NIM, and their similar semi-analytical background, it is desirable to investigate the common features in these schemes with the goal of providing insight for the development of improved schemes. The fact that both schemes rely on specialized procedures specific to the problem at hand necessitates that this exercise be carried out in the context of a specific problem. The FE is chosen here to be the model problem for such a comparison.

The FE

\[
\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} + \lambda u(x,t)(1 - u(x,t))
\]

describes the propagation of an advantageous gene in a one-dimensional infinite medium [17]. Kolmogoroff, Petrovsky, and Piscounov [18] studied this equation and showed, among other properties, that for all bounded initial conditions (ICs) in an infinite domain, the results remain bounded. Canosa [19] developed a second order perturbation solution for the FE for large characteristic speeds. Later, Gazdag and Canosa [20] used the accurate space derivative (ASD) technique [21] to numerically solve the FE and showed the evolution of various ICs into the traveling wave of minimal speed. Convergence of the ASD method required cutting off the right-hand tail of the wave moving toward the right. Moreover, the speed with which an IC evolved to the time-asymptotic minimum speed wave also depended upon the point at which the right-hand tail was cut off. As is shown below, the NIM does not have such restrictions. An excellent review of the FE (and other nonlinear diffusion problems), its properties, and its numerical solutions is given by Sachdev [22].

The rest of this paper is divided into five sections. The EFD and BFD schemes are briefly reviewed in section 2. The NIM is developed for the FE in section 3. The NIM scheme is compared in section 4 with the BFD scheme of Mickens [15], and similarities and differences between the two schemes are identified. Numerical results and discussion are in section 5. Section 6 summarizes the paper.

2. Review of EFDs and BFDs. This section is based on the material in [12, 15, 16]. Consider the following first and second order ODEs:

\[
\frac{dy(t)}{dt} = \mu y(t),
\]

\[
\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} + \lambda u(x,t)(1 - u(x,t))
\]
Various discrete approximations for the derivative in these equations lead to the standard FD schemes for the two equations. By standard FD schemes (SFD), we mean ones in which the derivatives are approximated by, for example, the backward, forward, or central difference formulas. With forward differences for the first derivative and central differences for the second derivative, the discrete forms of (2) and (3) are:

$$\frac{y_j - y_{j-1}}{\Delta t} = \mu y_{j-1}$$

and

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{(\Delta x)^2} + \nu y_i = 0,$$

where the subscript $i$ indicates the spatial grid points and the subscript $j$ indicates the time level. Later, for space- and time-dependent problems, the same subscripts, separated by a comma, will be used. Equations (4) and (5) will be referred to as the SFD schemes for (2) and (3), respectively. But, given the fact that the exact solution of (2) and (3) is known to any sophomore, one can easily construct the exact FD schemes for them by first (exactly) solving the differential equations with the corresponding initial and boundary conditions, and then by rewriting the solution in the same format as (4) and (5) [12]. This leads to:

$$\frac{y_j - y_{j-1}}{\frac{e^{\mu \Delta t} - 1}{\mu}} = \mu y_{j-1}$$

and

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{(\Delta x)^2} + \nu y_i = 0,$$

The SFD schemes—(4) and (5)—and the EFD schemes—(6) and (7)—differ from each other only by the denominators in the approximations of the derivatives. However, the latter schemes have no restrictions on the size of the time step or grid size—the results will always be exact (to machine accuracy). On the other hand, restrictions on the size of these parameters for the SFD schemes are well known. Note that the approximations for the derivatives in the SFD schemes are functions of the discrete variables and the grid size ($\Delta t$ or $\Delta x$), whereas the “approximations” for the derivatives in the EFD schemes depend also on the system parameters ($\mu, \nu$).

This observation that the EFD schemes differ from the SFD schemes by so little (at least in these very simple cases), motivated a similar approach for real problems with no exact solution. As a generalization of the approximation for the first and second order derivatives, a general FD scheme has been suggested [15] in which the denominator in the FD approximations of the derivatives is generalized to functions of the grid size and problem parameters:

$$\frac{y_j - y_{j-1}}{\Psi(\Delta t, \mu)} = \mu y_{j-1}$$
and

\[ \frac{y_{i+1} - 2y_i + y_{i-1}}{\phi(\Delta x, \nu)} + \nu y_i = 0, \]

where \( \Psi(\Delta t, \mu) \) and \( \Phi(\Delta x, \nu) \) behave like

\[ \Psi(\Delta t, \mu) = (\Delta t) + O((\Delta t)^2), \]
\[ \Phi(\Delta x, \nu) = (\Delta x)^2 + O((\Delta x)^3). \]

The fact that (2) and (3) have known exact solutions made it easy, in fact possible, to find EFD schemes for them. For nonlinear ODEs that do not admit exact solutions, other conditions—some generic and some specific to each equation—are imposed to arrive at a BFD scheme. Consider the following equation:

\[ \frac{d^2 y}{dx^2} + \nu y(1 - y) = 0. \]

There is no EFD scheme for (12). Hence, a BFD scheme is developed by preserving the constant of motion of the above ODE (the energy, \( E \), of the nonlinear conservative oscillator) [13]. In arriving at the BFD scheme for (12), it is also required that the BFD scheme for the nonlinear problem must reduce to the EFD for the linear problem when the nonlinear term is absent. The details are given in [13, 16].

While the development of the EFD and BFD schemes for ODEs is seemingly straightforward, extensions to PDEs have relied on somewhat ad hoc methods. One approach is to first develop the EFD/BFD schemes for the subproblems of the PDE in question. Subproblems are simply obtained from the original PDE by considering, for example, the steady-state case, the space-independent case, the linear version of the PDE, etc. These schemes are then combined in such a way that the discrete representation of the PDE reduces to the discrete version of the appropriate continuous subproblem in the corresponding limit [15]. For example, the BFD scheme for the FE is obtained by combining the EFD scheme for the space-independent case \( \frac{d^2 u}{dx^2} = 0 \), the SFD scheme for the \( \lambda = 0 \) case, and the BFD scheme for the time-independent case \( \frac{du}{dt} = 0 \), (12). The BFD scheme for the FE is constructed such that in the appropriate limit the scheme reduces to the proper discrete model of the relevant subequation [16]. This leads to the following discretization for the FE:

\[ \frac{u_{i,j} - u_{i,j-1}}{\left( \frac{\epsilon^{\lambda \Delta t} - 1}{\lambda} \right)} = \frac{4}{\lambda} \left[ \sin \left( \frac{\sqrt{\lambda} \Delta x}{2} \right) \right]^2 \]
\[ + \lambda u_{i,j-1} - \lambda \left( \frac{u_{i+1,j} + u_{i,j} + u_{i-1,j}}{3} \right) u_{i,j-1}, \]

where \( i \) indicates the spatial grid point and \( j \) is the time step counter. Here, the first order time- and the second order space derivatives are approximated by nonstandard approximations similar to those in (6) and (7) for the linear equations with EFD schemes. The nonlinear term in the discretized FE is represented nonlocally, i.e., it is evaluated not at one grid point but rather as the product of the local population density at the previous time step and a population density averaged over the three consecutive grid points at the current time step. This feature—nonlocal evaluation of
the nonlinear terms—appears repeatedly in such schemes. Despite the implicit nature of the other terms, the linear term is evaluated at the previous time step, and so is one of the $u$ variables in the nonlinear ($u^2$) term. These features make this BFD scheme significantly different from SFD schemes. In the next section, where the NIM is developed for the FE, it is shown that the discrete set of equations for the NIM—obtained through a much more systematic procedure than those used to obtain the BFD scheme—also has many of the same features.

3. NIM formulation for the FE. The space-time domain is divided into layers of $n_x$ spatial elements, or nodes, each of width $2a$ in the horizontal (spatial) direction and of height $\Delta t$. Nonuniform nodes in space can easily be incorporated. A coordinate system local to each space-time node is defined with the origin at the bottom-center of the node. See Figure 1. Hence, $-a \leq x' \leq a$, $t_j \leq t' \leq t_j + \Delta t$. The space-averaged/time-dependent and time-averaged/space-dependent population densities over each node $(i, j)$ are defined as

$$\bar{u}_{x,i,j}(t') \equiv \frac{1}{2a} \int_{-a}^{+a} u(x', t') \, dx', \quad (14)$$

$$\bar{u}_{t,i,j}(x') \equiv \frac{1}{\Delta t} \int_{t_j}^{t_j + \Delta t} u(x', t') \, dt', \quad (15)$$

The discrete variables associated with the node $(i, j)$ are $\bar{u}_{x,i,j}(\equiv \bar{u}_{x,i,j}(t' = t_j + \Delta t))$ and $\bar{u}_{t,i,j}(\equiv \bar{u}_{t,i,j}(x' = +a))$. Having defined the transverse-averaged, local phase variables, the next step in the development of the NIM is to reduce the PDE to a set of ODEs—one for each independent variable, obtained by averaging over all independent variables except one. As explained in detail below, the ODEs are then solved, and the constant(s) are eliminated in favor of the discrete variables at node interfaces. A set of coupled algebraic equations for the discrete variables is then obtained by imposing appropriate interface conditions ($C^0$, $C^1$, etc.) at node interfaces.

In general, the ODEs for transverse-averaged variables cannot be solved exactly. Hence, all the terms that can lead to an exact homogeneous solution are retained on the left-hand side, while the other terms are lumped into what is often called the pseudosource term on the right-hand side of the transverse-integrated equations. Complete solutions of the ODEs are written as the sum of the homogeneous and particular solutions. The pseudosource terms, being a function of the dependent variables, must be approximated before the particular solutions for the ODEs can be explicitly written. The pseudosource terms are hence projected onto a complete set of basis functions and truncated at a desired order. The number of terms kept in the expansion determine the order of the numerical scheme [5]. Since the pseudosource terms are unknown, this projection is only formal, and a scheme must be identified to determine the coefficients. Nodal schemes vary based on how these coefficients are determined. One approach is to approximate the pseudosource terms using the discrete variables from the previous iteration [2]. A second approach involves the imposition of certain constraint conditions to arrive at additional algebraic equations to eliminate the coefficients [5]. This is the procedure used below in the development of the NIM for the FE.

The FE allows us the freedom to incorporate the linear term in either the solution of the time-averaged equation, or in the solution of the space-averaged equation, or in both. A priori it is difficult to decide exactly how the linear term must be “divided”
Fig. 1. Schematic diagram of the space-time nodes and discrete variables in the nodal integral method.

between the two ODEs for best results. Hence, we proceed with a general approach which allows us to numerically investigate the role of the linear term in each of the ODEs. The linear term in the FE is hence written as

$$\lambda u(x,t) \equiv \lambda (\alpha + \beta)u(x,t),$$

(16)

where \((\alpha + \beta) = 1\).

Operating on the FE by \(\frac{1}{\Delta t} \int_{t_j}^{t_{j+1}} dt'\), the equation for the time-step averaged, space-dependent, local population density becomes

$$\frac{d^2 \bar{u}'(x')}{dx'^2} + \lambda \bar{u}'(x') = \bar{S}'(x')$$

$$\equiv \frac{1}{\Delta t} \int_{t_j}^{t_{j+1}} \left( \frac{\partial u(x',t')}{\partial t'} - \lambda \beta u(x',t') + \lambda u^2(x',t') \right) dt',$$

and the nodal space-averaged, time-dependent equation—obtained by operating on the FE by \(\frac{1}{2a} \int_{-a}^{a} dx'\)—is
\[ \frac{d\bar{u}^x(t')}{dt'} - \lambda \beta \bar{u}^x(t') = \bar{S}^x(t') \]

\[ = \frac{1}{2a} \int_{-a}^{+a} \left( \frac{\partial^2 u(x', t')}{\partial x'^2} + \lambda \alpha u(x', t') - \mu u^2(x', t') \right) dx', \]

where the subscript \((i, j)\) has been omitted for convenience. The two ODEs are now solved. Note that different combinations of \(\alpha\) and \(\beta\) will yield different functional forms for node interior variation of the space-averaged/time-dependent and time-averaged/space-dependent population densities. Specifically, assuming \(\lambda\) is always positive, a positive, zero, or negative \(\alpha\) will yield (for zeroth order approximation for the pseudosource term), respectively, a trigonometric, quadratic, or exponential variation over the space dimension. Similarly, a positive/negative or zero \(\beta\) will yield, respectively, an exponential or linear variation for the space-averaged population density over time. In the development below, \(\alpha\) may be negative, and hence the trigonometric functions with complex arguments in those cases will actually be exponential (or hyperbolic) functions.

\[ A \ la \ nodal \ integral \ scheme \ [5], \ the \ pseudosource \ terms \ \bar{S}^t(x') \ and \ \bar{S}^x(t') \ in \ (17) \ and \ (18) \ are \ expanded \ in, \ say, \ Legendre \ polynomials, \ and \ truncated \ at \ the \ zeroth \ order—\textit{which} \ is \ known \ to \ lead \ to \ a \ second \ order \ scheme. \ Hence, \ \bar{S}^t(x') \cong \bar{S}^{t0} \ and \ \bar{S}^x(t') \cong \bar{S}^{x0}. \ Equations \ (17) \ and \ (18) \ are \ now \ solved \ over \ the \ node \ \((i, j)\) \ with initial \ and \ boundary \ conditions \ (Figure \ 1) \]

\[ \bar{u}^t(t' = t_j) = \bar{u}_{i,j-1}, \]
\[ \bar{u}^t(x' = -a) = \bar{u}_{i-1,j}, \quad \bar{u}^t(x' = a) = \bar{u}_{i,j}. \]

The results are

\[ \bar{u}^t(x') = \left[ \frac{\bar{S}_{i,j}^{t0}}{\lambda \alpha} \right] - \left[ \frac{2\bar{S}_{i,j}^{x0} - (\lambda \alpha)(\bar{u}_{i,j}^t + \bar{u}_{i-1,j}^t)}{2(\lambda \alpha) \cos(\sqrt{\lambda \alpha} a)} \right] \cos(\sqrt{\lambda \alpha} x') \]

\[ + \left[ \frac{(\bar{u}_{i,j}^t - \bar{u}_{i-1,j}^t)}{2 \sin(\sqrt{\lambda \alpha} a)} \right] \sin(\sqrt{\lambda \alpha} x') \]

and

\[ \bar{u}^x(t') = -\frac{\bar{S}_{i,j}^{x0}}{\lambda \beta} + \left[ \frac{\bar{S}_{i,j}^{x0}}{\lambda \beta} + \bar{u}_{i,j-1}^x \right] e^{\lambda \beta(t' - t_j)}, \]

where, again, it is understood that these are \textit{local} solutions within the space-time node \((i, j)\).

The discrete equation for the time-step-averaged population density, \(\bar{u}^t_{i,j}\), is obtained by requiring the first derivative of the time-step-averaged \(u\) to be continuous at the node interface (continuity of flux condition). Hence, two expressions are evaluated and equated for the derivative \(d\bar{u}^t(x')/dx'\) at the common interface between nodes \(i\) and \((i + 1)\), i.e., \((20)—which is for node \((i, j)\)—is differentiated and evaluated at \(x' = a\), and the result is equated to the derivative of the corresponding equation for the node \((i + 1, j)\) evaluated at \(x' = -a\). This yields the three point scheme that relates \(\bar{u}_{i-1,j}^t, \bar{u}_{i,j}^t, \) \(\), and \(\bar{u}_{i+1,j}^t; \)

\[ \bar{u}_{i+1,j}^t - 2\bar{u}_{i,j}^t + \bar{u}_{i-1,j}^t = \lambda \alpha \bar{u}_{i,j}^t \]

\[ \frac{4}{\lambda \alpha} \left[ \sin(\sqrt{\lambda \alpha} \Delta x) \right]^2 + \lambda \alpha \bar{u}_{i,j}^t = \frac{(\bar{S}_{i,j}^{t0} + \bar{S}_{i+1,j}^{t0})}{2}. \]
The discrete equation for the space-averaged population density for the node, \( \bar{u}^x_{i,j} \), is obtained by simply evaluating (21) at \( t' = (t_j + \Delta t) \):

\[
\frac{\bar{u}^x_{i,j} - \bar{u}^x_{i,j-1}}{e^{\lambda \beta \Delta t} - 1} - \lambda \beta \bar{u}^x_{i,j-1} = \bar{S}^{x0}_{i,j}.
\]

To eliminate the pseudosource terms \( \bar{S}^{t0}_{i,j} \) and \( \bar{S}^{x0}_{i,j} \), two conditions are imposed [5]. First the FE (1) is integrated over the space-time node

\[
\frac{1}{2a\Delta t} \int_{-a}^{+a} \int_{t_j}^{t_j+\Delta t} \left( \frac{\partial u(x',t')}{\partial t'} - \frac{\partial^2 u(x',t')}{\partial x'^2} \right) dx' dt' = 0,
\]

which, using the definitions of the pseudosource terms \( \bar{S}^{t0}_{i,j} \) and \( \bar{S}^{x0}_{i,j} \) from (17) and (18), becomes

\[
\bar{S}^{t0}_{i,j} = \bar{S}^{x0}_{i,j} + \lambda (\bar{u}^{xt}_{i,j})^2,
\]

where the average of the product has been approximated by the product of the averages, which is known to lead to a second order error [5], and the space-time-node-averaged velocity \( \bar{u}_{i,j}^{xt} \) is defined in (26). The second condition is obtained by requiring that the space-time-node-averaged population density obtained by first averaging in time and then in space should be equal to the average population density obtained by first averaging in space and then in time, i.e.,

\[
\bar{u}_t^{x} = \frac{1}{2a} \int_{-a}^{+a} \bar{u}_t(x') dx' = \frac{1}{\Delta t} \int_{t_j}^{t_j+\Delta t} \bar{u}^{x}(t') dt' \equiv \bar{u}^{xt}.
\]

Equation (26) is evaluated by substituting the expressions for \( \bar{u}_t(x') \) and \( \bar{u}^{x}(t') \) from (20) and (21), respectively.

The node-averaged population density and the pseudosource terms are eliminated using (25) and (26) from the set of discrete equations (22) and (23). Expressions for \( \bar{u}^{x}_{i,j} \) and \( \bar{u}_t^{x}_{i,j} \) obtained after eliminating the pseudosource terms, \( \bar{S}^{t0}_{i,j} \) and \( \bar{S}^{x0}_{i,j} \), are given in the appendix. Equations (22), (23), and (25)—with pseudo source terms—are, however, much more instructive in analyzing the discrete form of the FE for the NIM than those given in the appendix (with pseudosource terms eliminated). Here, to explicitly bring out the nonlinear terms in the discrete equations, (23) and (22) are combined with (25) and rewritten below.

\[
\frac{\bar{u}^{x}_{i,j} - \bar{u}^{x}_{i,j-1}}{e^{\lambda \beta \Delta t} - 1} - \lambda \beta \bar{u}^{x}_{i,j-1} + \lambda (\bar{u}^{xt}_{i,j})^2 = \bar{S}^{t0}_{i,j},
\]

\[
\frac{4}{\lambda \alpha} \left[ \sin \left( \frac{\sqrt{\lambda \alpha} \Delta x}{2} \right) \right]^2 + \lambda \alpha \bar{u}_t^{x}_{i,j} - \lambda \left[ \frac{(\bar{u}^{xt}_{i,j})^2 + (\bar{u}^{xt}_{i+1,j})^2}{2} \right] = \frac{(\bar{S}^{t0}_{i,j} + \bar{S}^{x0}_{i+1,j})}{2}.
\]
The structure of the discrete equations and their relationship to each other can now clearly be seen. Both (27) and (28) represent a discrete version of the FE. Hence, when compared with the FE, these equations’ RHSs must represent the terms missing on their LHSs. Equation (27) is missing the diffusion term and the $\alpha$-fraction of the linear term. The zeroth order approximation of the time-step-averaged pseudosource term, RHS of (27), indeed represents these terms missing from the LHS of (27); see (17). Equation (28), on the other hand, is missing the time derivative and the $\beta$-fraction of the linear term. Equation (18) shows that the RHS of (28) indeed represents the terms missing on the LHS, calculated in an average sense over the nodes on both sides of the surface on which the continuity of the derivative condition ($C^1$) is being imposed. Additional comments on the structure of these discrete equations are made in the next section.

4. Comparison of the BFD scheme and the NIM. The most obvious difference between the NIM and the BFD scheme (or the FD schemes in general) is that unlike point values in the FD schemes, the discrete variables in the NIM are the transverse-averaged variables at node surfaces. The number of discrete unknowns per node in the NIM is equal to the number of independent variables. Consequently for the FE, while there is only one unknown, the population density $u_{i,j}$, per grid point in the FD schemes, there are two unknowns (and hence two equations) for each of the space-time node, $(i, j)$, in the NIM: the space-averaged population density at the top surface $\bar{u}_{x,i,j}$ and the time-averaged population density at the right surface $\bar{u}_{t,i,j}$. Hence, care should be exercised when comparing the two schemes.

The implicit BFD scheme for the FE is given by (13). Corresponding discrete equations for the NIM are (27) and (28), which clearly show the similarities with the BFD scheme. In the discrete equation for $\bar{u}_{x,i,j}$, (27), the time-derivative for the space-averaged population density is represented by the nonstandard form, as is the second derivative with respect to $x$ in the discrete equation for the time-averaged population density $\bar{u}_{t,i,j}$, (28). The linear term in the discrete equation for $\bar{u}_{x,i,j}$ (27) is, as in the BFD scheme, evaluated at the previous time step. On the other hand, the linear term in (28) (second term on the LHS) is, in terms of the only appropriate discrete variable, the time-averaged population density at the point where the derivative is being evaluated. For comparison, the (entire) linear term in the BFD scheme is evaluated at the previous time step.

As stated previously, one of the characteristics of the BFD schemes is that the nonlinear terms in the discrete schemes are evaluated nonlocally. In fact, nonlocal evaluation of the nonlinear terms is considered to be essential in a BFD scheme [15]. Precisely how the nonlinear term must be evaluated is not known a priori and varies from one problem to another. For the FE, the $u^2$ term is represented by the product of the local $u$ variable at the previous time step and the average of the population density at three grid points at the current time step. As in the BFD scheme, the NIM also leads to a discrete set of equations that requires nonlocal evaluation of the nonlinear terms. Moreover, the form of the nonlinear terms in the NIM has a precise physical meaning—each of the $u$ variables is simply the average $u$ over the immediate space-time domain that influences the discrete variable being evaluated. Marching in time—given $\bar{u}_{x,i,j-1}$, find $\bar{u}_{t,i,j}$—involves only a single node, and hence the nonlinear term in (27) is simply the square of the average population density in that node, $(i, j)$. See Figure 1. On the other hand, evaluation of the time-step-averaged population density, $\bar{u}_{t,i,j}$ (28), depends upon two nodes, $(i, j)$ and $(i+1, j)$, the unknown being at the interface of these two nodes. The nonlinear term is hence approximated nonlocally.
as the arithmetic average of the square of the space-time-averaged population density in the neighboring nodes on each side.

Both schemes preserve some of the constants of motion. While only the time-independent subproblem of the BFD scheme conserves energy, the general space- and time-dependent NIM does satisfy the original PDE over each space-time node in an integral sense—a direct consequence of one of the conditions imposed to evaluate expressions for the pseudosource terms.

The systematic approach of the NIM for PDEs clearly shows that FD-type schemes that have the properties of the BFD schemes can be developed via a transverse integration process. This systematic approach of the NIM is in contrast with the combining process of the BFD schemes that requires the assembly of the FD schemes for subproblems such that the full model reduces to the BFD or EFD model of the subproblems in the appropriate limits [16].

5. Results and discussion. Four numerical examples are presented. The first example is used to compare the BFD scheme and the NIM. This example is also used to carry out parametric studies on time step size, grid/node size, optimum values of $\alpha$ and $\beta$, etc. The other three problems are chosen to investigate the evolution from different ICs, representing symmetric and asymmetric initial distributions of the population density, leading to the asymptotic solution. Neither the BFD scheme nor

Example 1. The initial population density is 1 for $x < 0$ and zero for $x > 0$. Boundary conditions are set at 0 for $x \rightarrow \infty$, and 1 for $x \rightarrow -\infty$. The initial step-profile in this case evolves to a front with (minimum) wave speed of $c = 2$ and propagates to the right [19]. Boundary conditions for the numerical calculations are specified at $x = -20$ and $x = 80$. The calculations were repeated with boundary conditions specified at $x = -10$ and $x = 30$, and no noticeable differences were found in the results. Results of the BFD scheme at $t = 10$ for $\Delta t = 0.01$ and for various spatial grid sizes are shown in Figure 2a. At a grid size of about 0.333, the solution reaches its asymptotic behavior, and there is no noticeable change in the solution for $\Delta x = 0.25$. The profile compares very well with the second order asymptotic solution given by Canosa [19]. There are no wiggles in the solution even at very coarse grid sizes. However, the wave speed is clearly much higher than the minimum speed of 2 for simulations with large $\Delta x$. The original motivation for the BFD schemes was to take advantage of the EFD schemes of similar equations and develop FD schemes that will be free of elementary instabilities [16]. That goal for simulations with large $\Delta x$ is achieved for the FE, so it seems, only by sacrificing the correct propagation speed. The effect of the time step size on accuracy is reported in Figure 2b. The BFD scheme yields fairly good results even with $\Delta t = 0.05$, and the profile obtained using $\Delta t = 0.01$ is essentially indistinguishable from that obtained with $\Delta t = 0.005$. The population density profiles at different times, obtained with $\Delta x = 0.5$ and $\Delta t = 0.01$, are presented in Figure 2c. As expected, after the initial transient, the front moves with the minimum speed of 2 to the right.

Corresponding results for the NIM are shown in Figures 3 and 4. For all NIM results in this paper, values of the time-step-averaged $u$ variable $\bar{u}_{t,j}$ are plotted at discrete values of the $x$ coordinate. Recall that these are $u$ values at discrete $x$ coordinates but are averaged over the $j$th time step. For the NIM, the role of $\alpha$ and $\beta$ on the accuracy of the results is first investigated with $\Delta t = 0.01$ and a relatively coarse spatial grid size of $\Delta x = 1$ (All combinations of $\alpha$ and $\beta$ studied resulted in
very accurate results at fine mesh sizes.) Results in Figure 3, when compared with the fine grid solution of the BFD scheme (as well as the fine grid NIM solutions), show that the combination \((\alpha, \beta) = (-1, 2)\) yields the most accurate solution. Notice that this means that the node interior spatial solution for the time-step-averaged population density is being represented by hyperbolic functions. It is believed that this choice is dictated by the fact that local spatial segments of the propagating front are better represented (modeled) by hyperbolic functions than by trigonometric functions. Hence, for \(\alpha = -1\), the (local) solution for \(\bar{u}(x')\) is of the form

\[
\bar{u}(x') = -\frac{S_{\text{int}}}{\lambda} + C_1 \sinh(\sqrt{\lambda} x') + C_2 \cosh(\sqrt{\lambda} x').
\]

For problems with a more wavy (oscillatory) spatial solution, a positive value of \(\alpha\) is expected to be optimal. For the rest of the calculations reported in this paper we used \((\alpha, \beta) = (-1, 2)\).

The effect of node size on the results of the NIM is shown in Figure 4a. Comparison of results in Figures 2a and 4a clearly shows that the NIM—though very slightly contaminated by an undershoot for the very large node size of 2.0—yields the same level of accuracy with \(\Delta x = 1\) as the BFD scheme yields with \(\Delta x = 0.25\). Recalling that there are two unknowns in the NIM for each node, compared to the single unknown per grid point for the BFD scheme, the above comparison shows that for the same number of unknowns, the results obtained using the NIM with \(n_x/2\) nodes are comparable in accuracy to the results from the BFD scheme with \(n_x\) grid points.

The time step can similarly be rather large in the NIM. As shown in Figure 4b, for \(\Delta t\) as large as 0.2, the NIM yields very good accuracy. The "error" in the simulation
Fig. 3. Parametric study to determine the effects of the parameters $\alpha$ and $\beta$ on the accuracy of the numerical result for the nodal integral method. $\bar{u}^t_{i,j}$ is plotted at $t = 10$ for different combinations of $\alpha$ and $\beta$.

Fig. 4. Parametric studies for the nodal integral method. Shown are values of $\bar{u}^t_{i,j}$ at discrete values of the $x$ coordinate: (a) Grid effect, (b) time step size effect, (c) propagating front starting from a step function.
with an even larger time-step of $\Delta t = 0.5$ is not as big as it might appear from Figure 4b. Recall that for the NIM, the discrete variable being plotted here is the $u$ variable averaged over the last time-step. Hence, $\bar{u}_{t,j}$ for different $\Delta t$ cases are averaged over different time segments: over $9.99 < t < 10.0$ for the $\Delta t = 0.01$ case, and over $9.5 < t < 10$ for the $\Delta t = 0.5$ case. Consequently, with a propagating speed of 2, the front for the latter case is expected to be about 0.5 units behind the former. Figure 4c shows the traveling front profile at different times obtained using the NIM. As in the BFD case, the front moves with a velocity of 2 to the right after the initial transient.

Results obtained using the BFD scheme and the NIM are compared with their corresponding reference results in Figure 5. For the BFD scheme, the population density $u$ obtained using $\Delta t = 0.1$ and $\Delta x = 0.5$ is plotted at $t = 10$. The corresponding reference solution was obtained using the BFD scheme with $(\Delta x, \Delta t) = (0.25, 0.01)$. For the NIM, the time-step averaged population density is calculated with $\Delta t = 0.1$ and $\Delta x = 1.0$, leading to the same number of discrete unknowns as those in the BFD calculation. The reference result for the NIM was calculated with $(\Delta x, \Delta t) = (0.5, 0.01)$. (See the comment made above in reference to Figure 4b when comparing the results obtained using the NIM with two different time steps.) The propagating front calculated using the BFD scheme is moving faster than the reference solution. The NIM results, however, match very well with the corresponding reference results.

**Examples 2–4.** Evolution of three different ICs is studied in these problems using the NIM. All problems were solved with $\Delta x = 1.0$, $(\alpha, \beta) = (-1, 2)$, and with zero boundary conditions specified at $x = -40$ and $x = 40$. 
The evolution of the initially concentrated population density of the advantageous gene, \( u(x,0) = 1 \) for \(-1 \leq x \leq 1\) and zero elsewhere, is shown in Figure 6a. As expected, strong diffusion initially causes the population density to drop at the site of its initial concentration, but it recovers with time as a result of the (nonlinear) generation term. As time increases, two fronts of the advantageous gene, symmetric about the origin, travel to the left and right with the minimum speed.

To study the interaction of two wave fronts approaching each other, the FE is solved with ICs that are symmetric or asymmetric about the origin. The interaction of two symmetric concentrations of the population density is studied with the IC \( u(x,0) = 1 \) for \(-5 \leq x \leq -4\) and \(4 \leq x \leq 5\), and zero elsewhere. The symmetric evolution of the initial profile is shown in Figure 6b. To study the asymmetric IC and its effect on front propagation, the FE was solved with \( u(x,0) = 1.0 \) for \(4 \leq x \leq 5\) and \(u(x,0) = 0.5\) for \(-5 \leq x \leq -4\), and \(u(x,0) = 0\) elsewhere. The resulting population density profiles at different times are shown in Figure 6c. An interesting feature in the asymmetric IC problem is that at large times \((t > 10)\), the effect of the initial asymmetry disappears and the left moving front and the right moving front have shapes and positions that are almost mirror images of each other (Figure 6c) and, more importantly, are almost the same as those at the corresponding time for the symmetric IC problem; see Figure 6b. For the asymmetric problem, the right moving front—while maintaining the evolution of its own shape and speed that matches with the right moving front in the symmetric problem—helps the left moving front, which is initially smaller, to gain its amplitude. This is accomplished by the asymmetry at the origin which causes diffusion from the right to the left. Being a nonzero-sum game—due to the generation term—the shape and speed of the right moving front is little affected by this generosity.

6. Summary and conclusions. An NIM has been developed for the FE and compared with the corresponding NSFD scheme. It was shown that the nodal integral approach is relatively more systematic than the rather ad hoc development of the NSFD scheme. The discrete variables in the two schemes are different: there are point values in the NSFD scheme and locally averaged variables in the case of the NIM. This, for the FE, leads to twice as many discrete unknowns in the NIM for the same number of grid points as in the NSFD scheme. A higher number of discrete unknowns per node, however, does not pose a limitation on the NIM due to its high accuracy even on coarse meshes.

There are many similarities in the final sets of discrete equations obtained via the two significantly different approaches. Specifically, a rearrangement of the set of discrete equations for the NIM—which is developed without explicitly approximating the derivatives as is common in the FD-type schemes—showed that the first order time- and second order space-derivatives in this approach are indeed approximated by nonstandard representations similar to those used in the NSFD scheme. Moreover, it was shown that the nodal integral scheme has some of the desirable features of the NSFD schemes such as the nonlocal evaluation of the nonlinear terms.

In reference to other possible applications, it must be pointed out that extension of the NIM to higher dimensions is fairly straightforward. Moreover, it has already been applied to sets of PDEs \([2, 5, 7]\). The major drawback of the (standard) NIM is that the scheme is limited to geometric domains that can be formed by a union of rectangles. This limitation results from the transverse-integration step that is used to reduce a PDE in \(N\) independent variables to a set of \(N\) ODEs. Recently developed hybrid nodal schemes for the heat conduction equation \([23]\) and for the
Fig. 6. Evolution from different initial conditions (NIM results): (a) A single lump of concentrated gene at and around the center, (b) two symmetric lumps of concentrated gene, (c) two asymmetric lumps of concentrated gene.
multidimensional, convection-diffusion equation [24] have, however, relaxed this restriction. Hybrid schemes applicable in irregular geometries for other sets of PDEs are under development.

Numerical results presented for the FE for various symmetric and asymmetric ICs showed that both schemes are very accurate on fine mesh sizes. The NIM, however, yields very accurate results even for a relatively coarse mesh size. In fact, results obtained using the NIM with half as many grid points (nodes) as those used in the NSFD scheme—leading to the same number of discrete unknowns in both schemes—were better than the corresponding results obtained using the NSFD scheme.

Appendix. The expressions for $\bar{u}^x_{i,j}$ and $\bar{u}^t_{i,j}$ are given by

$$\bar{u}^x_{i,j} = \frac{f_1 \left( \bar{u}^t_{i-1,j} + \bar{u}^t_{i+1,j} \right) / 2 - f_{10} \bar{u}^t_{i+1,j} - \lambda \left( \bar{u}_{i,j}^{avg} + \bar{u}_{i+1,j}^{avg} \right) - (g_i + g_{i+1})}{f_{12}}$$

where

$$f_1 = \frac{\lambda \alpha}{\sin^2 (\sqrt{\lambda \beta} \alpha)} , \quad f_2 = e^{2 \lambda \beta \tau} , \quad f_3 = \frac{f_2 - 1}{2 \lambda \beta \tau} ,$$

$$f_4 = \frac{\tan (\sqrt{\lambda \beta} \alpha)}{\sqrt{\lambda \beta} \alpha} , \quad f_5 = 2 \tau , \quad f_6 = f_1 - 2 \lambda \alpha ,$$

$$f_7 = \frac{f_5 - 1}{\lambda \beta} , \quad f_8 = \frac{f_4 - 1}{\lambda \alpha} , \quad f_9 = f_7 + f_8 ,$$

$$f_{10} = \frac{f_4}{2 f_9} , \quad f_{11} = -\lambda f_8 , \quad f_{12} = f_1 - 2 \lambda \alpha + f_{10} ,$$

$$g_i = \frac{f_4 \bar{u}^t_{i-1,j} / 2 + f_{11} u_{i,j}^{avg} - f_3 \bar{u}^x_{i,j-1}}{f_9} , \quad \bar{S}^0_{i,j} = f_{10} \bar{u}^t_{i,j} + g_i ,$$

$$\bar{u}_{i,j}^{avg} = \frac{f_3 \bar{u}^x_{i,j-1} + f_7 \left( f_{10} \bar{u}^t_{i,j} + f_4 \bar{u}^t_{i-1,j} - f_3 \bar{u}^x_{i,j-1} \right)}{1 \left( f_7 f_{11} / f_9 \right) \bar{u}_{i,j}^{avg}} .$$

Acknowledgment. The author would like to acknowledge the support provided by the Center for Simulation of Advanced Rockets, University of Illinois at Urbana-Champaign. The Center is supported by the US Department of Energy through the University of California under subcontract B341494.

REFERENCES


