CONF-900418--1

DE89 016859

Convergence Properties of Iterative Algorithms For Solving the Nodal Diffusion Equations

Y. Y. Azmy and Bernadette L. Kirk

Oak Ridge National Laboratory*

Oak Ridge, TN 37831

Paper prepared for International Conference on the

Physics of Reactors: Operation, Design, and Computation

Marseille, France

April 23-27, 1990

*Operated by Martin Marietta Energy Systems, Inc., for the U.S. Department of Energy under Contract No. DE-AC05-84OR21400.

CONVERGENCE PROPERTIES OF ITERATIVE ALGORITHMS FOR SOLVING THE NODAL DIFFUSION EQUATIONS

Y. Y. Azmy and Bernadette L. Kirk
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6363

ABSTRACT

We derive the five point form of the nodal diffusion equations in two-dimensional Cartesian geometry and develop three iterative schemes to solve the discrete-variable equations: the unaccelerated, partial Successive Over Relaxation (SOR), and the full SOR methods. By decomposing the iteration error into its Fourier modes, we determine the spectral radius of each method for infinite medium, uniform model problems, and for the unaccelerated and partial SOR methods for finite medium, uniform model problems. Also for the two variants of the SOR method we determine the optimal relaxation factor that results in the smallest number of iterations required for convergence. Our results indicate that the number of iterations for the unaccelerated and partial SOR methods is second order in the number of nodes per dimension, while, for the full SOR this behavior is first order, resulting in much faster convergence for very large problems. We successfully verify the results of the spectral analysis against those of numerical experiments, and we show that for the full SOR method the linear dependence of the number of iterations on the number of nodes per dimension is relatively insensitive to the value of the relaxation parameter, and that it remains linear even for heterogenous problems.

I. INTRODUCTION

Mostly all practical applications involving the solution of the neutron diffusion equations require implementation of an iterative scheme which operates successively on an initial guess until it converges to the solution. Occasionally, situations arise where such iterative algorithms converge extremely slowly (or sometimes diverge altogether) in which case, the development of effective acceleration methods can be crucial for the success of the calculation.

In Sect. II of this paper, we develop an iterative scheme (unaccelerated) for solving the nodal diffusion equations in the five-point form, as well as a partial Successive Over Relaxation (SOR), and full SOR methods. In Sect. III, we show via a spectral analysis of these methods performed on an infinite medium, homogeneous, model problem that the first two require a number of iterations that is second order in the number of nodes per dimension, while this relation is first order for the full SOR. Repeating the analysis on a finite medium, homogenous, model problem for the unaccelerated and partial SOR methods shows a reduction in the number of iterations, but retains its second order dependence on the number of nodes per dimensions. The spectral analysis also yields expressions for the optimal relaxation factor for the two variants of the SOR method. Finally in Sect. IV, we present the results of several numerical experiments performed with codes implementing the three iterative schemes, which we use to verify the spectral analysis.

II. A FIVE-POINT NODAL INTEGRAL METHOD FOR THE NEUTRON DIFFUSION EQUATION

The nodal integral method[1] has been developed for a wide class of PDEs, and has been applied[1] to the neutron diffusion equation resulting in a weighted difference form for the nodal balance equation that is much simpler than previous derivations of equivalent methods.[2,3] However, the questions of evaluating the transverse-leakage terms and closing the system of algebraic equations with the appropriate continuity conditions in this formulation have not been addressed until very recently,[4] where a five-point scheme was derived via the nodal integral method for the two-dimensional neutron diffusion equation. In this section, we briefly review this derivation for fixed source, steady state, monoenergetic problems in two-dimensional Cartesian geometry. Then we present the iterative methods used to solve these equations,[4-6] which are analyzed in the remainder of this paper. Generalization of the five-point scheme presented here to an analogous seven-point scheme in three-dimensional Cartesian geometry is straightforward, and iterative procedures to solve them can be developed by direct analogy. Multigroup and/or criticality (eigenvalue) problems can be solved using the standard inner/outer iterative procedure through which the calculation is broken-up into a sequence of fixed source calculations, updating the source every iteration. Hence the method presented here can be viewed as the "kernel" for more general, production type calculations.

The continuum diffusion equation in the (x,y) plane is given by,

$$-\frac{\partial}{\partial x}\,D\,\frac{\partial \phi}{\partial x}-\frac{\partial}{\partial y}\,D\,\frac{\partial \phi}{\partial y}+\sigma\,\phi = S,\ (x,y)\in[0,X]\times[0,Y]\ , \tag{1}$$

where D and σ are the diffusion coefficient and the macroscopic removal cross section, respectively, ϕ is the scalar flux, and S is the fixed, i.e. nonhomogeneous, source. Equation (1) is normally augmented with a set of boundary conditions specific to the physical problem being solved, and in general represents a linear combination of the flux and net current on the edges of the domain of the problem. The initial step in the nodal integral method is to divide the problem domain into I×J rectangles of the form $[x_{i-1}, x_i] \times [y_{j-1}, y_j]$, i=1,..., I, and j=1, ..., J, where $x_o=0=y_o$, and $x_I=X$, $y_J=Y$. The nuclear parameters D and σ, and the source S are considered to be constant over each computational cell, or "node," so that they are globally piecewise constant.

The discrete-variables employed in nodal diffusion methods are node-averaged quantities and transverse-averaged, surface-evaluated quantities. It has been shown that these can be fluxes, net, or partial currents, all resulting in mathematically equivalent methods.[1] Here we use as discrete-variables the node-averaged flux, defined by,

$$\bar{\bar{\phi}}_{ij} \equiv \frac{1}{(x_i - x_{i-1})(y_j - y_{j-1})}\int_{x_{i-1}}^{x_i} dx \int_{y_{j-1}}^{y_j} dy\ \phi(x,y)\ , \tag{2}$$

the x-averaged flux evaluated at the surface y_j, defined by,

$$\bar{\phi}^{x}_{ij} \equiv \frac{1}{(x_i - x_{i-1})}\int_{x_{i-1}}^{x_i} dx\ \phi(x,y_j)\ , \tag{3}$$

and an analogously defined y-averaged flux evaluated at the surface x_i, denoted by $\bar{\phi}^y_{ij}$. The nodal integral method prescription for deriving the nodal diffusion equations from Eq. (1) consists of the following steps.[1] First Eq. (1) is integrated over the volume of node i,j, and we apply the piecewise-constant property of D and σ, to obtain the nodal balance equation relating the node-averaged flux to the transverse-averaged net currents evaluated on the four surfaces bounding node i,j. Second, we transverse-average Eq. (1) once with respect to x, then replace the x-leakage term by its average value over the node to obtain a second order ODE in the x-averaged, y-dependent flux. These are solved exactly in terms of the eigenfunctions of the one-dimensional diffusion operator, i.e. hyperbolic sines and cosines for subcritical systems, and the arbitrary constants are expressed as combinations of $\bar{\phi}^x_{i,j-1}$ and $\bar{\phi}^x_{ij}$. The resulting expression is integrated once with respect to y to yield the node-averaged and x-averaged fluxes; then it is differentiated once with respect to y and evaluated at y_{j-1} and y_j to yield a relation between the x-averaged fluxes and currents on the x=constant surfaces of the node. Analogous steps are performed on Eq. (1) in the y-direction. All these expressions are combined to result in an expression for each of the transverse-averaged net currents at the node surfaces in terms of the node averaged flux and the transverse-averaged flux in the same direction. For example the x-averaged y-currents evaluated within node i,j, as y approaches the surfaces y_j and y_{j-1} have the form,

$$-D_{ij}\left.\frac{d\bar{\phi}^x}{dy}\right|^{\pm}_{ij} = -D_{ij}\left[(1\pm\omega^y_{ij})\bar{\phi}^x_{ij} - (1\pm\omega^y_{ij})\,\bar{\phi}^x_{i,j-1} \mp 2\omega^y_{ij}\,\bar{\bar{\phi}}_{ij}\right]/P^y_{ij}\,(y_j - y_{j-1}) \quad , \tag{4}$$

respectively, where we have defined the piecewise constant parameters,

$$P^y_{ij} \equiv \frac{\tanh\left[\gamma_{ij}(y_j - y_{j-1})/2\right]}{\gamma_{ij}(y_j - y_{j-1})/2} \quad , \tag{5.a}$$

$$\omega^y_{ij} \equiv \frac{\tanh^2\left[\gamma_{ij}(y_j - y_{j-1})/2\right]}{(1 - P^y_{ij})} \quad , \tag{5.b}$$

and $1/\gamma_{ij} \equiv \sqrt{D_{ij}/\sigma_{ij}}$ is the diffusion length.

Now the transverse-averaged net currents can be eliminated from the nodal balance equation described above to yield,

$$-\frac{D_{ij}}{2}\left\{\left(\frac{2\gamma_{ij}P^x_{ij}}{1 - P^x_{ij}}\right)\left(\bar{\phi}^y_{ij} - 2\bar{\bar{\phi}}_{ij} + \bar{\phi}^y_{i-1,j}\right) + \left(\frac{2\gamma_{ij}P^y_{ij}}{1 - P^y_{ij}}\right)\left(\bar{\phi}^x_{ij} - 2\bar{\bar{\phi}}_{ij} + \bar{\phi}^x_{i,j-1}\right)\right\} + \sigma_{ij}\bar{\bar{\phi}}_{ij} = S_{ij} \quad , \; i=1,\ldots,I,\; j=1,\ldots,J \quad . \tag{6}$$

Clearly, Eq. (6) is a weighted difference form of the original PDE, Eq. (1). Continuity of the net currents across node boundaries (and possibly their discontinuity at internal surface sources for example) is enforced through the condition,

$$D_{ij} \frac{d\bar{\phi}^x}{dy} \Bigg|_{ij}^{+} = D_{i,j+1} \frac{d\bar{\phi}^x}{dy} \Bigg|_{i,j+1}^{-}, \quad i=1,....I, \; j=1,....,J-1, \tag{7}$$

where the net currents are given by Eq. (4). An analogous condition in the other direction guarantees the continuity of the x-current across x=constant node boundaries. Equations (6), (7), and its analogue constitute (3IJ-I-J) linear equations each involving five unknown variables. These are augmented by 2I and 2J general boundary conditions on the x and y=constant global boundaries thus bringing the number of algebraic equations to (3IJ+I+J), the same number of unknown variables, $\bar{\bar{\phi}}_{ij}$, $\bar{\phi}^x_{ij}$, and $\bar{\phi}^y_{ij}$. Direct methods can be used to solve this system, but for most practical applications iterative methods are essential due to memory size and execution time limitations. In the remainder of this section we present an iterative method previously developed and implemented for solving this system,[4-6] then we present a partial Successive Over Relaxation (SOR) scheme that has been used to accelerate convergence,[5,6] and finally we present a full SOR scheme which more effectively reduces the number of iterations. Stability of the three iterative methods will be analyzed and verified in the remainder of this paper.

II.1. The Iterative Method for Solving the Nodal Method Equations

A careful examination of the nodal integral method balance and current continuity equations reveals a very loose coupling between the three sets of equations that has been exploited into an iterative scheme to solve them.[4-6] The current continuity conditions for each row or column is completely uncoupled from those for other rows or columns, respectively; however, they are coupled to those for other columns or rows, respectively and to the balance equations via the node-averaged fluxes. Hence, if the latter quantities are iterated upon in the balance equation, Eq. (6), each set of row or column current continuity equations will form a tridiagonal system of equations that is completely uncoupled from the rest of the system. To be more specific, let the left superscript n indicate the n-th iterate of the node- or transverse-averaged flux. Then the iterative procedure is represented by,

$$\begin{aligned} &-\beta^y_{ij}(1-\omega^y_{ij})\,{}^n\bar{\phi}^x_{i,j-1} + (\beta^y_{ij}+\beta^y_{i,j+1})(1+\omega^y_{ij})\,{}^n\bar{\phi}^x_{ij} \\ &-\beta^y_{i,j+1}(1-\omega^y_{i,j+1})\,{}^n\bar{\phi}^x_{i,j+1} = 2\beta^y_{ij}\omega^y_{ij}\,{}^{n-1}\bar{\bar{\phi}}_{ij} + 2\beta^y_{ij+1}\omega^y_{i,j+1}\,{}^{n-1}\bar{\bar{\phi}}_{i,j+1}, \end{aligned} \tag{8}$$

and an analogous equation for the x-current, and

$${}^n\bar{\bar{\phi}}_{ij} = \left[\frac{S_{ij}}{\sigma_{ij}} + \pi^x_{ij}\left(\frac{{}^n\bar{\phi}^y_{ij} + {}^n\bar{\phi}^y_{i-1,j}}{2}\right) + \pi^y_{ij}\left(\frac{{}^n\bar{\phi}^x_{ij} + {}^n\bar{\phi}^x_{i,j-1}}{2}\right)\right] / (1+\pi^x_{ij}+\pi^y_{ij}), \quad n\geq 1, \tag{9}$$

where ${}^0\bar{\bar{\phi}}_{ij}$ is a specified initial guess; and

$$\beta^y_{ij} \equiv D_{ij}/P^y_{ij}(y_j - y_{j-1}), \tag{10.a}$$

$$\pi^y_{ij} \equiv P^y_{ij}/(1-P^y_{ij}), \tag{10.b}$$

with analogous definitions for β_{ij}^{x} and π_{ij}^{x}. Eq. (8) represents (J-1) equations for each column of nodes which can be solved using an efficient tridiagonal solver routine, such as DGTSL of LINPACK.[7] Similarly its x-currents analogue represents a tridiagonal system of order (I-1) for each row of nodes that can be solved using DGTSL. Updating the nodal flux via Eq. (9) is straightforward as it does not involve solving simultaneous equations.

II.2 The Partial SOR Iterative Method

Convergence of the iterative method presented above can be significantly accelerated by applying the SOR technique. Initial development of this technique concentrated on relaxing only the node-averaged fluxes,[4-6] but not the transverse-averaged fluxes (hence the term partial). This approach optimizes memory size requirements, as it avoids storage of any additional arrays beyond the unaccelerated method. The partial SOR iterative procedure is represented by the tridiagonal systems, Eq. (8) and its x-current analogue, and the balance equations,

$$\overset{n=}{\phi}_{ij} = (1-\Omega)\overset{n-1=}{\phi}_{ij} + \Omega\left[\frac{S_{ij}}{\sigma_{ij}} + \pi_{ij}^{x}\left(\frac{\overset{n-y}{\phi}_{ij} + \overset{n-y}{\phi}_{i-1,j}}{2}\right)\right. \tag{11}$$

$$\left. + \pi_{ij}^{y}\left(\frac{\overset{n-x}{\phi}_{ij} + \overset{n-x}{\phi}_{ij-1}}{2}\right)\right] /(1+\pi_{ij}^{x} + \pi_{ij}^{y}),\ n \geq 1,$$

where Ω is the relaxation parameter, $0 < \Omega < 2$. This iterative method has been previously shown to result in a large reduction in the total number of iterations at no virtual cost to the memory requirement or the CPU execution time per iteration;[4-6] clearly the total execution time is drastically reduced.

II.3 The Full SOR Iterative Method

The motivation for developing the full SOR technique for the nodal diffusion method is the experimentally observed $O(I^2)$ behavior of the number of iterations for a "square" (i.e. J=I) test problem, which is contrary to the usual O(I) behavior for the SOR method.[8,9] In this method, the transverse-averaged fluxes are also relaxed with the same relaxation parameter as that for the node-averaged flux. This method is represented by the tridiagonal systems,

$$-\beta_{ij}^{y}(1-w_{ij}^{y})\overset{n-x}{\phi}_{i,j-1} + (\beta_{ij}^{y}+\beta_{i,j+1}^{y})(1+w_{i,j+1}^{y})\overset{n-x}{\phi}_{ij} - \beta_{i,j+1}^{y}(1-w_{ij}^{y})\overset{n-x}{\phi}_{i,j+1}$$

$$= (1-\Omega)\left[-\beta_{ij}^{y}(1-w_{ij}^{y})\overset{n-1-x}{\phi}_{i,j-1} + (\beta_{ij}^{y}+\beta_{i,j+1}^{y})(1+w_{ij}^{y})\overset{n-1-x}{\phi}_{ij}\right.$$

$$\left. - \beta_{i,j+1}^{y}(1-w_{i,j+1}^{y})\overset{n-1-x}{\phi}_{i,j+1}\right] + 2\Omega\left[\beta_{ij}^{y}\, w_{ij}^{y}\overset{n-1=}{\phi}_{ij} + \beta_{i,j+1}^{y} w_{i,j+1}^{y}\overset{n-1=}{\phi}_{i,j+1}\right], \tag{12}$$

and its x-current analogue for calculating the transverse-averaged fluxes, and Eq. (11) for updating the nodal flux. Clearly, this method would require storing the arrays of x-averaged and y-averaged fluxes, which have sizes I(J+1) and J(I+1), respectively, between iterations. However, this is a very mild price to pay compared to the tremendous reduction in the number of iterations as shown in the following sections.

III. SPECTRAL ANALYSIS OF THE ITERATIVE METHODS FOR SOLVING THE NODAL EQUATIONS

Spectral, or Fourier mode, analysis methods have often been used to establish the stability of iterative methods for solving linear systems of equations, and to determine the effectiveness of acceleration methods in reducing the number of iterations required for convergence.[8,9] Such analysis has been used extensively in the nuclear field to evaluate the convergence properties of several transport methods and Diffusion Synthetic Acceleration methods.[10-13] For elliptic systems, Fourier analysis has been used in studying the convergence of mostly all classical iteration strategies,[8,9] and several modern strategies[14] for solving the discrete-variable form of model elliptic PDEs. In this section, we evaluate the spectral radius for the three iterative methods developed in Sect. II for solving the nodal diffusion equations. Due to similarity of the analyses of the three methods we will first detail the analysis of the unaccelerated method, then briefly outline the procedure for the partial and full SOR methods, stressing the differences between the three derivations and presenting the final expressions for the spectral radius.

III.1 Spectral Analysis of the Unaccelerated Method

The spectral analysis is concerned with estimating the smallest reduction per iteration of the error in the variables iterated on; hence we define the node-averaged flux-difference,

$$\overset{n=}{\Phi}_{ij} \equiv \overset{n+1=}{\phi}_{ij} - \overset{n=}{\phi}_{ij}, \tag{13}$$

and analogous definitions for $\overset{n-x}{\Phi}_{ij}$ and $\overset{n-y}{\Phi}_{ij}$. Evaluating Eqs. (8), its x-current analogue, and (9) at iterations (n+1) and n, then subtracting the resulting expressions yields three corresponding equations in which each ϕ is replaced by Φ, and S_{ij} is set to zero. Furthermore, the model problem used in the analysis has a uniform material composition, and uniform x and y dimensions of the computational cells, 2a and 2b respectively. Therefore, the node indices on the parameters ω and π are superfluous, so we suppress them, and the parameters β factor out so that without loss of generality we set them to unity. The analysis is based on the ansatz that the difference quantities are completely decomposable into their Fourier modes,

$$\overset{n=}{\Phi}_{ij} = {}^{n}\epsilon \exp\left[i(\lambda_x x_i + \lambda_y y_j)\right] , \tag{14.a}$$

$$\overset{n-x}{\Phi}_{ij} = {}^{n}\zeta_y \exp\left[i\lambda_x x_i + i\lambda_y (y_j + b))\right] , \tag{14.b}$$

$$\overset{n-y}{\Phi}_{ij} = {}^{n}\zeta_x \exp\left[i\lambda_x (x_i + a) + i\lambda_y y_j)\right] , \tag{14.c}$$

where λ_x and λ_y are the Fourier variables. Substituting Eqs. (14) into the equations involving the flux-difference quantities described above results in,

$$ {}^{n}\zeta_y = {}^{n-1}\epsilon w^y \cos(\lambda_y b)/\left[w^y \cos^2(\lambda_y b) + \sin^2(\lambda_y b)\right] , \tag{15.a} $$

$$ {}^{n}\zeta_x = {}^{n-1}\epsilon w^x \cos(\lambda_x a)/\left[w^x \cos^2(\lambda_x a) + \sin^2(\lambda_x a)\right] , \tag{15.b} $$

$$ {}^{n}\epsilon = \left[{}^{n}\zeta_x \pi^x \cos(\lambda_x a) + {}^{n}\zeta_y \pi^y \cos(\lambda_y b)\right]/(1 + \pi^x + \pi^y) . \tag{15.c} $$

It follows immediately from Eqs. (15) that ${}^{n+1}\zeta_y/{}^{n}\zeta_y = {}^{n+1}\zeta_x/{}^{n}\zeta_x = {}^{n}\epsilon/{}^{n-1}\epsilon \equiv \epsilon_u$, where ϵ_u is the constant eigenvalue of the unaccelerated iterations; thus without loss of generality we set ${}^{n}\epsilon = (\epsilon_u)^n$.

Solving Eqs. (15) simultaneously for the iteration eigenvalue we obtain,

$$ \epsilon_u(\lambda_x, \lambda_y) = \left[\frac{\pi^x w^x \cos^2(\lambda_x a)}{w^x \cos^2(\lambda_x a) + \sin^2(\lambda_x a)} + \frac{\pi^y w^y \cos^2(\lambda_y b)}{w^y \cos^2(\lambda_y b) + \sin^2(\lambda_y b)}\right]/(1 + \pi^x + \pi^y) . \tag{16} $$

Examining Eq. (16) yields four important properties of the eigenvalue in the Fourier plane:

i - ϵ_u is periodic in λ_x and λ_y with periods π/a and π/b, respectively;
ii - ϵ_u is symmetric about the λ_x and λ_y axes;
iii - ϵ_u is positive definite over the entire Fourier plane for all physically acceptable parameter values;
iv - ϵ_u is monotonically decreasing over the rectangle $[0,\pi/2a] \times [0,\pi/2b]$ in the Fourier plane.

From these properties, the definition of the spectral radius of the unaccelerated method for the infinite medium model problem reduces to,

$$ \rho_u = \max_{\substack{0 \le \lambda_x \le \pi/2a \\ 0 \le \lambda_y \le \pi/2b}} \epsilon_u(\lambda_x, \lambda_y) = \epsilon_u(0,0); \tag{17} $$

that is,

$$ N_u = \log(E)/\log(\rho_u) , \tag{18} $$

In order to achieve convergence within E of the iteration limit, therefore, requires,

$$ \rho_u = (\pi^x + \pi^y)/(1 + \pi^x + \pi^y) . \tag{19} $$

iterations, which is second order in the larger of $1/\gamma a$ and $1/\gamma b$, similar to the results of spectral analyses of conventional finite-difference approximations of elliptic equations.

This analysis can be refined by using a finite size model problem.[8,9] In this case, only a finite number of Fourier modes will be available, and the largest eigenvalue will correspond to the mode closest to the origin in the Fourier plane, $\lambda_x = \pi$, $\lambda_y = \pi$, by the periodic property of ϵ_u. In this case, the spectral radius for the finite medium model problem is

$$\bar{\rho}_u = \left[\frac{w^x \pi^x}{w^x + \tan^2(\pi a)} + \frac{w^y \pi^y}{w^y + \tan^2(\pi b)}\right] / (1 + \pi^x + \pi^y) < \rho_u \ . \tag{20}$$

which requires fewer iterations than the infinite medium case: however, the number of iterations is still quadratic in the largest of the number of nodes in the x or y directions.

III.2 Spectral Analysis of the Partial SOR Method

Rewriting the equations for this method, Eqs. (8), its x-current analogue, and Eq. (11) in terms of the flux-difference quantities, then using the Fourier mode decomposition, Eqs. (14) yields the infinite medium, partial SOR, iteration eigenvalue,

$$\epsilon_p(\lambda_x, \lambda_y; \Omega) = 1 - \Omega + \Omega \ \epsilon_u(\lambda_x, \lambda_y) \ . \tag{21}$$

Equation (21) shows that ϵ_p shares with ϵ_u the periodic, symmetry, and monotonic properties mentioned before. The relaxation paramater, Ω, is chosen so as to minimize the partial SOR spectral radius,

$$\Omega_p = \left[1 - \frac{(\pi^x + \pi^y)/2}{(1 + \pi^x + \pi^y)}\right]^{-1} , \tag{22}$$

which yields the minimum spectral radius,

$$\rho_p = (\pi^x + \pi^y)/(2 + \pi^x + \pi^y) \ . \tag{23}$$

In the limit of very fine meshes $\Omega_p \rightarrow 2$, as previously observed in numerical tests,[4,5] while the number of partial SOR iterations required for convergence

$$N_p \longrightarrow \frac{3(a^2 + b^2)}{2(\gamma a b)^2} \log(1/E) \ , \tag{24}$$

which is half the number of unaccelerated iterations, but still second order in I, where without loss of generality we have assumed I≥J.

Analysis of the finite medium model problem yields a relation between ϵ_p and ϵ_u that is analogous to Eq. (21), which can be used to evaluate the optimum relaxation parameter and spectral radius. As expected, the optimum spectral radius is smaller than for the infinite medium partial SOR method case, but the number of iterations is similarly second order in I. In the special case I=J the resulting expressions for the optimum relaxation parameter and spectral radius are,

$$\bar{\Omega} = \left[1 - \left(\frac{w^x \pi^x}{1 + 2\pi^x}\right)\left\{\frac{1}{w^x + \tan^2(\pi a)} + \frac{1}{w^x + \cot^2(\pi a)}\right\}\right]^{-1} , \tag{25}$$

$$\bar{\rho} = \left(\frac{w^x \pi^x \bar{\Omega}}{(1 + 2\pi^x)}\right)\left|\frac{1}{w^x + \tan^2(\pi a)} - \frac{1}{w^x + \cot^2(\pi a)}\right| . \tag{26}$$

III.3 SPECTRAL ANALYSIS OF THE FULL SOR METHOD

Repeating the same procedure for the full SOR method, Eqs. (12), its x-current analogue, and (11), produces a quadratic equation for the iteration eigenvalue,

$$(\epsilon_f + \Omega - 1) \;=\; \epsilon_f(\Omega^2 \epsilon_u)\,. \tag{27}$$

Comparing the two branches of $\epsilon_f(\lambda_x, \lambda_y; \Omega)$ that satisfy Eq. (27) shows that the eigenvalue with the largest magnitude is given by,

$$\max|\epsilon_f(\epsilon_u,\Omega)| = \left|1 - \Omega + \frac{\Omega^2\epsilon_u}{2} \;+\; \sqrt{[1 - \Omega + \frac{\Omega^2\epsilon_u}{2}]^2 \;-\; (1-\Omega)^2}\right|,$$

$$\text{if } \Omega \le \frac{2 - 2\sqrt{1-\epsilon_u}}{\epsilon_u}\,,$$

$$= \Omega - 1\,, \text{ if } \Omega > \frac{2 - 2\sqrt{1-\epsilon_u}}{\epsilon_u}\,, \tag{28}$$

where $\epsilon_u\,(\lambda_x, \lambda_y)$ is given by Eq. (16). This expression depends on λ_x and λ_y only through ϵ_u, therefore $\max|\epsilon_f|$ is periodic, and symmetric like ϵ_u, and is monotonically decreasing with increasing ϵ_u. Hence the slowest converging mode corresponds to $\lambda_x=\lambda_y=0$, and its eigenvalue is monotonically decreasing (increasing) with increasing Ω such that $\Omega \le [2\text{-}2\sqrt{1\text{-}\rho_u}]/\rho_u$ ($\Omega > [2\text{-}2\sqrt{1\text{-}\rho_u}]/\rho_u$) respectively. The optimal relaxation parameter therefore becomes,

$$\Omega_f \;=\; \left[2 - 2\sqrt{1-\rho_u}\right]/\rho_u\,, \tag{29}$$

and the full SOR spectral radius is.

$$\rho_f \;=\; \frac{2 - 2\sqrt{1-\rho_u}}{\rho_u} - 1\,. \tag{30}$$

In the limit of very fine meshes, the number of full SOR iterations required for convergence in the infinite medium case is,

$$N_f \rightarrow \frac{\sqrt{3(a^2+b^2)}}{2\gamma ab}\log\,(1/E)\,, \tag{31}$$

which is first order in the number of computational cells in each direction, consistent with classical results.[8,9]

IV. NUMERICAL RESULTS

The three iterative methods developed in Sect. II and analyzed in Sect. III were implemented in computer codes.[4-6] In this section, we verify the spectral analysis results by comparing actual numbers of iterations required for convergence to the solution of a homogeneous problem by each method to those derived by the spectral analysis. Then we consider an inhomogeneous problem and show that if the relaxation parameter is chosen close

to the value based on the longest diffusion length in the system, the number of iterations retains its first order dependence on the number of unknowns per dimension even though it is not optimal.

The homogeneous test problem is a unit square region divided into I×I computational cells (I even) each of dimension 2a × 2a, where a=1/2I. Dirichlet boundary conditions are imposed on all four external surfaces, and the fixed source is unity in the square [0..5] × [0..5] and zero otherwise. The nuclear properties are represented by uniform $\gamma=10$, and the number of iterations required by each method to achieve convergence within $E=10^{-4}$ of the solution is measured as a function of I. These results are plotted in Fig. 1 in comparison with the analytical expressions derived in Sect. III for the infinite and finite medium model problems. For the partial and full SOR methods the theoretically predicted optimal relaxation parameter is used in the numerical experiments. The good agreement between the observed and theoretically predicted behavior is apparent from Fig. 1 in particular for the unaccelerated and partial SOR methods. The discrepancy in the case of full SOR is due to the fact that the relaxation factor used in the numerical experiments is not optimal since it is based on the infinite medium analysis, thus resulting in a larger number of iterations than predicted by the analysis. However, as clear from the results, the number of iterations remains linear in I, in spite of the lack of optimality of the relaxation factor.

Finally, a heterogeneous test problem with the same geometry, external source, and boundary conditions as above was solved using the full SOR method. The nuclear properties of the four quadrants were chosen to be $\gamma=10$ in two diagonally-opposite quadrants, and $\gamma=5$, and 20 in the two other quadrants. The infinite medium model problem with uniform $\gamma=5$ and I=10, 20, 30, and 40 has optimal relaxation factors 1.82, 1.90, 1.93, and 1.95, respectively, by Eq. (29), which when used in the code converges to the solution in 70, 129, 186, and 262 iterations, respectively, close to linear in I. Furthermore, for these four cases, the actual optimal relaxation factors were determined experimentally to be 1.70, 1.83, 1.88, and 1.91, and the corresponding optimal number of iterations required for convergence were found to be 39, 78, 120, and 153, respectively.

We conclude that the full SOR method is very effective in reducing the number of iterations necessary for solving the nodal diffusion equations at a very low additional CPU cost per iteration and the storage of two additional arrays. The behavior of the number of iterations as a function of the number of nodes per dimension was shown to be linear even when the relaxation factor is not optimal, or the material composition is not uniform. Because the additional computational cost expended in the acceleration is minuscule, the full SOR may indeed require shorter CPU time to converge the nodal diffusion method equations than other more sophisticated methods, such as multigrids.

REFERENCES

1. Y. Y. AZMY, "Nodal Methods for Problems in Fluid Mechanics and Neutron Transport," PhD Thesis, University of Illinois, Urbana, 1985. See also Y. Y. AZMY and J. J. DORNING, "A Nodal Integral Approach to the Numerical Solution of Partial Differential Equations," *Advances in Reactor Computations*, p. 893, American Nuclear Society, 1983.

2. J. DORNING, "A Review of Local Green's Function Coarse-Mesh and Nodal Methods for the Numerical Solution of Fluid Flow Problems," *Advances in Mathematical Methods*

for the Solution of Nuclear Engineering Problems, Vol. 1, p. 437, American Nuclear Society, 1981.

3. R. D. LAWRENCE, "Progress in Nodal Methods for the Solution of the Neutron Diffusion and Transport Equations," *Prog. Nucl. Energy*, 17, 271 (1986).

4. B. L. KIRK and Y. Y. AZMY, "A Parallel Approach to the Nodal Method Solution of the Two-Dimensional Neutron Diffusion Equation," *Advances in Nuclear Engineering Computation and Radiation Shielding*, Vol 1, 23, American Nuclear Society, 1989.

5. B. L. KIRK and Y. Y. AZMY, "Hypercube Applications of the $x - y$ Geometry Nodal Method for the Neutron Diffusion Equation," *Trans. Am. Nucl. Soc.* 57, p. 104, 1988.

6. B. L. KIRK and Y. Y. AZMY, "An Iterative Algorithm for Solving the Multidimensional Neutron Diffusion Nodal Method Equations on Parallel Computers," Submitted for publication in *J. Comput. Phys.*

7. JACK DONGARRA, LINPACK Subroutines, Argonne National Laboratory, Argonne, Illinois, 1978.

8. E. L. WACHSPRESS, *Iterative Solution of Elliptic Systems*, Prentice-Hall, 1966.

9. RICHARD S. VARGA, *Matrix Iterative Analysis*, Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962.

10. E. M. GELBARD and L. A. HAGEMAN, "The Synthetic Method as Applied to the S_n Equations," *Nucl. Sci. Engr.*, 37, 288 (1969).

11. E. W. LARSEN, "Unconditionally Stable Diffusion-Synthetic Acceleration Methods for the Slab Geometry Discrete Ordinates Equations. Part I: Theory," *Nucl. Sci. Engr.*, 82, 47 (1982).

12. WARREN F. MILLER, JR. and EDWARD W. LARSEN, "Modified Diffusion Synthetic Acceleration Algorithms," *Nucl. Sci. Engr.*, 92, 403 (1986).

13. Y. Y. AZMY and E. W. LARSEN, "Fourier Analysis of the Diffusion Synthetic Acceleration Method for Weighted Diamond-Differencing Schemes in Cartesian Geometries," *Nucl. Sci. Engr.*, 95, 105 (1987).

14. TONY F. CHAN AND HOWARD C. ELMAN, "Fourier Analysis of Iterative Methods for Elliptic Problems," *SIAM Review*, 31, 20, 1989.

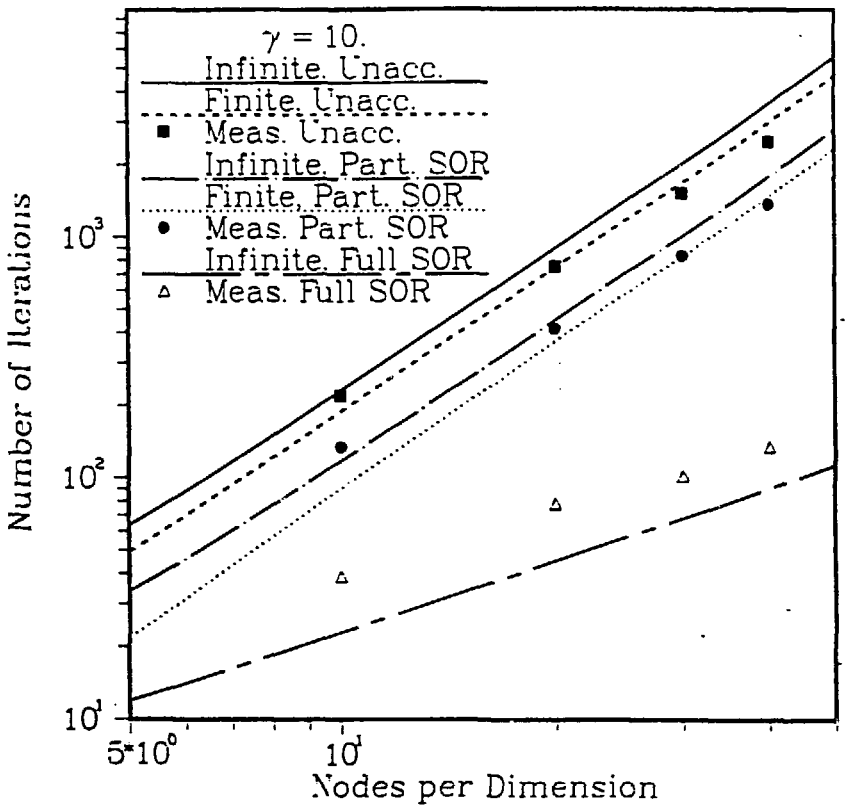

Fig. 1. Comparison of measured and theoretically predicted numbers of iterations required by the three iterative methods to solve the uniform model problem, with 10^{-4} convergence criterion.