A Numerical Assessment on Water Quality Model Using the Half-Sweep Explicit Group Methods

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ABSTRACT

Presently, there are many science and engineering problems described in mathematical models. The solutions to these problems can be obtained analytically or numerically. Thus, the aim of this paper is to assess the water quality model using full- and half-sweep finite-difference approximation equations. The 2, 3 and 4-point of Full-Sweep Explicit Group (FSEG) and Half-Sweep Explicit Group (HSEG) iterative methods together with the Red-Black (RB) ordering strategy were also presented to solve the systems of linear equations. Finally, a number of numerical experiments were conducted in order to show the effectiveness of the HSEG methods with RB ordering in computing numerically.

Keywords: *numerical assessment, water quality model, half-sweep iteration, Crank-Nicolson scheme*

Introduction

The numerical techniques such as the finite difference, finite element, finite volume and boundary methods have been used by many researchers to gain approximate solutions. Those methods are some of the most efficient approximate techniques for solving a wide variety of science and engineering problems. This paper focuses on the effectiveness of using the full- and half-sweep finite difference approximation solver by using the Explicit Group (EG) iterative method (Yousif 1984; Evans 1985; Arsmah 1993). Besides EG iterative methods, two ordering strategies; lexicography (NA) and red-black (RB), are considered in solving any system of linear equations. This is because the combination of iterative schemes and ordering strategies, which have been proven, can accelerate the convergence rate (see Parter 1988; Evans & Yousif 1990; Zhang 1996).

Let us consider the water quality model given as

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + E\frac{\partial^2 C}{\partial x^2}, \qquad x \in [0,1], t \geq 1. \qquad (1)$$

subject to the initial condition

$$C(x,0) = \rho_0(x), \; a \leq x \leq b$$

and the boundary conditions

$$\left.\begin{aligned} C(a,t) &= \rho_1(t), \\ C(b,t) &= \rho_2(t), \end{aligned}\right\}, \; t \geq 0$$

where,

U = Mean velocity (m/s)
E = Dispersion coefficient (m^2/s)
x = Distance downstream (m)
t = Time (s)
C = Concentration of Dissolved Oxygen (DO) ($mg/\,l$)

To facilitate in formulating the full- and half-sweep finite difference approximation equations for problem (1), we shall restrict our further discussion in the next sections onto uniform node points only. Therefore, we assume the solution domain (1) can be uniformly divided into $m = 2^p$, $p \geq 2$ and R subintervals in the x and t directions. The subintervals in the x and t directions are denoted Δx and Δt respectively, which are uniformed and defined as

$$\left.\begin{aligned} \Delta x &= \frac{(b-a)}{m} = h, \quad m = n+1 \\ \Delta t &= \frac{(T-0)}{R} \end{aligned}\right\} \qquad (2)$$

The Half-Sweep Crank-Nicolson Finite Difference Approximation

Referring to Figure 1, the finite grid networks show the distribution of uniform node points to be considered in implementing the half- and full-sweep iterative methods. Before further explanation on the implementation of iterative process, the half- and full-sweep iterative methods will be used to compute approximate values onto node points of type only until the convergence criterion is reached. Then solutions of the other remain points are computed directly (see Abdullah 1991; Ibrahim & Abdullah 1995; Yousif & Evans 1995; Abdullah & Ali 1996).

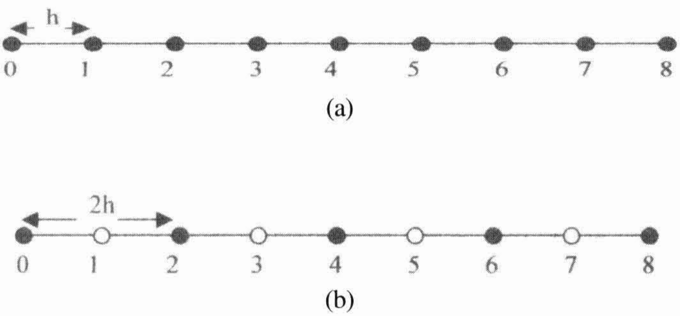


Figure 1: (a) and (b) Shows the Distribution of Uniform Node Points for the Full- and Half-sweep Cases, Respectively

Using the θ iterated scheme, the general approximation equation for problem (1) can be written as

$$-(\alpha\theta + \beta\theta)C_{i-1,j+1} + (1 + 2\alpha\theta)C_{i,j+1} - (\alpha\theta - \beta\theta)C_{i+1,j+1} = f_{i,j+1} \qquad (3)$$

where,

$$\alpha = \frac{E\Delta t}{(h)^2}, \quad \beta = \frac{U\Delta t}{(2h)},$$

$$f_{i,j+1} = (\alpha(1-\theta) + \beta(1-\theta))C_{i-1,j} + (1-2\alpha(1-\theta))C_{i,j} - (\alpha(1-\theta) - \beta(1-\theta))C_{i+1,j}$$

The values of θ in Eq. (3), correspond to 0, 1, and $\frac{1}{2}$, represents the expilicit (classical), fully implicit and the Crank-Nicolson (CN) schemes, respectively. It can be shown that the truncation errors for each scheme are $O\left((\Delta x)^2+(\Delta t)\right)$, $O\left((\Delta x)^2+(\Delta t)\right)$, and $O\left((\Delta x)^2+(\Delta t)^2\right)$, respectively. In this paper, the CN scheme is mainly considered due to its high accuracy. Similarly using the same way to derive Eq. (3) and by substituting $\theta=\frac{1}{2}$, we can express full- and half-sweep CN approximation equations as stated in the following equation

$$-C_{i-1,j+1}+\rho C_{i,j+1}-\phi C_{i+1,j+1}=f^{*}_{i,j+1} \tag{4}$$

where,

$$\eta=\frac{E\Delta t}{2(ph)^2},\quad \upsilon=\frac{U\Delta t}{4(ph)},$$

$$\rho=\frac{1+2\eta}{\eta+\upsilon},\quad \phi=\frac{\eta-\upsilon}{\eta+\upsilon},\quad \gamma=\frac{1-2\eta}{\eta+\upsilon},$$

$$f^{*}_{i,j+1}=C_{i-1,j}+\gamma C_{i,j}+\phi C_{i+1,j}$$

The values of p, which correspond to 1 and 2, represents the full- and half-sweep cases respectively. Thus, the computational molecule for equation (3) is shown in Figure 2 and the corresponding system of linear equations can be stated as

$$A\underset{\sim}{C}=\underset{\sim}{b} \tag{5}$$

where,

$$A=\begin{bmatrix} \rho & -\phi & & & \\ -1 & \rho & -\phi & & \\ & \vdots & \vdots & \vdots & \\ & & -1 & \rho & -\phi \\ & & & -1 & \rho \end{bmatrix}_{\left(\left(\frac{m}{p}\right)-p\right)x\left(\left(\frac{m}{p}\right)-p\right)}$$

$$\underset{\sim j+1}{f}=\left[f^{*}_{1p,j+1}+C_{0,j+1}\quad f^{*}_{1p,j+1}\quad f^{*}_{2p,j+1}\quad\cdots\quad f^{*}_{m-p,j+1}+\phi C_{m,j+1}\right]^{T}$$

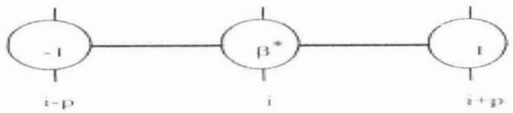


Figure 2: Computational Molecule of the Full- and Half-sweep CN Finite Difference Approximations for Problem (1)

The Half-Sweep Explicit Group Iterative Methods

In this paper, the approximate solutions of the system of linear equations are restricted to the 2, 3 and 4-point block schemes.

The 2-Point FSEG and HSEG Schemes

Considering Figure 2, the 2-Point FSEG and HSEG schemes using Eq. (4) generally can be shown as (Yousif 1984; Arsmah 1993),

$$\begin{bmatrix} \rho & -\phi \\ -1 & \rho \end{bmatrix} \begin{bmatrix} C_{i,j+1} \\ C_{i+p,j+1} \end{bmatrix} = \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} \tag{6}$$

where,

$$S_1 = f^*_{i,j+1} + C_{i-p,j+1}, \quad S_2 = f^*_{i+p,j+1} + \phi C_{i+2p,j+1}.$$

Determining the inverse matrix of the coefficient system, (6), both schemes can generally be written as

$$\begin{bmatrix} C_{i,j+1} \\ C_{i+p,j+1} \end{bmatrix} = \frac{1}{\rho^2 - \theta} \begin{bmatrix} \rho & \phi \\ 1 & \rho \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} \tag{7}$$

The 3-Point FSEG and HSEG Schemes

These schemes involve a pair of three points accordingly in order to generate a system of linear equations, (3 x 3). From Eq. (4), both schemes can be represented in the following system of linear equations

$$\begin{bmatrix} C_{i,j+1} \\ C_{i+p,j+1} \\ C_{i+2p,j+1} \end{bmatrix} = \frac{1}{\psi} \begin{bmatrix} \rho^2 - \phi & \phi\rho & \phi^2 \\ \rho & \rho^2 & \phi\rho \\ 1 & \rho & \rho^2 - \phi \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \\ S_3 \end{bmatrix} \tag{8}$$

where,

$$\psi = \rho^3 - 2\phi\rho,$$

$$S_1 = f^*_{i,j+1} + C_{i-p,j+1}, \quad S_2 = f^*_{i+p,j+1}, \quad S_3 = f^*_{i+2p,j+1} + \phi C_{i+3p,j+1}.$$

To reduce the complexity of computations in system (8), the technique of doing one computation and its value stored in one variable will be used into the system. As a result, the value can be used repeatedly for other computations (see Jumat and Abdul Rahman 1998). Generally the implementation of the system can be represented as follows,

$$\left. \begin{aligned} C_{i,j+1} &= \phi S_a + {S_1}/{\rho} \\ C_{i+p,j+1} &= \rho S_a \\ C_{i+2p,j+1} &= S_a + {S_3}/{\rho} \end{aligned} \right\} \tag{9}$$

where,

$$S_a = (S_1 + \rho S_2 + \phi S_3)/\psi$$

The 4-Point FSEG and HSEG Schemes

By using the same way to formulate scheme (9), it can be shown that the 4-Point FSEG and HSEG are stated as

$$\begin{bmatrix} C_{i,j+1} \\ C_{i+p,j+1} \\ C_{i+2p,j+1} \\ C_{i+3p,j+1} \end{bmatrix} = \frac{1}{\psi} \begin{bmatrix} \rho\nu_2 & \phi\nu_1 & \phi^2\rho & \phi^3 \\ \nu_1 & \rho\nu_1 & \phi\rho^2 & \phi^2\rho \\ \rho & \rho^2 & \rho\nu_1 & \phi\nu_1 \\ 1 & \rho & \nu_1 & \rho\nu_2 \end{bmatrix} \begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \end{bmatrix} \tag{10}$$

where,

$$\psi = \rho^4 - 3\phi\rho^2 + \phi^2, \quad \nu_1 = \rho^2 - \phi, \quad \nu_2 = \rho^2 - 2\phi$$
$$S_1 = f^*_{i,j+1} + U_{i-p,j+1}, \quad S_2 = f^*_{i+p,j+1},$$
$$S_3 = f^*_{i+2p,j+1}, \quad S_4 = f^*_{i+3p,j+1} + \phi U_{i+4p,j+1}.$$

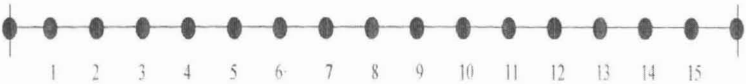
Referring to Eq. (10), its coefficient matrix can be separated into two parts by a dot line. Applying the same technique as mentioned in the previous section, generally both methods can be implemented iteratively as follows

$$\left.\begin{aligned} C_{i,j+1} &= \phi S_a + \nu_a S_1 \\ C_{i+p,j+1} &= \rho S_a + \nu_b S_1 \\ C_{i+2p,j+1} &= \rho S_b + \phi \nu_b S_4 \\ C_{i+3p,j+1} &= S_b + \nu_a S_4 \end{aligned}\right\} \qquad (11)$$

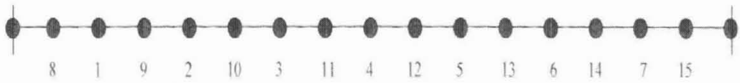
where,

$$\nu_a = \rho\left(\rho^2 - 2\phi\right)/\psi, \quad \nu_b = \left(\rho^2 - \phi\right)/\psi,$$
$$S_a = \left(\left(\rho^2 - \phi\right)S_2 + (\phi\rho)S_3 + \left(\phi^2\right)S_4\right)/\psi, \quad S_b = \left(S_1 + \rho S_2 + \left(\rho^2 - \phi\right)S_3\right)/\psi,$$

In this section, two ordering strategies such as lexicography (NA) and red-black (RB) are carried out. Consequently, the application of the RB strategy applied into the FSEG and HSEG iterative methods will be indicated as FSEG-RB and HSEG-RB methods, repectively. The location of numbers 1p, 2p, 3p, ... , *m-p* shows how the implementation of full- and half-sweep iterative methods either by using the NA or RB ordering, where it can be computed by starting at number 1 and ending at number *m-p*, see Figures 3 and 4.

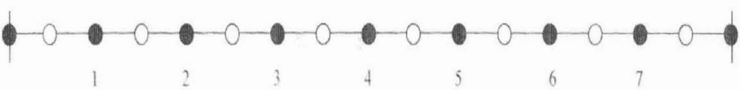


(a)

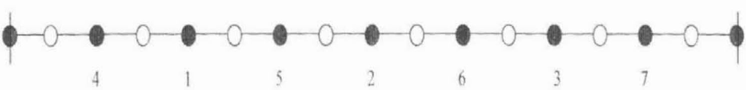


(b)

Figure 3: (a) and (b) Shows the NA and RB Ordering Strategies Respectively in the Full-sweep Case



(a)



(b)

Figure 4: (a) and (b) Shows the NA and RB Ordering Strategies Respectively in the Half-sweep Case

Computational Experiments

To indicate the effectiveness of the numerical assessment using the full- and half-sweep finite difference approximation equation in (5), there are three parameters considered in numerical comparison such as the number of iterations, execution time and maximum absolute error. In this section, the following is a water quality model stated as

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + E\frac{\partial^2 C}{\partial x^2}, \qquad x \in [0,1], t \geq 1. \tag{12}$$

Then boundary conditions and the exact solution of the problem (12) were defined by

$$C(x,t) = \frac{500}{2\sqrt{\pi E t}} e^{\left(\frac{-(x-Ut)^2}{4Et}\right)}, \qquad 0 \le x \le 1, t \ge 1. \tag{13}$$

All the results of numerical experiments, obtained from implementation of the GS, 4 Point FSEG-RB and HSEG-RB methods, are recorded in Table 1. In the implementation mentioned above, the convergence test considered the tolerance error $\varepsilon = 10^{-10}$. Figures 5 and 6 show the number of iterations and the execution time versus mesh size.

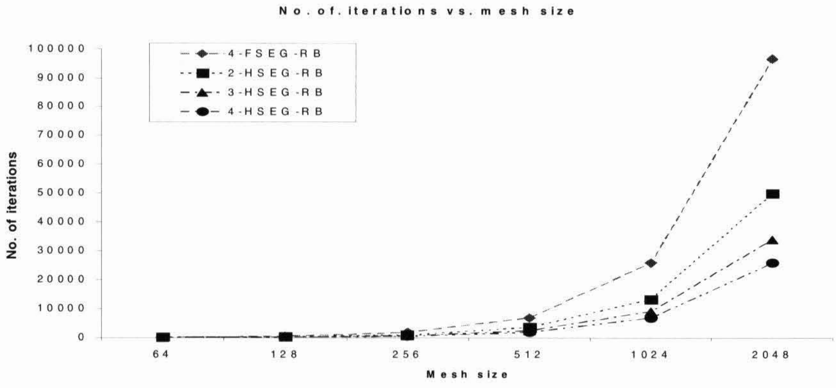


Figure 5: Number of Iterations Versus Mesh Size of the 4 Point FSEG-RB and HSEG-RB Methods

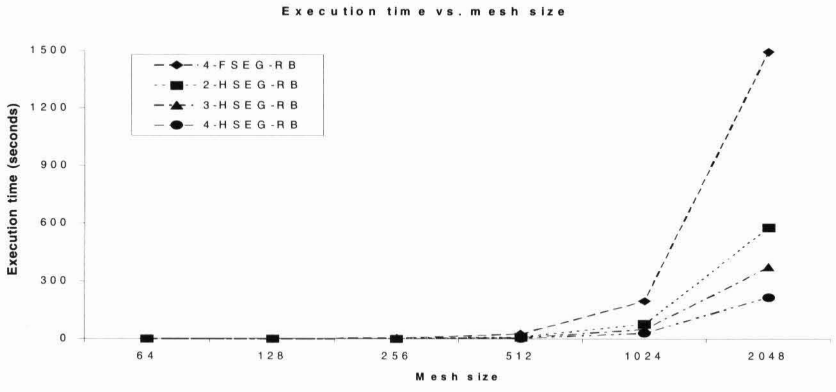


Figure 6: The Execution Time (seconds) Versus Mesh Size of the 4 Point FSEG-RB and HSEG-RB Methods

Table 1: Comparison of Number of Iterations, the Execution Time (Seconds) and Maximum Errors for the Iterative Methods

$a = 0,\quad b = 1,\quad R = 100,\quad T = 0.0488,$

$h^{-1} = 128, 256, 512, 1024, 2048, 4096,\quad \varepsilon = 10^{-10}$

No. of Iterations

Methods	Mesh size					
	64	128	256	512	1024	2048
GS	496	1844	6915	25902	96659	358915
2-FSEG-RB	257	952	3568	13387	50066	186395
3-FSEG-RB	178	649	2425	9097	34056	126967
4-FSEG-RB	139	496	1845	6916	25905	96666
2-HSEG-RB	73	257	952	3568	13387	50066
3-HSEG-RB	54	178	649	2425	9097	34056
4-HSEG-RB	44	139	496	1845	6916	25905

Execution time (Seconds)

Methods	Mesh size					
	64	128	256	512	1024	2048
GS	0.31	2.23	16.52	121.25	923.07	6840.65
2-FSEG-RB	0.25	1.54	11.32	82.96	639.66	4923.53
3-FSEG-RB	0.17	1.11	7.84	58.40	444.35	3468.46
4-FSEG-RB	0.10	0.49	3.57	25.95	197.70	1493.57
2-HSEG-RB	0.06	0.19	1.34	9.74	76.58	578.54
3-HSEG-RB	0.04	0.13	0.85	6.29	49.72	375.01
4-HSEG-RB	0.02	0.12	0.55	3.90	29.05	218.90

Maximum Absolute Errors

Methods	Mesh size					
	64	128	256	512	1024	2048
GS	2.659e-5	1.139e-5	2.110e-5	2.446e-5	2.902e-5	4.506e-5
2-FSEG-RB	2.660e-5	1.135e-5	2.093e-5	2.380e-5	2.637e-5	3.445e-5
3-FSEG-RB	2.660e-5	1.134e-5	2.088e-5	2.358e-5	2.549e-5	3.092e-5
4-FSEG-RB	2.660e-5	1.133e-5	2.085e-5	2.346e-5	2.505e-5	2.916e-5
2-HSEG-RB	1.781e-4	2.660e-5	1.135e-5	2.093e-5	2.380e-5	2.637e-5
3-HSEG-RB	1.781e-4	2.660e-5	1.134e-5	2.088e-5	2.358e-5	2.549e-5
4-HSEG-RB	1.781e-4	2.660e-5	1.133e-5	2.085e-5	2.347e-5	2.505e-5

Conclusion

The findings in Figures 5 and 6 show that the number of iterations and the execution time for the 4 Point HSEG-RB have declined by 68.34 – 73.32% and 75.51 – 85.34%, respectively compared with the 4 Point FSEG-RB method. Thus, the HSEG-RB methods are far better than the FSEG-RB method in terms of a number of iterations and the execution time. This is attributed to the computational complexity of the HSEG-RB methods, which is 50% less than the FSEG-RB methods.

In terms of the half-sweep approximation equations, the 4 Point HSEG-RB is the best scheme among the HSEG methods. For instance, the 4 Point HSEG-RB method has reduced its number of iterations and the execution time by 18.51 – 23.97% and 36.84 – 66.66% respectively compared with the 2 Point HSEG-RB method.

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