Optimum extrapolated ADI iterative difference schemes for the solution of Laplace’s equation in three space variables

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This paper describes the application of the extrapolated ADI methods for the numerical solution of Laplace’s equation over the open unit cube under ‘model problem’ boundary conditions. Three different approximating difference formulae are considered and each one of the resulting extrapolated ADI schemes is treated by using the set of Douglas parameters in two different ways. In addition a comparison of the two methods is made and optimum extrapolated ADI schemes are given.

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1. Introduction
A rather extensive literature concerning the numerical solution of the 3-dimensional Laplace’s equation under ‘model problem’ boundary conditions using either Alternating Direction Implicit (ADI) methods or Extrapolated (E) ADI ones already exists. In brief we mention the works by Douglas and Rachford (1956), Douglas (1962), Samarskii and Andreyev (1963) and (1964), Fairweather and Mitchell (1965), Guittet (1967), Fairweather, Gourlay, and Mitchell (1967) and Hadjidimos (1968a) and (1969).

In this paper we follow the analysis given in Hadjidimos (1970) as far as the solution of Laplace’s equation over the open unit cube is concerned by considering three different types of difference formulae. It is then our purpose to examine in the light of EADI methods, all the possible cases arising and find the best EADI iterative difference scheme to use in each specific case for each value of $N(N \geq 3$ is the number of mesh subdivisions in each co-ordinate direction).

In the text which follows, Laplace’s equation is considered to be approximated (i) by a 7-point difference equation (ii) by a 19-point difference equation and (iii) by a 27-point difference equation. In each case the set of Douglas parameters is applied to the resulting iterative difference scheme following (a) the method of Douglas and (b) the method of Samarskii and Andreyev in the way these two methods have been implemented by the present author. In all six cases optimum numerical results have been obtained for $N = 10(10)100$ as well as for $N \to \infty$. It has been found that some of the results corresponding to the special limiting case of $N \to \infty$ are already known. However, all the other optimum results are new, although it should be pointed out that some of the results as well as part of the analysis of this present paper have already been given in Hadjidimos (1968b).

As one can see from the Tables given in the text, EADI schemes treated by Douglas’ straightforward method seem to give poorer optimum theoretical convergence rates than by being treated by Samarskii and Andreyev’s method for all values of $N$. In spite of this fact Tables 1 and 2 are displayed, for we think that Douglas’ method should not be discarded before very much more practical experience has been gained.

2. General considerations
We start with Laplace’s equation (2.1)

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} = 0 \quad (x_1, x_2, x_3) \in \mathcal{R}$$

over the open unit cube $\mathcal{R}(x_i | i = 1, 2, 3$ are the space variables) where the unknown function $u = u(x_1, x_2, x_3)$ is prescribed on the boundary $\partial \mathcal{R}$ of $\mathcal{R}$. To solve (2.1) numerically we impose a uniform mesh spacing of length $h$ in each co-ordinate direction on $\mathcal{R}$ and employ the notation

$$u(i_1 h, i_2 h, i_3 h) = u_{i_1 i_2 i_3}, \quad 0 \leq i_1, i_2, i_3 \leq N \left( \equiv \frac{1}{h} \right)$$

The difference equation used to approximate (2.1) is of the general form below

$$\left\{ \sum_{i=1}^{3} \frac{\delta x_i^2}{\delta x_i^2} + k \sum_{j>i}^{3} \delta x_i \delta x_j + l \prod_{i=1}^{3} \delta x_i \right\} u_{i_1 i_2 i_3} = 0$$

(2.2)

where $u_{i_1 i_2 i_3}$ denotes now an approximate solution of (2.1) at the corresponding nodal point. In (2.2) $\delta x_i | i = 1, 2, 3$ is the central difference operator in the $x_i$-direction and $k$ and $l$ are constants. In particular for $k = l = 0$ (7-point difference formula) equation (2.2) is 2nd order correct in $h$ when it is used to approximate (2.1) while for $k = 1/6$ and $l = 0$ (19-point difference formula) it is 4th order correct in $h$ and for $k = 1/6$ and $l = 1/30$ (27-point difference formula) it is 6th order correct in $h$.

When we are using EADI methods to solve (2.2) the following iterative scheme is produced (see Hadjidimos, 1970).
If we start with
\[3 \prod_{i=1}^{N-1} (1 - r_{m+1} \delta_{m+1}^i) u_{i|j,i}^{(m+1)} = \left\{3 \prod_{i=1}^{N-1} (1 - r_{m+1} \delta_{m+1}^i) + \omega r_{m+1} F\right\} u_{i|j,i}^{(m)}\]
\[l \leq i_1, i_2, i_3 \leq N-1\] (2.3)
where \(u_{i|j,i}^{(m)}\) is the \(m\)th iteration approximation to \(u_{i|j,i}^{(0)}\) (\(a_{i|j,i}^{(0)}\) arbitrary), \(r_{m+1}\) is a sequence of positive iteration parameters, \(\omega\) is the extrapolation parameter and \(F\) is the difference operator involved in (2.2) that is given by
\[F \equiv \sum_{i=1}^{N-1} \delta_{m+1}^i + k \sum_{i=1}^{N-1} \delta_{m+1}^i \delta_{m+1}^{i+1} + l \sum_{i=1}^{N-1} \delta_{m+1}^i\]

Because of the 'model problem' boundary conditions the different matrices arising in solving (2.2) using EADI methods commute and by virtue of that fact it can readily be seen that the amplification factor associated with (2.3) is given by
\[\rho_{i,k,i,k}^{(m+1)}(r_{m+1}, \omega) = 1 - \alpha f(r_{m+1}, a_1, a_2, a_3)\] (2.4)
where
\[f(r_{m+1}, a_1, a_2, a_3) = \frac{r_{m+1} [a_1 + a_2 + a_3 - k(a_1 a_2 + a_2 a_3 + a_3 a_1) + l a_1 a_2 a_3]}{\sum_{i=1}^{N-1} (1 + r_{m+1} a_i)}\] (2.5)
with \(a_i = 4 \sin^2 k_i \pi / 2N (i = 1, 2, 3\) and \(k_i = 1, 2, \ldots, N - 1\).

3. Optimum EADI schemes
To begin with let us consider the set of Douglas parameters which is defined as follows (see Hadjidimos, 1970).

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<th>Table 1</th>
<th>Optimum parameters (Straightforward method, (k = 0, l = 0))</th>
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\[\lambda_n = \mu \left(\frac{\mu}{v}\right)^{-1} \sin^{-1} \frac{\pi}{2N} \text{ for } n = 1, 2, \ldots, n_0 \] (3.1)

where \(\mu\) and \(v\) are constants to be determined satisfying
\[0 < \mu \leq \mu_0 \leq v \text{ and } \frac{\mu}{v} > t \] (3.2)

\(\mu_0\) and \(v_0\) are two prescribed constants, \(t = \tan^2 \frac{\pi}{2N}\) and \(n_0\) is such that
\[\ln \left(\frac{\mu}{v}\right) + v < n_0 < \ln \left(\frac{\mu}{v}\right) + 1. \] (3.3)

The set of Douglas parameters can be applied either straightforward (Douglas’ method) or by using the method proposed by Samarskii and Andreyev.

(a) Straightforward method
In this case the prescribed constants used in (3.2) assume the values \(\mu_0 = \cos^2 \frac{\pi}{2N}\) and \(v_0 = 1\). Therefore (3.2) becomes
\[0 < \mu \leq \cos^2 \frac{\pi}{2N} < 1 \leq v \text{ and } \frac{\mu}{v} > t \] (3.4)

If we put
\[a_i = 4\xi_i \quad i = 1, 2, 3 \text{ and } \]
\[\lambda_n = 4r_n \quad n = 1, 2, \ldots, n_0 \] (3.5)

then (2.6) can be written as
\[\left(1 - 4k\right) \frac{\lambda_4}{3} \left(1 + \lambda_4 \xi_4\right) \leq f \leq \left(1 - 4k\right) \frac{\lambda_4}{3} \left(1 + \lambda_4 \xi_4\right) \] (3.6)

Thus the sequence of Douglas parameters can be applied with
\[r_{m+1} = r_n = \frac{\lambda_2}{4} \quad n = 1, 2, \ldots, n_0 \text{ and }\]
\[n = (m+1) - n_0 \text{ enter (m/n_0)} \] (3.7)

provided that \(\omega\) has been chosen appropriately.

As is known if we iterate \(n_0\) times with the parameter sequence (3.7) there exists a value of \(n = n^* \quad n = 1, 2, \ldots, n_0 \) for which
\[\mu \leq \lambda_n \xi_n \leq v \text{ and } \mu \leq \lambda_n \xi_n \leq v \quad (i \neq j \text{ and } i, j = 1, 2, 3) \] (3.8)

while for all \(n \neq n^*\) the following inequalities hold
\[\mu \leq \lambda_n \xi_n \leq \mu t \quad i = 1, 2, 3 \text{ and } n \neq n^* \] (3.9)

Having in mind (3.6) we can find (see Hadjidimos, 1968b) that
\[f_M = \frac{2\mu + v}{(1 + \mu)^2(1 + v)} \]
\[f_m = \min \left\{ \left(1 - 4k\right) \frac{2\mu + v}{(1 + \mu)^2(1 + v)}, \left(1 - 4k\right) \frac{3v}{(1 + v)^3} \right\} \] (3.10)

\[f_{M*} = \frac{2\mu + \mu t}{(1 + \mu)^2(1 + v)} \]

where \(f_m\) and \(f_{M*}\) are the maximum and the minimum values of the upper and the lower bounds of \(f\) given by (3.6) under the restrictions (3.8) while \(f_{M*}\) is the maximum value of the upper bound of \(f\) under the restrictions (3.9).

To simplify the subsequent analysis we equate the two terms giving the minimum in (3.10). In this way we provide the parameters \(\mu\) and \(v\) with the extra relationship
\[\frac{2\mu + v}{(1 + \mu)^2(1 + v)} = \frac{3v}{(1 + v)^3} \equiv \Psi(v) \] (3.11)

which yields the following equation in \(v\)
\[\Psi(v) = (2\mu + v)^3 + 3(2\mu + v)^2v + 3[(2\mu + v)\left(1 + (1 + \mu)^2\right) + (2\mu + v) = 0 \] (3.12)

In order to be allowed to use (3.11) or equivalently (3.12) in the sense that neither of these relations violates the restrictions imposed on \(\mu\) and \(v\) by (3.4) it should be proved that either of these relationships gives at least one pair \((\mu, v)\) for each \(t\) such that all the restrictions (3.4) are satisfied. The proof is as follows: We first observe that equation (3.12) has three real roots belonging to the intervals \((-\infty, -1), (0, \frac{1}{2})\) and \((\frac{1}{2}, +\infty)\) respectively for any \(\mu(0, \cos^2 \frac{\pi}{2N} = 1/1 + t)\) and any \(N\) (or \(t < 0 \leq 1/3\)). We restrict ourselves to considering the root \(v_1\) belonging to the third interval since we must have \(v \geq 1\). By studying the functions \(q_1(\mu)\) and \(q_2(\mu)\) defined by (3.11) we can easily find out that \(q_1(\mu)\) strictly increases in \((0, 1/1 + t)\) while \(q_2(\mu)\) strictly decreases in \((1, +\infty)\) for any fixed \(t(0 < t \leq 1/3)\). In addition to the above we can find that
\[q_1(0) = 0 \quad q_1\left(\frac{1}{1+t}\right) > \frac{3}{8} \] (3.13)

\[q_2(1) = \frac{3}{8} \quad q_2(+\infty) = 0 \]

Because of the range of values of \(q_1(\mu)\) and in view of the fact that \(q_1(\mu)\) is a strictly increasing function in the interval mentioned previously there exists just one value of \(\mu = \mu_1\) for which \(q_1(\mu_1) = 3/8\). Therefore for any \(\mu(\mu_0, c(0, 1/1 + t))\) the corresponding \(v_1\) is \(\geq 1\). Consequently all pairs \((\mu, v)\) formed in this way satisfy the restrictions imposed on \(\mu\) and \(v\) by the first part of (3.4). Among all these pairs there exists at least one which satisfies the further restriction \(\mu/v > t\). E.g. for \(\mu = \mu_1\) when \(v_1 = 1\) we have \(\mu/v = \mu_1/v_1 = \mu_1/1 > t\), for it can be proved that \(q_1(t) < q_1(\mu_1) = 3/8\).

As is known (see Hadjidimos, 1970) the optimum extrapolation parameter \(\omega\) is given by
\[\omega = \min(\omega_1, \omega_2) \text{ with } \omega_1 = \frac{2}{f_{M*}} \text{ and } \omega_2 = \frac{2}{f_M + f_m} \] (3.14)

where in order to find the optimum values for the parameters \(\mu\) and \(v\) and consequently the optimum values for all the other parameters involved we have to maximise computationally the function
\[z = \ln p(\mu, v) \ln(\mu/v) \]

for all possible pairs \((\mu, v)\) for each value of \(N\) where
\[p(\mu, v) = 1 - \omega f_m \]

The optimum numerical results found for each \(N = 10(10)100\) and \(\mu = 0.01(0.01)\mu_1\) are given in Tables 1 and 2. In the last rows of these Tables the limiting values of the different optimum parameters as \(N \to \infty\) are also given.

As it comes out of Table 1 the optimum EADI scheme for \(k = l = 0\) tends to the well-known Douglas' scheme as \(N \to \infty\) while Table 2 shows that for \(k = 1/6\) and \(l = 1/30\) the corresponding optimum EADI scheme tends to the Improved Douglas one as \(N \to \infty\).

(b) Samarskii and Andreyev's method
In this case both constants \(\mu_0\) and \(v_0\) are equal to \(\frac{1}{6}\) so (3.2) becomes
\[0 < \mu \leq \frac{1}{6} \leq v \text{ and } \frac{\mu}{v} > t \] (3.4)
If we put
\[ a = \frac{a_1 + a_2 + a_3}{3} = \frac{4\xi_1 + 4\xi_2 + 4\xi_3}{3} = 4\xi \]
and
\[ \lambda_n = 4r_n \quad n = 1, 2, \ldots, n_0 \]
then because of the following relationships which are always valid
\[
1 + 3r_{m+1}a < \prod_{i=1}^{3}(1 + r_{m+1}a) \leq (1 + r_{m+1}a)^3
\]
(2.6) becomes
\[
(1 - 4k) \frac{3\lambda_n}{(1 + \lambda_n^2)} \leq f \leq \frac{3\lambda_n}{1 + 3\lambda_n^2}
\]
corresponding to (3.6).

The set of Douglas parameters can be applied again with (3.7) and a suitable value for \( \rho \).

The relationships which now correspond to (3.8) are
\[
\mu \leq \lambda_n^2 \xi \leq \nu \quad \text{for } n = n^* \tag{3.8}'
\]
while (3.9) still remain the same except that \( \xi \) is replaced by \( \xi \).

The values which are assumed by \( f_M, f_n \) and \( f_m^* \) under the corresponding restrictions (3.8)' and (3.9) can be found to be
\[
f_M = \frac{3\nu}{1 + 3\nu}
\]
\[
f_m = \min\left\{(1 - 4k) \frac{3\mu}{(1 + \mu)^3}, (1 - 4k) \frac{3\nu}{(1 + \nu)^3}\right\}
\]
\[
f_m^* = \frac{3\mu}{1 + 3\mu}
\]
If, for the sake of convenience, we take the two terms giving the minimum in (3.10)' equal, we obtain

It can readily be seen that the positive root \( v \) of (3.12)' always satisfies the restriction \( \frac{1}{2} < v < \nu \) for any \( \mu(0, \frac{1}{2}) \). Moreover the restriction \( \mu(0, \frac{1}{2}) > t \) is also satisfied provided that the inequality \( \sigma(\mu) \equiv (1 + t)^3 + 3t\mu^2 - t^2 > 0 \) holds for any \( (0 < t \leq 1/3) \). \( \sigma(\mu) \) has one real root only, say \( \mu_1 \), such that \( 0 < \mu_1 < \frac{1}{2} \) for any \( t \) in the range above. It can be shown then that all possible pairs \( (\mu, v) \) consisting of any \( \mu(\mu, \frac{1}{2}) \) \( C(0, \frac{1}{2}) \) and the corresponding \( v_1 \) satisfy all the restrictions imposed on \( \mu \) and \( v \) by (3.4)

The subsequent analysis as far as the choice of the optimum parameters is concerned is still the same as in the previous straightforward case. Thus Tables 3 and 4 have been constructed in the same way as Tables 1 and 2 (with the obvious slight modifications) and give the optimum numerical values of the different parameters involved. To differentiate the results of this present method from the previous one bars have been added to the different parameters.

We notice from Table 4 that the corresponding optimum EADI scheme tends to that one given by Samarskii and Andreyev as \( N \to \infty \).

### Table 3: Optimum parameters (Samarskii and Andreyev's method, \( k = 0, l = 0 \))

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<th>( N )</th>
<th>( \bar{\mu} )</th>
<th>( \bar{v} )</th>
<th>( \bar{\omega}_1 )</th>
<th>( \bar{\omega}_2 )</th>
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### Table 4: Optimum parameters (Samarskii and Andreyev's method, \( k = 1/6, l = 0 \) and \( 1/30 \))

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of $N$. It is clear that the best method for a given $N$ is the one which corresponds to the largest of $z$ and $\tilde{z}$.

As one can readily see from Tables 1 and 3 as well as from Tables 2 and 4 the results obtained by the method of Samarskii and Andreyev are better than the corresponding ones obtained by the straightforward method of Douglas for all values of $N$.

References


