On a generalised alternating direction implicit method for solving Laplace's equation

By Apostolos Hadjidimos*

This paper describes a generalized A.D.I. scheme involving an extra parameter which is equivalent to Guittet's scheme for solving Laplace's equation over an m-dimensional supercube. In addition the 'model problem' in the 3-dimensional case is treated but the method using the alternative generalisation is applied with the parameter sequence of Douglas, unlike Guittet's which has a fixed parameter.

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1. Introduction

For the numerical solution of the model problem many alternating direction implicit methods have been proposed. Among these there are those of Peaceman–Rachford (1955), Douglas–Rachford (1956), and Douglas (1962). Peaceman and Rachford solved the problem in the 2-dimensional case by using a parameter r varying during the iterations. Douglas and Rachford solved the problem in the 2-dimensional case as well as in the 3-dimensional one, although their iterative method was inferior to that of Peaceman–Rachford's as far as the 2-dimensional case was concerned. Finally, Douglas proposed a method to solve the problem in the 3-dimensional case by using a set of iteration parameters. It must be mentioned that either Douglas–Rachford's method or Douglas' method is convergent for any fixed $r > 0$ in the m-dimensional case ($m \geqslant 2$) and that Douglas' method is superior to that of Douglas–Rachford's for at least $m = 2$ and 3. Moreover, Douglas' method is equivalent to that of Peaceman–Rachford's when $m = 2$.

Samarskii and Andreyev (1963 and 1964) solved the same problem in the 2 and 3-dimensional case by considering different difference equations to approximate Laplace's equation, and used sets of iteration parameters based on the idea given by Douglas.

Recently Guittet (1967) generalised the methods of Douglas–Rachford and Douglas in the m-dimensional case ($m \geqslant 2$) by introducing an extra parameter. He also found optimum values of that extra parameter as well as of the fixed parameter r for all values of m. Here it must be stressed that Guittet's scheme is not a natural generalisation of Douglas–Rachford's and Douglas' scheme, as far as each individual step of an iteration is concerned. The generalisation is in the sense that the iterative matrix in Guittet's scheme is a generalised version of the iterative matrices involved in the other two schemes.

Another recent paper devoted to the solution of Laplace's equation is that by Fairweather, Gourlay and Mitchell (1967). They proposed the so-called 'Improved Douglas scheme' which is of an order of accuracy higher than all the corresponding ones in the previous papers, and used the set of iteration parameters of Douglas as it had been implemented by Samarskii and Andreyev (1963).

In the present paper we propose an equivalent scheme to that proposed by Guittet which is an actual generalisation of Douglas–Rachford's and Douglas' schemes. With either Guittet's scheme or ours we work out the model problem in the 3-dimensional case by using the set of iteration parameters proposed by Douglas (1962). Moreover, a comparison of the number of calculations needed to solve the 3-dimensional model problem shows that the method we propose is always superior to Douglas' and when the number of mesh subdivisions is large (approximately $\geqslant 17$) it is superior to Guittet's.

It is intended that a comparison of the methods of Samarskii and Andreyev (1964), Fairweather, Gourlay and Mitchell (1967) and the one we propose will be given in a forthcoming paper.

2. General scheme proposed

Our problem is to find numerically the solution of the equation

$$u_{x_1x_1}(x_1, x_2, \ldots, x_m) + u_{x_2x_2}(x_1, x_2, \ldots, x_m) + \ldots + u_{x_mx_m}(x_1, x_2, \ldots, x_m) = 0 \qquad (2.1)$$

with $(x_1, x_2, \ldots, x_m) \epsilon R$, where R is the unit supercube (unit square or unit cube when $m = 2$ or 3 respectively) with boundary Γ and $u(x_1, x_2, \ldots, x_m)$ is prescribed on Γ.

We suppose there are $N \equiv \frac{1}{h}$ equal subdivisions in each co-ordinate direction. As is known, this problem can be transformed into a matrix problem which approximates (2.1) with a $(2m + 1)$-point formula. The arising matrix problem is of the form

$$(X_1 + X_2 + \ldots + X_m)u = g \qquad (2.2)$$

where u is the approximating solution $(N - 1)^m$-dimensional vector, g is a known $(N - 1)^m$-dimensional vector which comes from the boundary conditions and

* *Department of Computational and Statistical Science, The University, Liverpool*, 3.

$X_i | i = 1, 2, \ldots, m$ is real symmetric positive definite $(N-1)^m \times (N-1)^m$ matrix which after suitable permutation transformations is the direct sum of tridiagonal matrices (see Varga, 1962).

We propose the following generalised iterative scheme for solving (2.2)

$$(I + r_{p+1}X_1)u^{(p+1/m)} = [(I + r_{p+1}X_1) - \omega r_{p+1}\sum_{i=1}^{m} X_i]u^{(p)} + \omega r_{p+1}g$$

$$(I + r_{p+1}X_j)u^{(p+j/m)} = u^{(p+(j-1)/m)} + r_{p+1}X_j u^{(p)} \text{ for } j = 2, \ldots, m \qquad (2.3)$$

where $u^{(p)}$ are the vector iterates of u, $r_{p+1} > 0$ constant during an iteration, I the identity matrix and ω a constant to be defined. The proposed iterative scheme (2.3) simply reduces to the Douglas–Rachford iterative scheme for $\omega = 1$, while for $\omega = 2$ it reduces to the corresponding Douglas scheme.

Under the boundary conditions mentioned above all X_i's$|i = 1, 2, \ldots, m$ commute. Thus if we put $r = r_{p+1} > 0$ then from equations (2.3) by solving we can get after some elementary matrix operations.

$$u^{(p+1)} = T_r u^{(p)} + \omega r(I + rX_m)^{-1} \ldots (I + rX_2)^{-1}(I + rX_1)^{-1}g \qquad (2.4)$$

where

$$T_r \equiv I - \omega r(I + rX_m)^{-1} \ldots (I + rX_2)^{-1}(I + rX_1)^{-1}\sum_{i=1}^{m} X_i \qquad (2.5)$$

is the iterative matrix of the procedure (exactly the same as in Guittett's scheme).

If now scheme (2.3) is convergent then for p large any intermediate solution $u^{(p+j/m)}|j = 0, 1, \ldots, m$ is an approximating solution of (2.2). This does not happen in Guittet's scheme where only for $j = 0$ and m is $u^{(p+j/m)}$ an approximating solution of (2.2).

From (2.5) one can readily see that the eigenvalues of T_r are

$$t_{f_1 f_2 \ldots f_m} = 1 - \omega r \frac{\sum_{i=1}^{m} x_{if_i}}{\prod_{i=1}^{m}(1 + rx_{if_i})} \qquad (2.6)$$

where the x_{if_i}'s are the $(N-1)^m$ eigenvalues of X_i. Therefore for the convergence of T_r we must have

$$-1 < t_{f_1 f_2 \ldots f_m} < 1. \qquad (2.7)$$

It is clear that ω must be positive for otherwise the eigenvalues of T_r would be greater than 1.

As one can see from the above, $\omega > 0$ is a necessary and sufficient condition for $t_{f_1 f_2 \ldots f_m} < 1$. Therefore for specific values of m and r one perhaps can find a value of $\omega > 0$ for which (2.7) is valid and, moreover, for which either the asymptotic rate of convergence is a maximum (this is what has been done by Guittet) or the number of calculations needed to reduce the norm of the matrix operator that maps the error vector $e^{(0)}$ to the error vector $e^{(p)}$ below a preassigned $\epsilon > 0$ is a minimum (this is what we shall do in the following as far as the 3-dimensional case is concerned).

3. 3-dimensional case ($m = 3$)

In this case the eigenvalues of the iterative matrix T_r are

$$t_{f_1 f_2 f_3} = 1 - \omega \frac{r_{p+1}(x_{1f_1} + x_{2f_2} + x_{3f_3})}{(1 + r_{p+1}x_{1f_1})(1 + r_{p+1}x_{2f_2})(1 + r_{p+1}x_{3f_3})} \qquad (3.1)$$

where

$$x_{1f_1} = 4\sin^2\frac{\pi q_1}{2N},\ x_{2f_2} = 4\sin^2\frac{\pi q_2}{2N},\ x_{3f_3} = 4\sin^2\frac{\pi q_3}{2N} | 1 \leqslant q_1, q_2, q_3 \leqslant N-1. \qquad (3.2)$$

Let us put

$$\zeta = 4r_{p+1},\ \xi_{q_i} = \sin^2\frac{\pi q_i}{2N} \text{ for } i = 1, 2, 3 \text{ and} \qquad (3.3)$$

$$a = \zeta\xi_{q_1},\ b = \zeta\xi_{q_2},\ c = \zeta\xi_{q_3}. \qquad (3.4)$$

Because of (3.3) and (3.4), (3.1) takes the form

$$\rho \equiv \rho(a, b, c) \equiv t_{f_1 f_2 f_3} = 1 - \omega\frac{(a + b + c)}{(1 + a)(1 + b)(1 + c)}. \qquad (3.5)$$

We use, instead of a fixed ζ, the sequence of parameters $\{\zeta_n\} n = 1, 2, \ldots, n_0$ defined by Douglas (1962) in the following way:

$$\zeta_n = \mu\left(\frac{\mu}{v}\right)^{n-1}\sin^{-2}\frac{\pi}{2N} | n = 1, 2, \ldots, n_0 \qquad (3.6)$$

where n_0 is such that

$$\left(\frac{v}{\mu}\right)^{n_0-1}\sin^2\frac{\pi}{2N} < \cos^2\frac{\pi}{2N} \leqslant \left(\frac{v}{\mu}\right)^{n_0}\sin^2\frac{\pi}{2N} \qquad (3.7)$$

and

$$0 < \mu \leqslant \cos^2\frac{\pi}{2N} < 1 \leqslant v \ (\mu, v \text{ constants to be determined}). \qquad (3.8)$$

Consider now any triple (a, b, c) for which say $a \geqslant b \geqslant c$. If we iterate n_0 times with the parameter sequence (3.6) then for at least one value of $n = n^* | n = 1, 2, \ldots, n_0$ we shall have

$$\mu \leqslant a \leqslant v$$

and therefore

$$c \leqslant b \leqslant a \leqslant v.$$

Moreover

$$b \geqslant c = \zeta_{n^*}\xi_{q_3} \geqslant \mu\left(\frac{\mu}{v}\right)^{n^*-1} \sin^{-2}\frac{\pi}{2N}\sin^2\frac{\pi}{2N}$$

$$\geqslant \mu\left(\frac{\mu}{v}\right)^{n_0-1} > \mu\tan^2\frac{\pi}{2N} \quad (3.9)$$

because of (3.7). Consequently if we consider all the possible permutations in the relationships $a \geqslant b \geqslant c$ then for an $n = n^*$ one of the following is satisfied

$$\mu \leqslant a \leqslant v,\ \mu\tan^2\frac{\pi}{2N} \leqslant b,\ c \leqslant v \quad \text{or}$$

$$\mu \leqslant b \leqslant v,\ \mu\tan^2\frac{\pi}{2N} \leqslant c,\ a \leqslant v \quad \text{or}$$

$$\mu \leqslant c \leqslant v,\ \mu\tan^2\frac{\pi}{2N} \leqslant a,\ b \leqslant v. \quad (3.10)$$

It is understood that for any $n \neq n^*$ the triple considered does not satisfy one of (3.10) any more. Instead we have

$$a, b, c = \zeta_n\xi_{q_i} \leqslant \mu\left(\frac{\mu}{v}\right)^{n-1} \sin^{-2}\frac{\pi}{2N}\cos^2\frac{\pi}{2N}$$

$$\leqslant \mu/\tan^2\frac{\pi}{2N} < v/\tan^2\frac{\pi}{2N}.$$

(We take $v/\tan^2\frac{\pi}{2N}$ as an upper bound for a, b, c instead of $\mu/\tan^2\frac{\pi}{2N}$ for $v/\tan^2\frac{\pi}{2N} > 1$ which facilitates the analysis in finding some extreme values of the function f later.)

A lower bound for a, b, c when $n \neq n^*$ can be found in the same way as in (3.9). Therefore for any $n \neq n^*$ we have

$$\mu\tan^2\frac{\pi}{2N} < a, b, c < v/\tan^2\frac{\pi}{2N}. \quad (3.11)$$

Let us call

$$f \equiv f(a, b, c) \equiv \frac{a+b+c}{(1+a)(1+b)(1+c)} > 0. \quad (3.12)$$

By taking derivatives we can very easily prove that the maximum value of f, when a, b, c satisfy (3.11), μ and v (3.8) and $N \geqslant 3$ is given by

$$f^*_{max} = \frac{2\mu\tan^2\frac{\pi}{2N} + v/\tan^2\frac{\pi}{2N}}{\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2\left(1+v/\tan^2\frac{\pi}{2N}\right)}. \quad (3.13)$$

In the same way we can prove that if a, b, c satisfy one of the conditions (3.10), μ and v satisfy (3.8) and $N \geqslant 3$ then the maximum and the minimum values of f are given by

$$f_{max} = max\left\{\frac{2\mu\tan^2\frac{\pi}{2N} + v}{\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2(1+v)}, \frac{\mu+\mu\tan^2\frac{\pi}{2N}+v}{(1+\mu)\left(1+\mu\tan^2\frac{\pi}{2N}\right)(1+v)}\right\}$$

$$f_{min} = min\left\{\frac{2\mu\tan^2\frac{\pi}{2N}+\mu}{(1+\mu)\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2}, \frac{3v}{(1+v)^3}\right\} \quad (3.14)$$

respectively, but

$$\frac{2\mu\tan^2\frac{\pi}{2N}+v}{\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2(1+v)} - \frac{\mu+\mu\tan^2\frac{\pi}{2N}+v}{(1+\mu)\left(1+\mu\tan^2\frac{\pi}{2N}\right)(1+v)}$$

$$= \frac{\mu\left(1-\tan^2\frac{\pi}{2N}\right)\left(v-1+\mu\tan^2\frac{\pi}{2N}\right)}{(1+\mu)\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2(1+v)} > 0.$$

Therefore

$$f_{max} = \frac{2\mu\tan^2\frac{\pi}{2N}+v}{\left(1+\mu\tan^2\frac{\pi}{2N}\right)^2(1+v)}. \quad (3.15)$$

For the sake of convenience we take the two expressions giving the minimum in (3.14) equal. Hence

$$f_{min} = \frac{\mu+2\mu\tan^2\frac{\pi}{2N}}{(1+\mu)\left(1+\mu\tan^2\frac{\pi}{2N}\right)} = \frac{3v}{(1+v)^3}. \quad (3.16)$$

We are now in a position to choose ω as a function of N, μ and v in such a way as to give an optimum result.

First of all we can observe that the possible range of ω is limited from the fact that we must have $-1 \leqslant \rho \leqslant 1$ for all the triples (a, b, c) which satisfy (3.11). This gives $-1 \leqslant 1 - \omega f \leqslant 1$ or

$$0 < \omega \leqslant 2/f^*_{max}. \quad (3.17)$$

With the above permissible range for ω one can easily see that $|\rho|$ is bounded by 1 for all the triples (a, b, c) which satisfy one of (3.10). It is clear that the greatest efficiency is achieved when $1 - \omega f_{min} = -(1 - \omega f_{max})$ that is when

$$\omega = 2/(f_{max} + f_{min}). \quad (3.18)$$

We distinguish two cases

Case 1 $2/(f_{max} + f_{min}) < 2/f^*_{max}$.

In this case ω is chosen as in (3.18) and satisfies (3.17).

Moreover we have

$$|\rho| \leqslant 1 - \omega f_{min} \equiv \rho(\mu, v). \tag{3.19}$$

Case 2 $2/f^*_{max} \leqslant 2/(f_{max} + f_{min})$.

With ω in the range defined by (3.17) we have $1 - \omega f_{min} > -(1 - \omega f_{max})$. Therefore $|\rho|$ satisfies the same inequality as in (3.19). The minimum value of the bound of $|\rho|$ takes place when ω is maximum. So

$$\omega = 2/f^*_{max}. \tag{3.20}$$

General conclusion from these two cases examined is that ω is given by

$$\omega = min\,\{2/f^*_{max},\ 2/(f_{max} + f_{min})\} \tag{3.22}$$

where $f^*_{max}, f_{max}, f_{min}$ are given by (3.13), (3.15) and (3.16), respectively, and that in either case the bound for $|\rho|$ is given by (3.19).

We come now to study a little more the relationship (3.16). By considering the function $y(v) = \dfrac{3v}{(1+v)^3}$ as a function of v we can form **Table 1**.

From the table we can see that for $N \geqslant 3$ and for all values of $\mu \in \left(0, \cos^2 \dfrac{\pi}{2N}\right]$ for which

$$0 < \frac{\mu + 2\mu \tan^2 \dfrac{\pi}{2N}}{(1+\mu)\left(1 + \mu \tan^2 \dfrac{\pi}{2N}\right)^2} \leqslant \frac{3}{8}$$

Table 1

v	$-\infty$		$-1-\epsilon$	$-1+\epsilon$		0		$\frac{1}{2}$		1		$+\infty$
$y(v)$	0	$\nearrow$	$+\infty$	$-\infty$	$\nearrow$	0	$\nearrow$	$\frac{4}{9}$	$\searrow$	$\frac{3}{8}$	$\searrow$	0
$y'(v)$			$+$					0	$-$			

the equation (3.16), where v is the unknown has three roots belonging to the intervals $(-\infty, -1)$, $(0, \frac{1}{2})$ and $[1, +\infty)$, respectively. We are only interested of course in that root belonging to the third interval.

It is known (see Douglas (1962)) that for a fixed $N \geqslant 3$ the number of calculations required to solve the model problem to a given accuracy is minimum for that pair (μ, v) for which $\log \rho(\mu, v) \log (\mu/v)$ is a maximum. By using the KDF9 computer of the University of Liverpool we have found for $N = 3(1)50$ and $\mu = 0{\cdot}01(0{\cdot}01)\cos^2 \dfrac{\pi}{2N}$ the corresponding values of v, $\omega_1 = 2/f^*_{max}$, $\omega_2 = 2/(f_{max} + f_{min})$, $\rho(\mu, v) = 1 - \min\{\omega_1, \omega_2\} f_{min}$ and $z = \log \rho(\mu, v) \log (\mu/v)$. From the results we have selected for each value of $N = 3(1)20$ and $N = 25(5)50$ those pairs (μ, v) for which the corresponding value of $z = \log \rho(\mu, v) \log (\mu/v)$ is a maximum. These selected results are set out in **Table 2**.

We now compare our method with Douglas' and Guittet's. We can very easily see that our method is better than that of Douglas for all values of $N \geqslant 3$. This is apparent from the fact that for the same values

Table 2

Optimum parameter values

N	μ	v	ω_1	ω_2	$\rho(\mu, v)$	z
3	0·29	1·35319559	2·86158800	2·33104028	0·27379785	1·99530706
4	0·32	1·47031830	2·45391131	2·30575465	0·32533689	1·71231595
5	0·35	1·47402177	2·29242497	2·28860084	0·33167970	1·58675371
6	0·37	1·46727495	2·20507063	2·27836085	0·35374694	1·43162689
7	0·35	1·57928583	2·13942520	2·27192443	0·40928135	1·34609891
8	0·35	1·60635042	2·10497610	2·26725868	0·42705848	1·29649021
9	0·34	1·66501886	2·07982656	2·26389304	0·45113357	1·26454932
10	0·34	1·67898437	2·06412969	2·26141422	0·45925271	1·24271198
11	0·34	1·68941145	2·05267780	2·25954529	0·46518236	1·22696254
12	0·34	1·69739646	2·04405921	2·25810397	0·46964866	1·21520718
13	0·34	1·70364351	2·03740629	2·25697043	0·47309862	1·20618849
14	0·34	1·70862096	2·03216110	2·25606363	0·47582004	1·19911149
15	0·34	1·71264989	2·02795119	2·25532731	0·47800528	1·19345223
16	0·33	1·75855916	2·02385689	2·25464255	0·49135927	1·18891171
17	0·33	1·76136377	2·02109969	2·25413486	0·49279073	1·18517218
18	0·33	1·76371842	2·01879573	2·25370796	0·49398720	1·18205306
19	0·33	1·76571428	2·01685057	2·25334565	0·49499757	1·17942372
20	0·33	1·76742058	2·01519323	2·25303557	0·49585860	1·17718631
25	0·33	1·77312163	2·00969299	2·25199731	0·49871727	1·16977974
30	0·33	1·77622830	2·00671970	2·25143013	0·50026332	1·16578781
35	0·33	1·77810487	2·00493181	2·25108705	0·50119324	1·16339136
40	0·33	1·77932419	2·00377338	2·25086394	0·50179587	1·16184020
45	0·33	1·78016076	2·00298007	2·25071078	0·50220861	1·16077865
50	0·33	1·78075947	2·00241306	2·25060112	0·50250364	1·16002027

μ and v, $\rho(\mu, v) < \rho_D(\mu, v)$ (D denotes Douglas) for it can be proved that $\omega = \min\{\omega_1, \omega_2\} > 2$. It is also obvious that as $N \to \infty$ then $\omega \to 2$ so our method tends to that of Douglas for very large values of N. The number of iterations needed to reduce the norm of the matrix which maps the error vector $e^{(0)}$ to the error vector $e^{(p)}$ below a preassigned $\epsilon > 0$ is given approximately by (see Douglas (1962))

$$P_H, P_D \simeq \frac{2 \log \tan \frac{\pi}{2N} \log \epsilon}{\log \rho(\mu, v) \log (\mu/v)}. \qquad (3.23)$$

in either our or Douglas' case, while the same number in Guittet's case is given by

$$P_G \simeq \log \epsilon / \log \rho^* \qquad (3.24)$$

where ρ^* is the amplification factor in Guittet's scheme given by

$$\rho^* = \frac{\left[1 - \left(\tan^2 \frac{\pi}{2N}\right)^{1/3}\right]^2 \left[1 + 2\left(\tan^2 \frac{\pi}{2N}\right)^{1/3}\right]}{1 + 3\left(\tan^4 \frac{\pi}{2N}\right)^{1/3} + 2 \tan^2 \frac{\pi}{2N}}$$

(see Guittet (1967) page 211.) (3.25)

By using the computer we have found that for $\mu = 0{\cdot}01$ (0·01) 1·00 the minimum P_D is achieved when $\mu = 0{\cdot}33$, where $v = 1{\cdot}78331472$,

$$\rho_D(\mu, v) = 0{\cdot}50375940 \text{ and}$$
$$\log \rho_D(\mu, v) \log (\mu/v) = 1{\cdot}15679610.$$

The insertion of the parameter ω with its optimum value for the chosen value of N does not substantially alter the number of calculations to be performed. Consequently we can suppose that the number of calculations needed to perform one iteration in any of the three schemes is the same (which is not far from the truth) then in order to compare these three methods it is sufficient to compare the numbers P_H, P_D and P_G or equivalently the numbers p_h, p_d and p_g where

$$p_h = -P_H/\log \epsilon,\ p_d = -P_D/\log \epsilon$$
$$\text{and } p_g = -P_G/\log \epsilon (\epsilon < 1). \qquad (3.26)$$

By using the computer once again we have found for $N = 3(1)20$ and $N = 25(5)50$ different values for these numbers which are presented in **Table 3.**

Table 3

Comparison of calculations in the three methods

N	p_h	p_d	p_g
3	0·55059810	0·94970262	0·38044178
4	1·02945206	1·52381839	0·59011434
5	1·41695237	1·94360478	0·80240989
6	1·83980604	2·27690584	1·02318241
7	2·19499821	2·55419663	1·25357223
8	2·49117333	2·79200616	1·49358114
9	2·74471725	3·00038211	1·74287160
10	2·96565909	3·18592021	2·00101165
11	3·16143766	3·35319732	2·26756054
12	3·33702673	3·50552603	2·54209959
13	3·49610919	3·64538459	2·82424212
14	3·64147289	3·77467731	3·11363503
15	3·77527084	3·89490024	3·40995723
16	3·89900442	4·00725073	3·71291673
17	4·01423369	4·11270240	4·02224762
18	4·12205871	4·21205786	4·33770713
19	4·22337501	4·30598674	4·65907291
20	4·31892626	4·39505361	4·98614075
25	4·72905431	4·78213223	6·70088982
30	5·05872546	5·09804665	8·53500483
35	5·33456539	5·36497943	10·4747261
40	5·57182050	5·59611590	12·5096571
45	5·78004000	5·79993918	14·6316260
50	5·96560479	5·98223185	16·8340134

As one can see from Table 3 Guittett's method is the best for $N \geqslant 3$ until approximately $N = 16$. But from approximately $N \geqslant 17$ the method we propose is the best.

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