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A variant of the residual correction method for the numerical solution of the Laplace and the Poisson equations*

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The high accuracy numerical solution of the Laplace or the Poisson equation is reduced to a sequence of the more simple finite difference problems of the second order accuracy. Some algorithms to realize effectively this scheme are discussed.

1. Introduction

Let us consider the classical problem: the approximate solution x_0 of the ordinary nonlinear equation $f(x) = 0$ is known, its deviation from the exact solution does not exceed h, but a more accurate approximation is wanted. There exists the following effective way to solve this problem: the function $f(x)$ in the vicinity of the point x_0 is approximated with the first order polynomial

$$p(x) = \varepsilon + f'(x_0)(x - x_0),$$

where the residual $\varepsilon = f(x_0)$, then the zero of this polynomial is the next approximation to the exact solution. Thus, the main part of the residual is cut off. Then the process is repeated if it is needed. It is the well-known linearization method which provides an accuracy $O(h^2)$ at each stage and, generally speaking, fast converges.

At the first sight, it seems that this method can be improved in such a straightforward way: replace $f(x)$ with a polynomial of a higher power (say, second or third) and then obtain a more accurate approximate solution from the arising algebraic equation. However, disadvantages of this approach are well-known.

Meanwhile, various analogies of the latter approach prevail in attempts to create effective methods for the numerical solution of the partial differential equations. These are so-called "high accuracy schemes", when a differential equation is replaced with a finite difference equation of as high order of accuracy as possible, and then one has to elaborate cumbersome algorithms to solve it.

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The aim of this work is to propose a variant of the analogue of the first above-mentioned approach to the numerical solution of the Laplace and the Poisson equations and to illustrate its advantages.

2. Outline of the approach

The following example exposes further the features of the proposed approach. Let us consider the Laplace equation

$$\Delta u = 0 \tag{1}$$

with the Dirichlet boundary condition, that is, the values of the unknown function u in all the boundaries are given.

Let us approximate equation (1) by the finite difference equation

$$L_n \tilde{u} = 0, \tag{2}$$

where $L_n \tilde{u}$ is the finite difference approximation of the nth order of accuracy for the Laplace operator.

The conventional algorithms to solve equation (2) are rather cumbersome, if n exceeds 2, therefore we shall attempt to try the following way:

First of all, let us put n equal to 2. It means that equation (2) is replaced with the difference equation of the second order of accuracy

$$L_2 u_0 = 0. \tag{3}$$

The solution of equation (3) may be obtained more or less easily with the accuracy $O(h^2)$, where h is a typical grid step.

The next stage is the calculation in each grid node the quantity $\rho_0 = L_n u_0$, which is further called the "computational charge". In other words, ρ_0 is the residual, which arises, when u_0 is substituted in (2).

Now, let us look for the solution of the difference Poisson equation

$$L_n \tilde{u}_0 = -\rho_0 \tag{4}$$

with zero boundary conditions. It means that the solution of (4) with these boundary conditions is equal to zero anywhere, if the source ρ_0 is absent.

It is obvious that the grid function $\tilde{u}_0 + u_0$ is the solution of (2).

But equation (4) may be approximately replaced in its turn with the equation of the second order of accuracy

$$L_2 u_1 = -\rho_1 \equiv -L_n \tilde{u}_0 \tag{5}$$

with zero boundary conditions as well. Thus, as a result we obtain a more accurate approximation:

$$\tilde{u}_2 = u_0 + u_1 + u_2,$$

where the prevailing part of the residual of the first approximation is cut off.

Then this approximate solution may be improved in the same way, etc.

Thus, we obtain a set of the difference equations with zero boundary conditions

$$L_2 u_k = -\rho_{k-1}, \tag{6}$$

where $\rho_{k-1} = L_n u_{k-1}$.

This process of the successive "cutting off" the residuals is quite similar to the linearization method for the numerical solution of the ordinary nonlinear equations. Hence, one may conclude that the limit of the sequence

$$u_0 + u_1 + u_2 + \ldots$$

should fast converge and this limit is the solution of (2).

Some remarks should be made here:

1. The same scheme works for numerical solution of the Poisson equation. The only distinction is that at the first stage the Poisson difference equation (instead of the Laplace equation) must be solved.
2. Residuals must be cut off not only in the equation, but also in the boundary conditions, if they are of the Neumann or of the third type. The same takes place for the inner boundaries, i.e., at the lines, which divide heterogeneous media.
3. The above approach essentially mollifies the difficulties, connected with possible peculiarities in the geometry of the problem. The reason of it is that the loss of accuracy of the computational schemes at the peculiar points originates the great computational charge which is then cut off. The possible irregularities in the computational charge distribution can be eliminated by smoothing procedures.

Thus, the numerical solution of the initial differential problem is reduced to a sequence of the finite difference problems of the second order of accuracy. Hence, it is necessary to have effective solvers for these problems which are well adapted to the algorithm as a whole. First of all, it implies that the solvers must take advantage of the existence of the good initial approximation which is the result of the previous stage of the proposed algorithm. Therefore, for instance, a well-known method of the incomplete factorization [1] is not suitable here, because it almost does not response to the quality of the initial approximation.

3. The second order scheme

The features of the proposed scheme may be shown using as an illustration the Laplace equation in axially symmetrical geometry within the rectangular calculation region

$$0 \le r \le R, \quad 0 \le z \le Z$$

The comparison of the numerical solution with the known analytical one

$$U(r,z) = \left(C_1 e^{-\lambda z} + C_2 e^{\lambda z}\right) J_0(\lambda z), \tag{7}$$

will show the effectiveness of the scheme. Here J_0 is the Bessel function and C_1, C_2, and λ are varying parameters.

It means that function (7) yields the boundary conditions for the numerical problem (except the axis), then the obtained numerical solution is to be compared with (7). The symmetry condition along the axis $r = 0$ further replaces here the Neumann boundary condition usually used in this case. All the parameters in (7) and grid parameters varied within the wide range, so that all the following conclusions were reliably checked.

For the sake of simplicity, we here consider only the uniform grids. In fact, this restriction does not matter, because only the form of the approximating operator L_n must be otherwise changed.

We set further $n = 4$, i.e., all the numerical derivatives in the operator L_n are determined by 5-point stencils.

Let us now list all the features of the proposed technique to numerically solve the Poisson equation with the second order scheme, because this problem arises at each stage of the general approach due to (6).

1. Averaging. Let the axially symmetric function $u(r,z)$ satisfy the Poisson equation in the 3D space

$$\Delta u = \rho. \tag{8}$$

and a node (r,z) be encircled with the 3D sphere of the radius r_s. This quantity will be further called "the radius of averaging".

Now let us carry out the following operations:

1. The known Green formula which relates the value of the function in the centre of the sphere to the volume and surface integrals

$$u = \frac{1}{4\pi r_s^2} \oint u \, dS + \frac{1}{4\pi r} \oint \frac{\partial u}{\partial n} \, dS - \frac{1}{4\pi r} \int \Delta u \, dV. \tag{9}$$

2. The transformation of the volume integrals in (9) into the surface ones and the numerical evaluation of the surface integral on the sphere with the known formula which has the form in the Cartesian coordinates

$$\frac{1}{4\pi r_s^2}\int u\,dS = \frac{1}{6}\Big(u(x+r_s,y,z)+u(x-r_s,y,z)+u(x,y+r_s,z)+$$
$$u(x,y-r_s,z)+u(x,y,z+r_s)+u(x,y,z-r_s)\Big). \quad (10)$$

The last two nodes of this quadrature do not belong to the plane (r,z), but they can be easily projected onto this plane due to the axial symmetry of our problem.

3. Because the nodes of quadrature (10) do not coincide with the grid nodes, the values of the function u in the quadrature nodes can be expressed by those in the adjacent grid nodes with the help of the quadratic interpolation.

All these are rather cumbersome, but straightforward transformations lead to the relation between the value of the grid function in (i,j)-node with the values in the adjacent nodes:

$$\alpha_{i,j}u_{i,j} = \alpha_{i+1,j}u_{i+1,j}+\alpha_{i-1,j}u_{i-1,j}+$$
$$\alpha_{i,j+1}u_{i,j+1}+\alpha_{i,j-1}u_{i,j-1}+\beta_{i,j}\rho_{i,j}. \quad (11)$$

Here all the coefficients depend on the averaging radius r_s, the grid steps and the distance r from the axis. Relation (11) is valid with the accuracy $O(h^4)$. Of course, the latter is true only for harmonic in the 3D space and axially symmetric functions u.

Relation (11) is the basic averaging formula. It is important that a variation of averaging radius r_s only slightly affects the accuracy of this relation. In other words, the change of r_s causes small changes of the coefficients in the formula which estimates the error of relation (11). The numerical experiments, where r_s varied from $0.05h$ to $2h$, confirmed this conclusion.

It is here worth to mention that for a "truly" 3D geometry (i.e., without axial symmetry), the formula of averaging is even simpler.

By the way, the use of the averaging algorithm provides an additional advantage: it gives the possibility to avoid troubles caused by the appearance of the small quantities in the dominators in the numerical axially symmetric Laplace operator near the axis. Of course, it is valid for the spherical coordinates, too.

2. The Seidel scheme and reordering of grid nodes. Formula (11) permits to use the well-known Seidel scheme (see, e.g., [2]), when one has to substitute into the right-hand side of (11) the values of the grid function, obtained at the previous stage of the iteration process, and to determine in such a way the more accurate value for $u_{i,j}$. These operations are to be carried out successively for all the nodes and then the process must be repeated again until the desired accuracy is attained.

This scheme provides the accuracy $O(h^2)$, is very simple and has an important advantage: a good initial approximation essentially decreases the number of needed iterations.

But the fault of this scheme is well-known, too: it converges, generally speaking, very slowly.

Some ways to overcome this fault are considered below.

First, it is useful to reorder grid nodes according to their distances to the nearest Dirichlet boundaries. The meaning of the reordering is clear, because the Seidel scheme realizes the "growing" of the Dirichlet boundary conditions inward the computational domain. Hence the reordering should essentially accelerate the calculation due to decreasing the share of the "blank" or almost "blank shots" in (11). Of course, this effect increases together with the total number of the nodes. For 60×80 grid the gain in the computer time due to the node reordering appeared to be about ten times.

Surely, the reordering itself must not be too expensive. A special technique for this purpose has been created and realized as a set of programs. This technique is effective for any 2D geometry of the computational domain, including multiply connected cases, because the number of operations for its realization is proportional only to the first power of the total number of nodes. For 60×80 grid the reordering takes no more than 2% of the total computer time of solving the whole problem. For larger grids a relative time of the reordering respectively drops. This technique will be described separately.

Unfortunately, this reordering algorithm cannot be directly applied to the case of the 3D geometry. It is the subject of the future work.

By the way, the reordering yields no gain, when the incomplete factorization method is used for the numerical solution of the same problems.

3. Embedded grids. The averaging method is sensitive to the quality of the initial approximation. It makes the embedded grids approach advantageous, when one firstly obtains the numerical solution on the sparse grid and then uses it as the initial approximation for the twice denser grid.

In our numerical experiments, the grid halving was performed twice. It gives the possibility to carry out the local Richardson extrapolation in each node (of course, in the grid version, when the extrapolation is performed to the numerical solution on the densest grid).

4. Successive over relaxation (SOR). It is possible to take the value $u_{i,j}$ "partially" from the previous iteration, having rewritten relation (11) in the form

$$\begin{aligned}(1-\gamma)\alpha_{i,j}u_{i,j} = {} & \alpha_{i+1,j}u_{i+1,j} + \alpha_{i-1,j}u_{i-1,j} + \alpha_{i,j+1}u_{i,j+1} + \\ & \alpha_{i,j-1}u_{i,j-1} - \gamma\alpha_{i,j} + \beta_{i,j}\rho_{i,j}. \qquad (12)\end{aligned}$$

It is known (see, e.g., [3]) that this technique can accelerate the convergence of an iteration process by several times. The only problem is a proper choice of the relaxation parameter γ. An improper choice can cause even the divergence of the process. It is impossible to estimate the optimal γ theoretically, especially in the cases of complicated geometries and non-uniform grids. Therefore a great number of numerical experiments, concerning this problem, were carried out for various grids and domain geometries, so that the following results are reliable and can be used in practice.

1. Increasing the relaxation parameter, starting with zero, accelerates the convergence until the optimal value is attained. The further growth abruptly leads to the divergence of iterations.
2. The halving of the grid almost does not change this optimal value. Probably, it is due to the chosen method of the node reordering.

Thus, we can propose a practical way to obtain nearly the best value of the parameter γ: we approach to it as near as possible on the sparsest grid (and, consequently, with low expenses) and then use the obtained parameter for the denser grids. The search for the best γ on the sparsest grid may be easily made automatically if one takes into account the first above-mentioned item.

In our numerical experiments, the SOR technique accelerated the convergence by 5–7 times.

The weak dependence of the result of the averaging on the averaging radius r_s makes it possible to use small r_s in the near-boundary nodes to avoid crossing the boundary. This gives the possibility to use for averaging in these cases not only the values of the grid function in the adjacent nodes, but in the nearest boundary points, too. It permits, in turn, to avoid a sophisticated procedure of the so-called local grid modification, i.e., to avoid the grid node transfer to the boundaries. The corresponding numerical experiments with "declined" boundaries appeared to be successful.

However it should be mentioned that the further improvements of the averaging technique require the quadratures on the sphere which include the irregularly located quadrature nodes. The same problem arises at the boundaries of the grid subdomains, where the grid becomes sparser or denser.

4. Some general remarks

The tests of the proposed method have revealed some peculiarities which may be used and are indeed used in real programs.

1. The loss of accuracy of the five-point stencils for the numerical derivatives in the difference Laplace operator at the boundaries does not cause the corresponding loss of accuracy of the numerical solution.

2. One may carry out the residual correction periodically, say, after 5, 10, or 20 SOR iterations. Let us call such a set of the SOR iterations "the big iteration step". Numerical experiments show that if the number of the big steps N is great enough, the deviation of the numerical solution $\tilde{u}_N$ from the exact one u after the Nth big step obeys the rule:

$$\tilde{u}_N - u \approx q(\tilde{u}_{N-1} - u), \quad q < 1 \tag{13}$$

and the decrements q in all the nodes tend to the same value.

This rule may be used to accelerate the convergence of the method. To this end let us store the grid functions on three successive big steps N, $N-1$, $N-2$. Then the increments q in each node may be easily estimated from the relation

$$q \approx \frac{\tilde{u}_N - \tilde{u}_{N-1}}{\tilde{u}_{N-1} - \tilde{u}_{N-2}}. \tag{14}$$

If the dispersion of this quantity in different nodes does not exceed, say, 10%, one can make the prognosis due to rule (13).

Since this decrement-analysis is seldom performed, it takes relatively small computer time, but provides an essential gain in the total computer time, up to 2–3 times.

On the whole, the numerical experiments show that the proposed approach with all the described improvements yields the solution with an accuracy up to 6th decimal place on 60×80 grid about 500 time faster, than the incomplete factorization method with the conjugate gradients acceleration. The gain in required computer memory is about the same.

5. Verification of results

Some empirical facts are revealed in the described numerical experiments. Of course, it is necessary to be sure that they are reliable. A large number of special programs was worked out for this purpose. For example, the expected order of the accuracy was checked at least by three ways:

1. The direct comparison of the numerical solutions on three successive grids with the known analytical solution.
2. The comparison of the numerical solution on the densest grid with the Richardson extrapolation from two previous grids, assuming the order of accuracy n to be equal to 4.
3. Finally, the order of the accuracy was estimated directly from the data on all three successively twice denser grids:

$$\frac{u^{(1)} - u^{(2)}}{u^{(2)} - u^{(3)}} \approx 2^n.$$

The thus obtained values n deviate from 4 not more than by 5% in all the nodes.

Another example: the analysis, which verifies the rules of the behaviour of the decrement q, was based on the estimation of the decrement in all the nodes from the data from three successive big iteration steps according to (14). Then the investigation was continued with the usual data processing technique: the determination of the mean value for q and the analysis of the distribution of deviations of the decrements from the mean value.

Thus, all the above facts are confirmed quite reliably and can be used in practice.

6. Prospects

Apparently, the most important problem now is to create an effective algorithm for reordering the grid nodes according to their distances to the nearest Dirichlet boundary in the 3D geometry. It will give us the hope to effectively solve the 3D problems, because the above algorithm provides fairly high accuracy and requires little computer memory. Probably, it will open the way to get over the "fatality of the dimension".

Another important problem is to apply the approach to the numerical solution of the Helmholtz equation and to the systems of these equations. It is of great interest for Geophysics.

References

[1] Il'in V.P. Iterative Incomplete Factorization Methods. – Singapore: World Sci. Publ. Co., 1992.

[2] Samarsky A.A., Andreev V.P. Finite Difference Methods for the Elliptical Equations. – Moscow: Nauka, 1976 (in Russian).

[3] Samarsky A.A., Nikolaev V.S. Methods of Solving Grid Equations. – Moscow: Nauka, 1978 (in Russian).