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AN EFFICIENT METHOD FOR SOLVING DIFFUSION EQUATIONS

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An algorithm for solving diffusion equations is described which has an arbitrary order of approximation in space variables, i.e., its accuracy is the higher, the smoother the solution in space variables. This provides an advantage over difference methods, which have a fixed order of approximation in space variables irrespective of the solution smoothness. In practice, this allows one (with smooth initial data) to carry out calculations on coarse space grids by an explicit scheme with applicable time steps. The method is competitive with difference methods in speed and the amount of information stored.

Introduction. Because of the problem of simulation of underground burial of liquid waste materials, interest has been recently rekindled in the development of algorithms for numerical calculation of diffusion equations. In practice, liquid waste materials are pumped into deep collector beds through several holes. If there is no groundwater motion, the impurity propagation is described by a diffusion equation. The initial impurity distribution after cessation of pumping is described by a function with large gradients over the space coordinates. This function may be thought of as smooth. Therefore, for discretization of a diffusion equation over space coordinates it is worthwhile to apply methods without saturation [1]. With respect to time, diffision is a very slow process, which is approximated by an explicit first-order scheme with an accuracy sufficient for practice. Moreover, the explicit scheme admits a simple realization on an electronic computer with several processors operating in parallel.

The classical technique for solving the diffusion equations is the difference method. Discretization by this method leads to a finite-dimensional problem with a "thinned" matrix. This allows one to organize efficient computations by an explicit scheme. Methods without saturation lead to a finite-dimensional problem with a completely filled matrix. However, in the case considered these matrices have a special structure [2], which makes it possible to organize computations economically and create a procedure that is competitive with difference methods in speed and memory needed, but exceeding them in accuracy (for smooth initial data).

1. Statement of the Problem and Discretization. We consider problem in a singly bound region $B \in R^2$ with a sufficiently smooth boundary ∂B:

$$\frac{\partial u(z, t)}{\partial t} = D\Delta u(z, t), \quad z \in B; \tag{1}$$

$$u|_{\partial B} = 0; \tag{2}$$

$$u|_{t=0} = u_0(z). \tag{3}$$

Here, D is the coefficient of diffusion and Δ is the Laplace operator. As an example, we consider the Dirichlet problem with zero boundary conditions (2). We shall see in what follows how the other boundary conditions can be considered. The function $u_0(z)$ is considered rather smooth.

Let $z = \varphi(\zeta)$, $|\zeta| \le 1$ be the conformal mapping of a single circle onto region B; then in the ζ plane we formally obtain the same relations (1)-(3), but with $u(z, t)$, $u_0(z)$ replaced by $u(z(\zeta), t)$, $u_0(z(\zeta))$ and D by $D|\varphi'(\zeta)|^{-2}$. Boundary condition (2) is now given at the boundary of the single circle, i.e., at $r = 1$.

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The discretization of the initial boundary-value problem (1)-(3) over space variables is reduced to discretization of the Laplace operator in a circle with the Dirichlet boundary-value condition. We will perform this discretization following the procedure described in [2]. Then, we obtain a discrete Laplacian in the form of an h-matrix:

$$H = \frac{2}{N} \sum_{k=0}^{n}{}' \Lambda_k \otimes h_k , \tag{4}$$

where $N = 2n + 1$ is the number of grid nodes over the circles R_ν, $\nu = 1, \ldots, m$; the sign $\otimes$ means the Kronecker product of matrices Λ_k of size $m \times m$ and matrices h_k of size $N \times N$; the prime at the summation sign means that the term at $k = 0$ is taken with the coefficient $1/2$. Here m is the number of the nodes of the grid on the radius of a single circle. The form of matrices h_k is described in [2]. To construct matrices Λ_k, $k = 0, \ldots, n$, it is necessary to perform discretization of the k-th Bessel equation on the grid R_ν, $\nu = 1, 2, \ldots, m$.

As nodes of the grid on the radius we select $R_\nu = 0.5(1 + r_\nu)$ and $r_\nu = \cos((2\nu - 1)\pi/2/m)$, $\nu = 1, 2, \ldots, m$. We obtain matrix Λ_0 by discretizing the zero Bessel equation following a procedure described in [3]. More precisely, using the BESSEL program published in [3], we calculate a matrix of size $m \times m$ and then calculate the reciprocal of that matrix. Thus, we obtain matrix Λ_0. Then, we select matrices $\Lambda_k = \Lambda_0 + S_k$, $k = 1, 2, \ldots, n$, as matrices Λ_k, where S_k are diagonal matrices with numbers $(k/R_\nu)^2$, $\nu = 1, 2, \ldots, m$ on the diagonal.

Thus the discretization of the operator $-\Delta$ constructed in a single circle satisfies the Dirichlet homogeneous boundary-value condition. To consider another boundary-value condition, it is necessary to construct a corresponding discretization of the Bessel equations.

We note that to save h-matrix H (4), it is necessary to save two files of Λ_0 numbers of size $m \times m$ and R_ν^{-2}, $\nu = 1, 2, \ldots, m$.

2. An Algorithm for Rapid Multiplication of h-Matrix by a Vector. For effective realization of the explicit difference scheme with respect to time of problem (1)-(3), we need a fast algorithm for multiplying h-matrix H by a vector. On the basis of theorem [2], matrix H is represented in the form

$$H = \begin{Vmatrix} h^{11} & h^{12} & \ldots & h^{1m} \\ h^{21} & h^{22} & \ldots & h^{2m} \\ \ldots & \ldots & \ldots & \ldots \\ h^{m1} & h^{m2} & \ldots & h^{mm} \end{Vmatrix} ,$$

where matrices $h^{\nu\mu}$, $\nu, \mu = 1, 2, \ldots, m$ of size $N \times N$ are symmetric circulants, i.e., matrices the first line of which has the form $a_0 a_1 \ldots a_n a_n a_{n-1} \ldots a_1$, and the remaining lines are obtained by permutation from the first cyclic one.

For matrices $h^{\nu\mu}$, $\nu, \mu = 1, 2, \ldots, m$ we have the following representation

$$h_{ij}^{\nu\mu} = \frac{2}{N} \sum_{k=0}^{n}{}' \lambda_k^{\nu\mu} \cos(k2\pi(i - j)/N) , \quad i, j = 1, 2, \ldots, N .$$

Here $\lambda_k^{\nu\mu}$, (ν, μ) is an element of matrix Λ_k, $\nu, \mu = 1, 2, \ldots, m$; $k = 0, 1, \ldots, n$; the prime at the summation sign means that the term at $k = 0$ is taken with the coefficient $1/2$.

In the case considered

$$\lambda_k^{\nu\mu} = \lambda_0^{\nu\mu} , \quad \nu \neq \mu ; \quad \lambda_k^{\nu\nu} = \lambda_0^{\nu\nu} + (k/R_\nu)^2 , \quad \nu = 1, 2, \ldots, m .$$

As a result, we obtain

$$h_{ij}^{\nu\mu} = \lambda_0^{\nu\mu} \delta_{ij} , \quad \nu \neq \mu , \quad i, j = 1, 2, \ldots, N ; \quad h_{ij}^{\nu\nu} = \lambda_0^{\nu\nu} \delta_{ij} + R_\nu^{-2} h_{ij}^{(1)} , \quad i, j = 1, 2, \ldots, N ,$$

where

$$h_{ij}^{(1)} = \frac{2}{N} \sum_{k=0}^{n}{}' k^2 \cos(k2\pi (i-j)/n), \quad i, j = 1, 2, ..., N,$$

i.e., $h^{(1)}$ is a symmetric circulant with eigenvalues k^2, $k = 0, 1, ..., n$; δ_{ij} is a unit matrix of size $N \times N$. Thus, for a rapid multiplication of h-matrix H (4) by a vector we need a fast algorithm for multiplication of a symmetric circulant $h^{(1)}$ by a vector. Such an algorithm was constructed in [4].

3. Counting the Number of Operations. In [4] the problem of rapid multiplication of a symmetric circulant by a vector is reduced to a problem of rapid calculation of sums of the form

$$A_q = \sum_{j=0}^{N-1} f_j \exp\left(2\pi i \frac{qj}{N}\right), \quad q = 0, 1, ..., 2n. \tag{5}$$

Let $N = 3^r$, $r = 1, 2, 3, ...$. Then, to calculate sums (3.1) we can use a fast Fourier transform algorithm [5]. This algorithm requires $4N \log_3 N - N + 1$ operations. The proof follows from an ordinary fast Fourier transform scheme if we take into account that some of the exponents by which multiplication is performed become equal to unity.

If only the Fourier coefficients at $q = 0, 1, ..., n$ are required (we will call such a transformation an incomplete Fourier transform), then the number of operations is reduced to $4N \log_3 N - 3N + 3$ operations.

To multiply a symmetric circulant by a vector, one incomplete Fourier transform and two complete transforms are required.

We will denote the number of nodes in a grid in a circle by $\Re = mN$. Then an accurate computation of the number of operations for multiplying h-matrix (4) by a vector yields

$$M = \Re (12 \log_3 N + 2(m-1)) + 5m$$

operations. Direct multiplication of a completely filled matrix of size $\Re \times \Re$ requires $2\Re^2 - \Re$ operations.

As an example, we will consider a grid in a circle of 10×27, i.e., consisting of 10 circles with 27 points in each circle. Then, using the algorithm for rapid multiplication of an h-matrix by a vector, the number of operations is reduced by a factror of 9.95 compared to direct multiplication of a matrix by a vector.

Calculations by the first-order explicit scheme require, in addition to (3.2), $3\Re + 1$ more operations in each time step.

4. Stability. In practical problems the value of the diffusion coefficient is very small. We assume that the characteristic time $T = 1$ is one year and the characteristic dimension is $L = 200$ m (the scale of the map). Then, the dimensionless diffusion coefficient D with which calculations were performed is $1.5768 \cdot 10^{-7}$. The stability of calculation by the explicit scheme is ensured if the condition $\tau < (D \operatorname{spr}(ZH))^{-1}$ is satisfied, where τ is the time step and Z is a diagonal matrix with numbers $z_i = |\varphi'(\zeta_i)|^2$, $i = 1, 2, ..., \Re$ on the diagonal (ζ_i, $i = 1, 2, ..., \Re$ are the nodes of the grid in a circle). In practical calculations we performed direct computation of the spectral radius of matri ZH, and the conditions of the time stability of calculation were obtained: for $\tau < 3.34$ for a grid 10×27; $\tau < 0.2036$ for a grid of 20×27, and $\tau < 4.00 \cdot 10^{-2}$ for a grid of 30×27. Thus, the stability conditions are not burdensome and allow one to carry out fast calculations.

Conclusion. The described algorithm for solving diffusion equations has an arbitrary order of approximation in space variables, i.e., its accuracy is the higher, the smoother the solution in space variables. This follows from the algorithm for solving the Bessel equations to construct the cells Λ_k, $k = 0, 1, ..., n$ of h-matrix H. This offers an advantage over difference methods, which have a fixed order of approximation over space variables irrespective of the smoothness of the solution. In practice, this allows (with smooth initial data) calculations on coarse space grids. We note that spr (ZH) grows rapidly with an increase in $\Re$, and this makes it necessary to decrease the time step to ensure stability.

In speed and the amount of information stored, the method is competitive with difference methods.

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