ON APPLICATION OF MONTE CARLO METHOD FOR POISSON PROBLEM SOLVING

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Abstract

The paper presents the application of random grid walk for Dirichlet problem solving for Poisson equation. Boundary value problem is discretized and reduced to the system of linear algebraic equations. The matrix of this system is used for stochastic matrix constructing. Thus, there is a possibility of Markov chains obtaining. The special random value is defined on Markov chain trajectories; this value is used for approximation of the desired solution. The advantages of this method are discussed in the paper.

The algorithm is applied for electric potential calculation in the cell of support lattice of exit window in large-aperture electron accelerator.

DIRICHLET PROBLEM FOR POISSON EQUATION

Consider the Dirichlet problem for electric potential. Poisson equation for unknown potential $u(x,y)$ has the form

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=\tilde{f}(x,y),\quad (x,y)\in G \tag{1}$$

with boundary conditions

$$u\big|_{\Gamma}=\varphi(x,y). \tag{2}$$

Here $G\subset R^2$ is some domain, Γ is the boundary of the domain G, $\tilde{f}(x,y)$ and $\varphi(x,y)$ are given functions.

Let us consider problem (1)-(2) discretization algorithm for the rectangle domain. The modification of this algorithm for the domain of any other form is given in the book [1].

For numerical solution of Dirichlet problem (1)-(2) we introduce sufficiently fine grid S with the step l: $S=\{s_{i,j}=(x_i,y_j):\ x_i=il,\ \ y_j=jl,\ \ i=\overline{0,L_x},\ \ j=\overline{0,L_y}\}$. We distinguish the set of boundary grid points $S_\Gamma=\{s_{i,j}=(x_i,y_j)\in S:\ \ i=0,L_x,\ j=0,L_y\}$. The internal grid points set is $S_G=S\setminus S_\Gamma$.

After that we introduce the following grid functions: $\{u_{i,j}=u(s_{i,j}):\ \ s_{i,j}\in S\}$, $\{\tilde{f}_{i,j}=\tilde{f}(s_{i,j}):\ \ s_{i,j}\in S_G\}$, $\{\varphi_{i,j}=\varphi(s_{i,j}):\ \ s_{i,j}\in S_\Gamma\}$.

Let us replace the equation (1) at internal grid points by the difference equation

$$u_{i,j}=(1/4)(u_{i-1,j}+u_{i+1,j}+u_{i,j-1}+u_{i,j+1}-l^2\tilde{f}_{i,j}). \tag{3}$$

At boundary grid points we assume

$$u_{i,j}=\varphi(x_i,y_j). \tag{4}$$

The solution of algebraic system (3)-(4) converges to the solution of Dirichlet problem (1)-(2) as $l\to 0$ [2,3].

Let us number all the grid points in any order (using one index) and rewrite the equations (3)-(4) in the same order. Now the grid S is described as follows: $S=\{(x_k,y_k),k=\overline{1,L}\}$, where $L=(L_x+1)(L_y+1)$. Let I_G and I_Γ be the sets of numbers of internal and boundary grid points correspondingly.

After that we introduce the grid functions $u=(u_1,...,u_L)$, $\tilde{f}=(\tilde{f}_1,...,\tilde{f}_L)$ and $\varphi=(\varphi_1,...,\varphi_L)$ representing the grid values of potential, right-hand part of equation (1) and boundary function correspondingly.

Now the system (3)-(4) takes the form

$$u=Au+f, \tag{5}$$

where A is $L\times L$ matrix of coefficients; L-vector f is determined as follows:

$$f_i=\begin{cases}(-1/4)l^2\tilde{f}_i, & i\in I_G\\ \varphi_i, & i\in I_\Gamma\end{cases}. \tag{6}$$

As for matrix A, when $i\in I_G$, the line $A_i=(a_{i,1},...,a_{i,L})$ contains four elements equal $1/4$ and other elements zero; if $i\in I_\Gamma$ the line A_i is zero.

"WALK-ON-GRID" METHOD

Stochastic Matrix

To obtain the solution of the system (5) we apply "walk-on-grid" algorithm.

Let us construct stochastic matrix P by the rule:

$$i\in I_G\Rightarrow\begin{Bmatrix}p_{i,j}>0\ \ if\ a_{i,j}>0\\ p_{i,j}=0\ \ if\ a_{i,j}=0\end{Bmatrix},\ j=\overline{1,L};\ \sum_{j=1}^{L}p_{i,j}=1;$$

$$i\in I_\Gamma\Rightarrow p_{i,j}=\delta_{i,j},\ \ j=\overline{1,L},$$

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where $\delta_{i,j}$ is Kronecker delta. Evidently, every line of matrix P presents the probability distribution. Besides, let us introduce initial probability distribution $p=(p_1,\ldots,p_L)$ ($\sum_{i=1}^{L} p_i=1,\quad p_i\geq 0$). Using the set $\{p,P\}$ we can simulate Markov chain; in this case p is initial states probability vector and P is transition matrix.

Markov chain simulation

Consider the problem of calculation of scalar product (h,u), where h is prescribed L-vector.

Markov chain may be considered to describe the evolution of the object called "particle". The particle changes its state in accordance with chain trajectory.

Let us assign the "weight" Q_k to moving particle. Suppose the "weight" to change in the process of particle movement. For "weight" determination let us introduce the values

$$q_i=\begin{cases} h_i/p_i, & p_i>0 \\ 0, & p_i=0 \end{cases},\quad q_{i,j}=\begin{cases} a_{i,j}/p_{i,j}, & p_{i,j}>0 \\ 0, & p_{i,j}=0 \end{cases}, \quad (7)$$

where $i,j=\overline{1,L}$.

The particle is "born" at some initial grid point; we obtain its number i_0 as a result of random variable simulation with probability distribution $p=(p_1,\ldots,p_L)$.

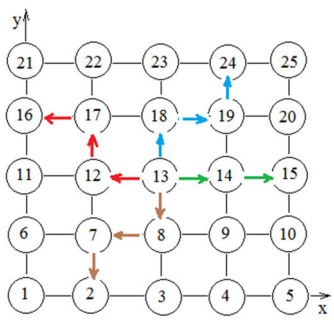

Figure 1: Random walk on grid (L=25)

The initial "weight" of particle is $Q_0=q_{i_0}$. We obtain next grid point number i_1 by random variable simulation with probability distribution $P_{i_0}=(p_{i_0,1},\ldots,p_{i_0,L})$; P_{i_0} is the line of stochastic matrix P. The particle passes to the point numbered i_1 with probability p_{i_0,i_1}. Particle "weight" becomes equal $Q_1=q_{i_0}\cdot q_{i_0,i_1}$, and so on. We calculate the "weights" by recurrent formula $Q_0=q_{i_0}, Q_m=Q_{m-1}\cdot q_{i_{m-1},i_m}$. If new particle state is boundary grid point with number i_μ, the particle stays at this point with probability $p_{i_\mu,i_\mu}=1$ and the chain terminates. Clearly, if one continues simulation, in view of Eq. 7 the result is $i_{\mu+1}=i_\mu$, $q_{i_\mu,i_{\mu+1}}=0$, $Q_{\mu+1}=0$ and so on. So in this case we obtain the chain of the length $\mu: i_0\to i_1\to\cdots\to i_\mu$. The example of Markov chains is depicted in Fig. 1, $L=25$.

Special random variable

Let us introduce random variable ξ_μ defined on the trajectories of the Markov chain of the length μ [1]:

$$\xi_\mu=\sum_{m=0}^{\mu} Q_m f_{i_m} \quad or \quad \xi_\mu=\sum_{m=0}^{\mu}\frac{h_{i_0}a_{i_0,i_1}\cdots a_{i_{m-1},i_m}}{p_{i_0}p_{i_0,i_1}\cdots p_{i_{m-1},i_m}}f_{i_m} \quad (8)$$

Here $f_{i_\mu}=\varphi_{i_\mu}$ in view of Eq. 6.

For internal grid points the matching conditions are satisfied:

$$p_i>0 \ \ if \ \ h_i\neq 0,$$
$$p_{i,j}>0 \ \ if \ \ a_{i,j}\neq 0.$$

Consequently, one can argue [1] that

$$M\xi_\mu \xrightarrow[\mu\to\infty]{} (h,u). \quad (9)$$

Consider N independent trajectories beginning at the point numbered i_0. If $h=\hat{h}=\left(0,\ldots,0,\underset{i_0}{1},0,\ldots,0\right)$, the scalar product provides the calculation of one component of the solution: $u_{i_0}=(h,u)$. In view of the statement (9) this component may be calculated by formula

$$u_{i_0}=(\hat{h},u)\underset{(9)}{\approx}M\xi_\mu\approx\frac{1}{N}(\xi_{\mu_1}+\cdots+\xi_{\mu_N}). \quad (10)$$

Consider the following particular case. Let us take $\hat{h}$ as initial distribution vector: $p=\hat{h}$ and assume $p_{i,j}=\begin{cases} a_{i,j}, & i\in I_G \\ \delta_{i,j}, & i\in I_\Gamma \end{cases}$, $j=\overline{1,L}$. In this case the "weights" along the trajectory are as follows: $Q_0=Q_1=\cdots=Q_\mu=1$ until the chain reaches the boundary; after that $Q_{\mu+1}=Q_{\mu+2}=\cdots=0$. Consequently, calculation of the values of random variable ξ_μ (See Eq. 8) becomes especially simple:

$$\xi_\mu=\left(f_{i_0}+\cdots+f_{i_{\mu-1}}+\varphi_{i_\mu}\right). \quad (11)$$

The formulae (10)-(11) provide the computational scheme for determination of one component of unknown vector u.

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NUMERICAL RESULTS

Electromagnetic fields determination in different devices and beam evolution modelling and investigation as well as optimization of beam dynamics and device parameters often includes boundary value problems solving for Poisson equation [4-26]. Monte Carlo method provides the simple and effective algorithms for computation and parallelization [1-2, 27-32].

This paper deals with application of "walk-on-grid" method to electric potential distribution determination in the cell of support lattice of exit window in large-aperture electron accelerator [27].

The application specifics of electron sources of large cross-section beams in gas laser or radiation-chemical technologies demands beam extraction from the vacuum into the gas at atmospheric pressure (or higher). Consequently, the obligatory component of such electron source construction is a window with thin metal foil and support lattice. The foil is impermeable to gas but quite freely passes the accelerated electrons [33].

The electron accelerator provides formation, acceleration and extraction of the electron beam in the workspace of gas discharge chamber. Particle beam energy is $150keV$, beam cross-section square is $700mm^2$, current density in stationary mode reaches $0.120\,mkA/mm^2$. Support lattice bar width is 1 mm, height is 12 mm, the distance between bars is 5 mm. Charge density value in the cell is calculated using the accelerator characteristics and equal $\rho_0 = 5.19 \cdot 10^{-9}\, C/m^3$.

Let us consider the potential calculation domain to be the rectangle $G = [0,a] \times [0,b]$. We suppose the potential distribution in any cross-section $z = const$ to be identical.

Electron beam moves through the side $y = b$, so the potential distribution is prescribed on this side. The potential on remaining sides of rectangle are supposed to be zero.

Boundary conditions are as follows:

$$u(0,y) = u(a,y) = 0, \quad 0 \le y \le b,$$

$$u(x,0) = 0,\ u(x,b) = \sin\frac{\pi}{a}x, \quad 0 \le x \le a.$$

The calculation was performed for various values of grid step l and trial number N .The results are presented for $l = 0.0024$, $N = 5000$. The potential was calculated by the formula (10). The potential distribution in the cell of support lattice of exit window in large-aperture electron accelerator is presented in Fig. 2.

PARALLEL PROCESSING

Monte Carlo methods allow the perfect parallelization of the computational process.

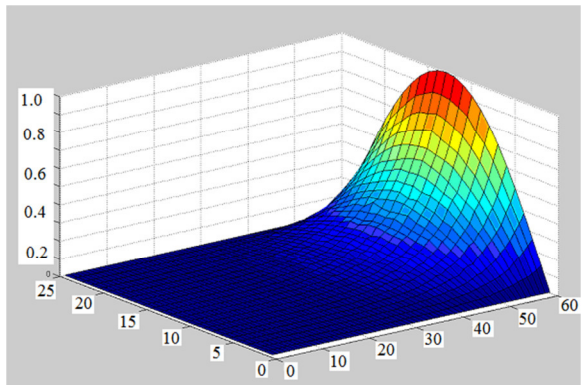

Figure 2: Potential distribution in the cell.

Parallel computing was performed for the problem under study. The numerical experiment shows that parallelization gives extremely low benefit for the grids with large step. Consequently, it is more efficient to use a fine grid.

The analysis of parallel processing efficiency is illustrated in Fig. 3. The graphs are presented for various number of threads and various number N of Markov chains. The best computing time result is achieved for 4 threads. Threads number increasing does not lead to appreciable time advantage.

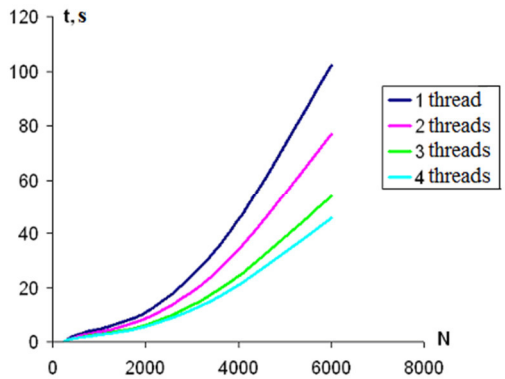

Figure 3: Parallel processing.

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