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PARALLEL ALGORITHM FOR THE LOCAL VARIATIONS METHOD*

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The behavior of the liquid meniscus near heterogeneous solid wall of a rectangular tank is of great interest now [5]. No numerical solution for the behavior of the liquid meniscus near randomly heterogeneous wall is obtained so far. We construct a parallel algorithm for the local variations method and we use it to obtain the equilibrium state of the liquid free surface for a liquid in a container with one randomly heterogeneous vertical wall.

The method of local variations (MLV) was developed by Chernousko [1]. With this method in [2] various variation problems were numerically investigated. We consider first the algorithm for the basic problem examined in [2]. It is necessary to find a function $u(x,y)$ in rectangular domain $D=\{0\le x\le x_0, 0\le y\le y_0\}$, satisfying some boundary conditions $u\in U$ and minimizing

$$J=\iint\limits_D f(x,y,u,\partial u/\partial x,\partial u/\partial y,\dots)\,dxdy. \tag{1}$$

In our case u describes the surface of a liquid and the set U is $U=\{u\ge 0\}$.

We use uniform mesh: $x_i=i\Delta$, $y_j=j\Delta$ supposing $x_0=N\Delta$ and $y_0=M\Delta$ We denote $u_{i,j}=u(x_i,y_j)$, $i=0,\dots,N; j=1,\dots,M$:

$$J\approx \sum_{i=1,N-1;j=1,M-1} F_{i,j}, \tag{2}$$

where

$$F_{i,j}=F(u_{ij},u_{i-1j},u_{i+1j},u_{ij-1},u_{ij+1},u_{i-1j-1},u_{i-1j+1},u_{i+1j-1},u_{i+1j+1},\Delta) \tag{3}$$

are local approximations for the functional J. We obtain them as shown in [7].

We start by specifying a certain initial approximation of the function $u^{(0)}_{i,j}, i=0,\dots,M$; $j=1,\dots,N$ and a certain value h for the variation of the values of u_{ij}. We enumerate all the nodes in a certain order Ψ. For example

$$\Psi=\{\Psi_0,\Psi_1,\dots,\Psi_N\};\quad \Psi_l=\{(x_l,y_0),(x_l,y_1),\dots,(x_l,y_M)\}. \tag{4}$$

We call Ψ_l a column. Then, we consider first node of Ψ (in our case (x_0,y_0)) and we put $u^{(1)}_{0,0}=u^{(0)}_{0,0}+h$ or $u^{(1)}_{0,0}=u^{(0)}_{0,0}-h$, if in one of these cases the value of the

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right-hand side of (2) decreases and $u_{0,0}^{(1)} \in U$. If this is not the case, then we leave $u_{0,0}^{(1)} = u_{0,0}^{(0)}$. Further we carry out a similar variation for the next node of Ψ (in our case $u_{0,1}^{(1)}$) and so on, until we arrive at the last node of Ψ that in our case is $u_{N,M}^{(1)}$. Thus the first approximation of the function $u \quad u_{i,j}^{(1)}, i = 0, \ldots, M;\ j = 1, \ldots, N$ has been constructed. Then, the procedure is repeated until all $u_{i,j}$ stop changing. Then we can decrease h, taking the obtained solution as the initial approximation, etc., until we attain a reasonable accuracy.

MLV is a convergent iterative algorithm as Jacobi, Gauss-Seidel, overrelaxation and Richardson algorithms. For MLV parallelization can be easily obtained [3,4]:

- The domain can be easily decomposed
- Variation of the interior points in each subdomain can be made to depend only on data residing on the same CPU
- Only the boundary points must depend on data from neighboring CPU so that during each iteration only data from the boundary points is needed to be exchanged.

We present realization of the parallel algorithm with column-wise decomposition. We use the enumeration (4) for the nodes. Than, the domain consists of $N+1$ columns $\Psi = \{\Psi_0, \Psi_1, \ldots, \Psi_N\}$. We denote by P the number of processors in use. For simplicity let us suppose that $Q = \dfrac{N+1}{P}$ is an integer. We divide the domain Ψ into P subdomains. The subdomain in each processor $L \in (0, 1, \ldots, P-1)$ consists of Q columns $= LQ, \ldots, LQ + Q - 1$. To compute $F_{LQ,j}$ and $F_{LQ+Q-1,j}$; $j = 0, \ldots, M$ on the L-th processor we need the value of u in the columns Ψ_{LQ-1} and Ψ_{LQ+Q} respectively. These columns are parts of the subdomains on the processors L-1 and L+1 respectively. Thus communications between consecutive processors are needed. Now we show how to avoid time loss because of data sending and receiving using non-blocking communications. We do this by the following steps :

1) On each processor L we first apply the MLV for the first column Ψ_{LQ}. For every column l we apply the MLV in the following order $(x_l, y_0), (x_l, y_1), \ldots, (x_l, y_M)$.

2) Then, we start sending the new values of u on the first column Ψ_{LQ} on the L-th processor to the previous processor L-1. As $(L-1)Q + Q = LQ \quad \Psi_{LQ}$ is the column needed on the previous processor to calculate the value of F on the last column.

3) During the process of exchanging information we apply the MLV for the columns $\Psi_{LQ+1}, \ldots, \Psi_{LQ+Q-2}$ consecutively. All of the processors calculate in the time of exchanging information as they have all the necessary data.

4) To apply the MLV for the last column on each processor we need the adequate values of u on the column Ψ_{LQ+Q} so we have to check if the sending-receiving process is over. The sending process will be over if the time for the calculations 3) is larger than the time for communications 2). If Q is large enough, this condition can be satisfied. As calculation and communications speeds are different for different multiprocessor machines the minimum value of Q satisfying the condition depends on the machine architecture.

5) After new values of u for the last column Ψ_{LQ+Q} on each processor L are obtained, we need to send them to the next processor $L+1$. This is because $(L+1)Q - 1 = LQ + Q - 1$ and thus u in the last column Ψ_{LQ+Q} is the data needed on processor L+1 to calculate F on its first column.

6) Then we repeat the same steps in reverse order applying MLV to columns Ψ_{LQ+Q-2}, $\ldots$, Ψ_{LQ}. We vary the columns in reverse order to execute calculations while data is being send.

Now we use this method to investigate the two-dimensional problem of the equilibrium of a capillary liquid under a gravity force $\mathbf{g} = -\operatorname{grad}(U_{gr})$. We work in Cartesian coordinates (x, y, z). We analyze water with free surface $\Sigma = \{x, y, u(x, y)\}$ in a vessel with vertical walls $\Sigma_1 = \{x = 0; 0 \leq y \leq y_0; z \geq z_0\}$, $\Sigma_2 = \{x = x_0; 0 \leq y \leq y_0; z \geq z_0\}$, $\Sigma_3 = \{y = 0; 0 \leq x \leq x_0; z \geq z_0\}$, $\Sigma_4 = \{y = y_0; 0 \leq x \leq x_0; z \geq z_0\}$ and rectangular bottom $D = \{0 \leq x \leq x_0, 0 \leq y \leq y_0; z = z_0\}$. Water surface tension and density are $\gamma = 72.5$ mJ/m^2 and $\rho = 1000$ kg/m^3 respectively. We assume $x_0 \gg l_c$, where $l_c = (\gamma/\rho g)^{1/2}$ is the capillary length. We suppose that the walls $\Sigma_2, \Sigma_3, \Sigma_4$ are homogeneous and liquid forms equilibrium contact angle of 90° with them. For the wall Σ_1 we suppose that it is chemically heterogeneous. On the bigger part of it the liquid forms equilibrium contact angle $\theta_{eq}(y, z) = 40°$. There are as well some randomly placed square "mesa" defects on this wall. The defects are with sides 10 μm and on them the liquid forms equilibrium contact angle $\theta_{eq}(y, z) = 30°$. The defects area is with fraction $f = 0.2$ (part of this wall is shown in Fig 2 where defects are depicted with dark squares). Recently this system was studied by David and Neumann [5] who used the corrugation energy approximation of the plate defects. In this paper we obtain full solution for the liquid meniscus equilibrium shape using the parallel algorithm for the MLV described in this article. We work in dimensionless units $x = x/l_c$, $y = y/l_c$, $z = z/l_c$, $x_0 = x_0/l_c$, $y_0 = y_0/l_c$. In a state of equilibrium the functional [6] (for simplicity we use the same symbols as for the dimensional variables)

$$(5)\quad J(u) = \iint\limits_D (z^2 + \sqrt{1 + u_x^2(x, y) + u_y^2(x, y)} + \lambda z)dxdy + \int\limits_0^{y_0} \int\limits_0^{u(0,y)} \cos\theta_{eq}(y, z)dzdy$$

reaches its minimum under boundary conditions $u_y(0, y) = u_y(x_0, y) = u_x(x, y_0) = 0$. Here λ is a Lagrange multiplier that determines the liquid volume. To investigate the same system as in [5] we choose the domain to be $D = \{0 \leq x \leq 7.3728,\ 0 \leq y \leq 0.37\}$ and $\lambda = 0$ (liquid level $u(\infty, y) = 0$ far away from the plate Σ_1). We use a modification of the MLV proposed in [7] in which the approximation (3) of the functional is performed. For the geometry considered in the present article MLV is tested in [8]. We use for the parameters of MLV the values from [8] that give reasonable accuracy. To find the minimum of J we have developed a C++ parallel computer program realizing the described parallel algorithm. To realize the communications between processors we used a library implementing MPI. This allowed us to make calculations on distributed memory systems. Calculations were performed on IBM Blue Gene/P situated in Sofia, Bulgaria. The domain D was divided on squares using $\Delta = 500$ nm which gives N=1999 and $M = 40959$. We have used $P = 2048$ cores, so $Q = 20$. This value of Q showed to be large enough that no extra time for communication is needed. We show in Fig. 1 a part of the obtained equilibrium liquid free surface close to the plate Σ_1.

The equilibrium state of the surface u may depend on the initial approximation $u^{(0)}$. For $u^{(0)}$ we have used the equilibrium liquid surface for homogenous wall Σ_1 on which the liquid forms equilibrium contact angle $\theta_{eq}(y, z) = 30°$. For this simpler case an analytical solution exists [9]. The behavior of the meniscus near a heterogeneous solid

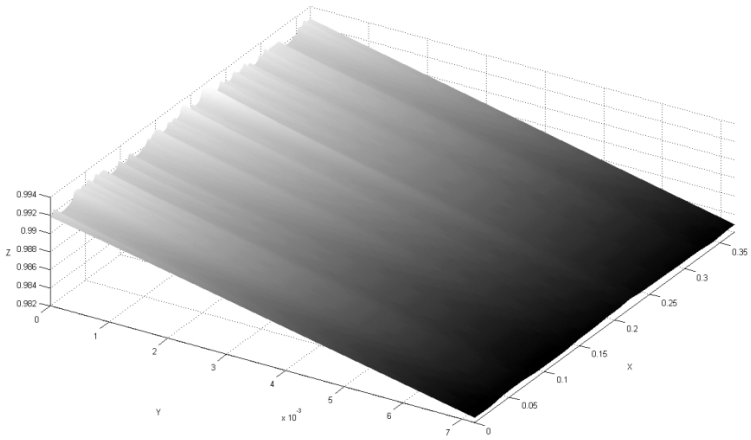

Fig. 1. A part of the obtained equilibrium liquid interface close to the plate Σ_1

plate is of great interest now [5]. We show the obtained contact line $u(x, 0)$ in Fig. 2.

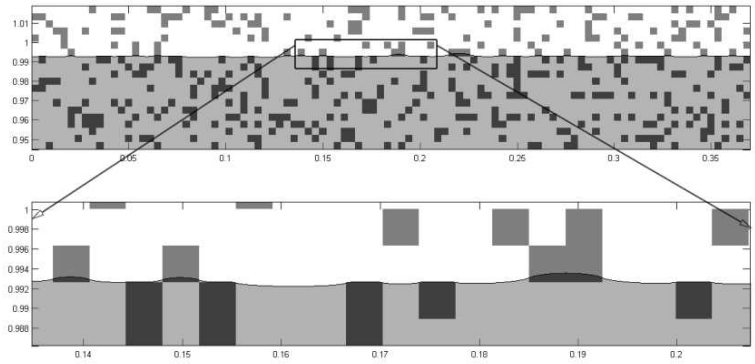

Fig 2. The contact line of the obtained solution on the randomly heterogeneous surface Σ_1. The total width of the wall Σ_1 in dimensional units is 1 mm. Gravity acts downward. Liquid is under the contact line

With the proposed algorithm many other equilibrium states may be obtained and other problems can be studied. Different area fraction of defects may be considered as well as different initial approximations. As defects are randomly placed, different distribution of defects may be also considered. That will allow us to make accurate investigation of the static contact angle hysteresis. This will be studied in a future work.

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ПАРАЛЕЛЕН АЛГОРИТЪМ ЗА МЕТОДА НА ЛОКАЛНИТЕ ВАРИАЦИИ

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Актуално е изследването на поведението на течен менискус в околността на хетерогенна стена. До сега няма получено числено решение за формата на менискуса около стена, която е с хаотична хетерогенност. В настоящата статия е разработен алгоритъм за метода на локалните вариации, който може да се използва на многопроцесорни системи. С този метод е получен за първи път профила на равновесен течен менискус около вертикална стена с хаотична хетерогенност.