CHAPTER 20

Algorithms of Box Domain Decomposition for Solution of 3-D Elliptic Problems

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Abstract. Three-dimensional elliptic finite element and finite difference problems are solved using the preconditioned conjugate gradient method (PCG). Preconditioners are constructed on the basis of box domain decomposition (decomposition with cross-points) using Poincaré-Steklov operators. The space of traces on subdomain boundaries is split into a sum of subspaces on which the preconditioners are easily invertible. The results of numerical experiments for linear and nonlinear problems are presented.

1. Introduction. The domian decomposition method for solving 2-D and 3-D elliptic problems has been considerably developed in recent years. Decomposition algorithms for 'strips'-type partitions were analysed in [1-4]. A family of preconditioners was constructed in [5-7] for 2-D finite element problems for decomposition by crossing boundaries. The first results for the three-dimensional case were obtained in [8].

Note that domain decomposition multigrid methods were analysed in [9,10] and the preconditioning technique with local grid refinement was developed in [11-12].

In Section 2 we have constructed a family of preconditioners for box decomposition in the three-dimensional case. The construction is based on splitting the original space of finite element basis functions into a direct sum of three subspaces of the sufficiently general form [13,14]. In Section 3 we have

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constructed preconditioners for 3-D finite difference problems. In Section 4 we use the box domain decomposition technique for solving three-dimensional quasi-linear equations in incomplete nonlinear formulation [13] for which the approximation of nonlinear effects is carried out on the coarse grid, which defines the decomposition of the domain $\Omega = \bigcup_i \Omega_i$.

2. Preconditioners for finite element elliptic systems. Let us consider the partitioning $\Omega = \bigcup_i \Omega_i$, $i = (i_1, i_2, i_3)$, of the parallelepiped $\Omega = \{0 \leqslant x_j \leqslant a_j,\ j = 1,2,3\}$ by using $n_k - 1$, $k = 1,2,3$, planes parallel to the planes $x_2 0 x_3$, $x_1 0 x_3$ and $x_1 0 x_2$, respectively, where $1 \leqslant i_k \leqslant n_k$, $k = 1,2,3$. Construct the box decomposition of the domain $\Omega = \Omega_B \cup \Omega_W$, where subdomains Ω_B and Ω_W are defined as

$$\Omega_B = \bigcup_{i \in I_B} \Omega_i, \qquad \Omega_W = \bigcup_{i \in I_W} \Omega_i \tag{2.1}$$

where $I_B = \{i\colon i_1 + i_2 + i_3 \text{ is even}\}$ and $I_W = \{i\colon i_1 + i_2 + i_3 \text{ is odd}\}$. Assume that the partitioning satisfies the condition

(A.1) There exists a constant $C_0 > 0$ such that for all i it satisfies the inequality $d/r_i \leqslant C_0$, where $d = \max_i(\operatorname{diam} \Omega_i)$, and r_i are radii of balls inscribed in Ω_i.

Introduce the notation $\Gamma_0 = \partial\Omega$, $\Gamma_i = \partial\Omega_i = \bigcup_{k=1}^{6} \Gamma_i^k$, $\partial\Gamma_i^k = \bigcup_{m=1}^{4} \Gamma_i^{km}$, $\Gamma = (\bigcup_{i \in I_B} \Gamma_i) \backslash \Gamma_0$, where Γ_i^k are sides, Γ_i^{km} are edges of parallelepipeds Ω_i and Γ is a set of internal boundaries. Define a finite-dimensional space Y_Γ of functions continuous on $\Gamma \cup \Gamma_0$ and equal to zero on Γ_0 as a direct sum of subspaces $Y_\Gamma = X_1 \oplus X_2 \oplus X_3$.

Definition 2.1. Denote by $\bar{X}_1 \subset \overset{\circ}{H}{}^1(\Omega)$ a family of first-order serendipity finite elements corresponding to the partitioning of the domain $\Omega = \bigcup_i \Omega_i$. In this case, we have $\dim \bar{X}_1 = \prod_{k=1}^{3} (n_k - 1)$. For X_1 we choose a space of traces of functions from $\bar{X}_1$ on Γ.

The space X_1 is used for the global information transfer among substructures Ω_i.

Let us consider the simplest case of choice of subspaces X_2 and X_3, which however reflects the main details of the approach. The general case was considered in [13,14]. Assume that we have prescribed compatible regular triangulations [17] $\Gamma_{i,h}^{km}$, $\Gamma_{i,h}^{k}$ and $\Omega_{i,h}$ of all edges, sides and subdomains, respectively, defined by the step size $h > 0$.

Consider the spaces $V(\Gamma_{i,h}^{km})$ of piecewise-linear elements and the spaces $V(\Gamma_{i,h}^{k})$ and $V(\Omega_{i,h})$ of linear elements, which correspond to these triangulations. The elements of these spaces have zero traces on Γ_0, and the inclusions $V(\Gamma_{i,h}^{km}) \subset \overset{\circ}{H}{}^{1/2}(\Gamma_i^{km})$ and $V(\Omega_{i,h})\big|_{\Gamma_i^k} \subset \overset{\circ}{H}{}^1(\Gamma_i^k)$ are valid. Define the space X_2.

Definition 2.2. Associate an arbitrary function $u \in V(\Gamma_{i,h}^{km})$ with four functions $\bar{u}_j$, $j = 1,2,3,4$, defined on the four sides having the common edge Γ_i^{km}. Assume that $u_j(x) = u$, $x \in \Gamma_i^{km}$, $j = 1,2,3,4$, and also $u_j = 0$ on the remaining three edges of the sides. Consider then, for example, a group of edges parallel to the axis $0x_3$. Define $\bar{u}_j$ at internal points of the sides parallel to the plane $x_2 0 x_3$ as a linear continuation of the function u on Γ_i^k, and for a pair of orthogonal sides define $\bar{u}_j$ as an h-harmonic continuation of u onto the domain Γ_i^k. We pursue the same arguments for the other two groups of edges parallel to the axes $0x_1$ or $0x_2$. Set $u_j = 0$ on the remaining part of Γ. The space of such functions will be denoted by $\bar{X}_i^{km}$. Then set

$$X_2 = \oplus \bar{X}_i^{km} \tag{2.2}$$

where the sum is extended to all internal sides $\Gamma_i^{km} \in \Gamma$.

Definition 2.3. Denote by $G(\Gamma_i^k)$ a subspace of functions from $V(\Gamma_{i,h}^k)$ which have zero traces on $\partial\Gamma_i^k$. Then define

$$X_3 = \oplus\, G(\Gamma_i^k), \qquad \Gamma_i^k \cap \Gamma_0 = \varnothing \tag{2.3}$$

where the sum is extended to all edges Γ_i^k.

Define the set of functions $Y_\Gamma = X_1 \oplus X_2 \oplus X_3$ given on Γ. Additionally assume that the elements from X_2 and X_3 are h-harmonically continued inside subdomains $\Omega_{i,h}$. Moreover, denote by $\bar{X}_2$ a set of finite elements on the grid $\Omega_{i,h}$ which have traces on Γ belonging to X_2, and also set $\bar{X}_3 = V(\Omega_{i,h})$. Denote by $Y_\Omega = \bar{X}_1 \oplus \bar{X}_2 \oplus \bar{X}_3$ the corresponding space of finite elements defined on the entire grid domain $\bigcup_i \Omega_{i,h}$.

Denote by $V_i^{1/2} \subset H^{1/2}(\Gamma_i)$ a space of traces of the functions $u \in Y_\Gamma$ on Γ_i. Consider two techniques for ordering elements from Y_Γ. Each function $u \in Y_\Gamma$ can be presented as a direct sum $u_B = \oplus\, u_i$ of components $u_i \in V_i^{1/2}$, $i \in I_B$, and similarly for subscripts $i \in I_W$. Denote by Y_B and Y_W the corresponding representations for Y_Γ and define the permutation operator T such that $T^*T = E$, $TY_B = Y_W$.

On $V_i^{1/2}$ define the Poincaré–Steklov operator $S_{\Delta,i}^{-1}$ mapping the function $u \in V_1^{1/2}$ onto the trace of the normal derivative of the function h-harmonic on $\Omega_{i,h}$ and having the value u on Γ_i. The element $v = S_{\Delta,i}^{-1}u$ belongs to $H^{-1/2}(\Gamma_i)$ and satisfies the condition $(v,1)_{\Gamma_i} = 0$ for all internal subdomains. Here and henceforth, $(\cdot\,,\cdot)$ is a scalar product in L_2. Define on Y_B and Y_W the operators $S_{B,\Delta}^{-1} = \oplus_{i \in I_B} S_{\Delta,i}^{-1}$ and $S_{W,\Delta}^{-1} = \oplus_{i \in I_W} S_{\Delta,i}^{-1}$, respectively. Denote $Y_B' = S_{B,\Delta}^{-1}(Y_B)$ and $Y_W' = S_{W,\Delta}^{-1}(Y_W)$, and define also diagonal operators

$$M_B = \underset{i \in I_B}{\oplus} \mu_i E_i, \qquad M_W = \underset{i \in I_W}{\oplus} \mu_i E_i \tag{2.4}$$

where E_i are identity operators on $V_i^{1/2}$ and $\mu_i > 0$ are given constants.

Construct the boundary operator $A_\Gamma = A_1 + A_2$, where

$$A_1 = M_B S_{B,\Delta}^{-1}, \quad A_2 = T^* M_W S_{W,\Delta}^{-1} T. \tag{2.5}$$

Let the function $\psi \in Y_B'$ be given which has the representation $\psi = \psi_1 + T\psi_2$, where $\psi_1 \in Y_B'$ and $\psi_2 \in Y_W'$. Let us consider two problems.

Problem (A): Find a function $u_\Omega \in Y_\Omega$ such that for all $\eta \in Y_\Omega$ we have

$$\sum_{i \in I_B \cup I_W} \mu_i \int_{\Omega_i} (\nabla u_\Omega \cdot \nabla \eta \, dx = \int_\Gamma \psi(S)\eta(S)\, dS. \tag{2.6}$$

The domain decomposition method equation in Problem (A) for decomposing $\Omega = \Omega_B \cup \Omega_W$ takes the form

Problem (B). Find a function $u_\Gamma \in Y_B$ such that

$$(A_\Gamma u_\Gamma, \eta) = (\psi, \eta), \quad \eta \in Y_B. \tag{2.7}$$

Note that the trace on Γ of the solution u_Ω to problem (2.6) satisfies (2.7) and the function which is an h-harmonic continuation of u_Γ inside all subdomains $\Omega_{i,h}$ satisfies (2.6). The operator A_Γ is symmetric, positive definite and defines the equivalent norm in Y_B.

On the subspace X_3 present the operator $S_{\Delta,i}^{-1}$ in the block form $S_{\Delta,i}^{-1}\{S_i^{km}\}$, $k,m = 1,\ldots,6$, according to the representation for $u \in V_i^{1/2}$ in the form $u = (u_1,\ldots,u_6)^{\mathrm{T}}$, $u_k \in G(\Gamma_i^k)$, $k = 1,\ldots,6$. On the subspace X_3 define the operator

$$\operatorname{diag} A_3 = M_B \bigoplus_{i \in I_B} \left[\bigoplus_{k=1}^{6} S_i^{kk} \right] + T^* M_W \bigoplus_{i \in I_W} \left[\bigoplus_{k=1}^{6} S_i^{kk} \right] T \tag{2.8}$$

where $\Gamma_i^k \cap \Gamma_0 = \varnothing$. Each function $u \in Y_B$ can be presented in the form $u = u_1 + u_2 + u_3$, $u_k \in X_k$, $k = 1,2,3$. Consider a family of preconditioners B_k, $u \in Y_B$, $k = 1,\ldots,5$, defined by the equalities [13,14]

$$(B_1 u, v) = (A_\Gamma u_1, v_1) + (A_\Gamma u_2, v_2) + (\operatorname{diag} A_3 u_3, v_3)$$

$$(B_2 u, v) = (A_\Gamma (u_1 + u_2), v_1 + v_2) + (\operatorname{diag} A_3 u_3, v_3)$$

$$(B_3 u, v) = (A_\Gamma u_1, v_1) + (\operatorname{diag} A_3 u_3, v_3)$$

for all $v \in Y_B$. The operator B_4 is defined by the equality

$$(B_4 u, v) = (A_\Gamma u_1, v_1) + (A_\Gamma u_2, v_2), \quad u,v \in X_1 \oplus X_2$$

and the operator B_5 is defined by the equality

$$(B_5 u, v) = (\operatorname{diag} A_2 u, v), \quad v,u \in X_2.$$

Here, $\mathrm{diag}A_2$ is the block-diagonal part of the operator A_Γ on X_2 corresponding to the splitting of X_2 of form (2.2). Note that the block dimension of A_Γ on X_2 is 13. It is obvious that the problem of inversion of the operators B_k, $k = 1,...,5$, on the corresponding subspace $D(B_k)$ is much easier than that for the operator A_Γ [13] and can be solved by special fast methods.

Denote by $æ_k = æ(B_k^{-1}A_\Gamma)$ the condition number of the operator $B_k^{-1}A_\Gamma$. Set $N = d/n$.

Lemma 2.1. The following estimates are valid:

$$æ_1 \leqslant C(1 + N^2\log^3 N), \qquad æ_4 \leqslant C(1 + N\log N)$$
$$æ_m \leqslant C(1 + N\log^2 N), \qquad m = 2,3,5 \tag{2.9}$$

where the constant C is dependent only on the form of subdomains Ω_i and independent of h, d and μ_i.

Estimates (2.9) imply [14]

Theorem 2.1. The solution of equation (2.7) by the PCG method with accuracy $\varepsilon = N^{-\nu}$, $\nu > 0$, by using preconditioner B_2 at the first level where the solution of auxiliarly problems on the subspaces $X_1 \oplus X_2$ and X_2 involves the use of preconditioners B_4 and B_5, respectively, requires $\mathcal{O}(n^{1/2}N_0^{5/2}\log^4 N)$ arithmetic operations with $\mathcal{O}(nN_0^2)$ numbers, where $N_0 = nN$, $n = \max_k n_k$, simultaneously stored.

3. Preconditioner for finite difference systems. Let us consider a finite difference problem. For the sake of simplicity, assume that Ω is a cube partitioned similarly to (2.1) into n^3 subdomains $\Omega_i = \{(i_k - 1)a \leqslant x_k \leqslant i_k a,\ i_k = 1,...,n,\ k = 1,2,3\}$, where a is the length of the edge of the subdomain Ω_i. Cover each subdomain Ω_i with the uniform grid $\bar{\omega}_i$ with the shift $h/2$ with respect to the boundaries of the subdomains, $\bar{\omega}_i = \{(i_k - 1)a + (s_k - 1/2)h,\ s_k = 0,...,N+1,\ k = 1,2,3\}$, $N = a/h$. By the trace γw of the grid function w on any of the sides Γ_i^j of the subdomain Ω_i we mean the average value of the two grid layers $w_{\Gamma+h/2}$ and $w_{\Gamma-h/2}$ between which Γ_i^j is located: $\gamma w = (w_{\Gamma+h/2} + w_{\Gamma-h/2})/2$, and by its external normal derivative we mean the value $\Delta w/\Delta n = (w_{\Gamma+h/2} - w_{\Gamma-h/2})/h$. Then by Γ_j^i we mean a grid domain on the side of Ω_i: $\{(i_k - 1)a + (s_k - 1/2),\ s_k = 1,...,N,\ k = 1,2\}$. Consider the problem of defining the grid function w:

$$\mu_i \Delta_h w = 0 \qquad \text{on } \omega_i$$
$$[\gamma w] = 0, \quad \left[\mu \frac{\Delta w}{\Delta n}\right] = \psi \qquad \text{on } \Gamma \tag{3.1}$$
$$\gamma w = 0 \qquad \text{on } \Gamma_0$$

where Γ is the internal adjacent boundary of grid subdomains $\bar{\omega}_i$:

$$\Gamma = \bigcup_{i \in I_B} \Gamma_i, \qquad \Gamma_i = \bigcup_{j=1}^{q} \Gamma_i^j. \tag{3.2}$$

In (3.2) $q = 6$ if the sides of the subdomian Ω_i do not lie at the boundary Γ_0 of the original domain Ω; otherwise $q = 5, 4$ or 3.

Let us consider a system of equations with respect to the trace $\varphi = \gamma W \in X(\Gamma)$ of the grid function w, which is equivalent to system (3.1) [16], $X(\Gamma)$ is a space of traces on Γ of h-harmonic functions on ω_i:

$$A_\Gamma \varphi \equiv \bigoplus_{i \in I_B} \mu_i S_i^{-1} \varphi + T^* \left[\bigoplus_{i \in I_W} \mu_i S_i^{-1} \right] T\varphi = \psi \tag{3.3}$$

where matrices $S_i^{-1} \{P_{kl}^i, k,l = 1,\ldots,q\}$ are finite difference counterparts [4,16] of the operators inverse to the Poincaré-Steklov operators. The operator A_Γ in (3.3) is symmetric and positive definite in $X(\Gamma)$ [16].

To construct the preconditioner B for the matrix A_Γ partition $X(\Gamma)$ into a sum of two spaces $X_0(\Gamma)$ and $X_L(\Gamma)$: for all $\varphi \in X(\Gamma)$ there exists $\varphi = \varphi_0 + \varphi_L$, $\varphi_0 \in X_0(\Gamma)$, $\varphi_L \in X_L(\Gamma)$. For the preconditioner we choose the operator B such that for all $\varphi, u \in X(\Gamma)$ we have

$$(B\varphi, u) = (B_0 \varphi_0, u_0) + (A_\Gamma \varphi_L, u_L)$$

where B_0 is the block-diagonal matrix

$$\begin{gathered} B_0 = \bigoplus_{i \in I_B} \mu_i \operatorname{diag} S_i^{-1} + T^* \left[\bigoplus_{i \in I_W} \mu_i \operatorname{diag} S_i^{-1} \right] T \\ \operatorname{diag} S_i^{-1} = \bigoplus_{k=1}^{q} P_{kk}^i . \end{gathered} \tag{3.4}$$

For $X_0(\Gamma)$ and $X_L(\Gamma)$ choose grid functions such that

$$\begin{gathered} X_L(\Gamma) = \left\{ \varphi_L = \bigoplus_{i \in I_B} \left[\bigoplus_{j=1}^{q} u_i^j \right], \ u_i^j = \text{const on } \Gamma_i^j \right\} \\ X_0(\Gamma) = \left\{ \varphi_0 = \bigoplus_{i \in I_B} \left[\bigoplus_{j=1}^{q} u_i^j \right], \ (u_i^j, 1) = 0 \text{ on } \Gamma_i^j \right\}. \end{gathered} \tag{3.5}$$

The preconditioner with the choice of spaces (3.5) is called PC3. The estimate of the condition number $\ae$ of the matrix $B^{-1} A_\Gamma$ satisfies the following statement.

Lemma 3.1 [16]. The PC3 preconditioner satisfies the inequality

$$æ \leqslant CN(1 + \ln N)^2$$

where C is independent of μ_l, n and N.

The computation of the vector $\varphi = B^{-1}\psi$ involves two stages:

(1) Solution of the problem

$$(A_\Gamma \varphi_L, v_L) = (\psi, v_L), \quad v_L \in X_L(\Gamma) \tag{3.6}$$

which is equivalent to the algebraic system $A_L c = \psi_L$ of dimension $3(n-1)n^2$ whose solution by the PCG method calls for

$$Q_L = \mathcal{O}(n^4(\mu_{\max}/\mu_{\min})^{1/2}) \tag{3.7}$$

operations.

(2) Solution of the problem

$$B_0\varphi_0 = f \equiv \psi - A_\Gamma \varphi_L. \tag{3.8}$$

The computation of the vector φ_0 consists of $3(n-1)n^2$ independent problems of definition of the function $u \equiv (\varphi_0)_i^j$ at the common boundary Γ_i^j of each two subdomains

$$\begin{gathered} \mu_{i_1} \operatorname{diag} S_{i_1}^{-1} u + \mu_i \operatorname{diag} S_i^{-1} u = f_i^j \\ i_1 \in I_B, \quad i \in I_W. \end{gathered} \tag{3.9}$$

The solution of problems (3.9) is carried out by the FFT method and the solution of (3.8) is thus carried out in $Q_0 = 3(n-1)n^2(CN^2 \log N + \mathcal{O}(N^2))$ operations.

Let the method from [18] be applied to solving partial problems in the subdomains. Then the following theorem is valid.

Theorem 3.1. The solution of problem (3.3) by the PCG method requires $\mathcal{O}(n^{1/2}N_0^{5/2}\log^3 N \cdot \log \varepsilon^{-1})$ arithmetic operations with $\mathcal{O}(nN_0^2)$ numbers, $N_0 = nM$ is the global number of variables in one direction, simultaneously stored.

It is worth noting that an increase in the number of subdomains n with a fixed N_0 can considerably complicate problem (3.6) according to estimate (3.7). In this case, to solve (3.6), it is necessary to use special methods [19].

Table 1 shows the results of numerical experiments illustrating Lemma 3.1. Problem (3.1) was considered in the cube partitioned into 27 subdomains Ω_{ijk}, $i,j,k = 1,2,3$; ρ_0 is the observed rate of convergence of the PCG method, n_ε is the number of iterations needed for achieving solution accuracy 10^{-4}. The column denoted by Δ shows the results for convergence for the Laplace equation, $\mu_i = 1$ for all i; the column μ shows the results of coefficients μ_i

strongly varying in passing over the subdomain boundaries. To make comparison, the column DD2 shows the similar results for the case μ where the preconditioner DD2 from [8] is used.

$\log N$	PC3				DD2	
	Δ		μ		μ	
	ρ_0	μ_0	ρ_0	μ_0	ρ_0	μ_0
1	0.13	5	0.19	7	0.39	11
2	0.20	7	0.28	9	0.55	16
3	0.25	8	0.38	12	0.64	21

Table 1. Results of numerical experiments illustrating Lemma 3.1.

4. Nonlinear problem. Let us consider problem (3.1) assuming that in some subdomains μ_i is nonlinearly dependent on the mean gradient of the solution in this subdomain Ω_i. To such problem we can reduce, in particular, magnetostatics problems (in incomplete nonlinear formulation [13]) where we can single out the nonlinearity domain $\Omega_F = \bigcup_{j=1}^{p} \Omega_F^j$ and the domain $\Omega_V = \bigcup_{j=1}^{q} \Omega_V^j$ with the constant coefficients μ. For simplicity, Figure 1 shows the two-dimensional case:

$$\Omega = \Omega_F \cup \Omega_V \cup \Gamma.$$

Denote $\vec{\mu} = (\mu_1,\ldots,\mu_p) \in R^P$, where μ_j in Ω_F^j, $j = 1,\ldots,p$, is a value to be determined. Then the nonlinear problem is equivalent to finding the steady-state point

$$\vec{\mu} = M(\vec{\mu}) \tag{4.1}$$

where the nonlinear operator $M(\vec{\mu})$ is defined by the following sequence of computations:

(a) for given $\mu_j = \text{const}_j$, $j = 1,\ldots,p$, linear problem (3.1) is solved; to this end, the algorithm from Section 3 is used;

(b) by using computed w find $\vec{\mu}_j' = M(\vec{\mu})$, $\mu_j' = \mu(y_j)$; $y_j = (\text{mes}\,\Omega_F^j)^{-1}(\int_{\Omega_F^j} |\nabla w|^2 dx)^{1/2}$.

We give the results of numerical experiments [20] of solution of problem (4.1) by the stationary Richardson method $\vec{\mu}_{n+1} = M(\vec{\mu})$:

(1) The computations were performed on the sequence of three grids

(12,14,14) → (24,28,28) → (48,56,56) with the partitioning of the nonlinearity domain Ω_F into 12 subdomains and 48 subdomains. This correspond to the partitioning of the entire domain Ω into 64 subdomains ($n_1 = n_2 = n_3 = 4$) and 150 subdomains ($n_1 = 5, n_2 = 6, n_3 = 5$).

(2) To solve (4.1) by the stationary Richardson method, it was sufficient to carry out $2-3$ iterations for obtaining the solution W with relative accuracy 10^{-4}.

(3) When using the sequence of grids the time of solution on the last one is approximately 8 minutes (IBM 370).

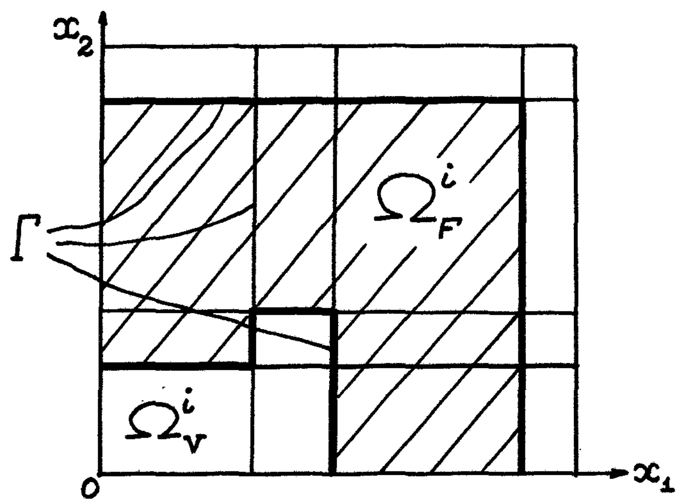

Figure 1. Two-dimensional case.

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