Geometric problems and algorithms in mathematical modeling

Valery Pavlovish Il'in
Institute of Computational Mathematics and Mathematical Geophysics, SBRAS
Novosibirsk, Russia,
{e-mail:ilin@sscc.ru}

Abstract

The issues of geometric modeling in the 3D numerical simulation problems are considered, including description of complicated computational domains and mathematical statements, automatical construction of algorithms, postprocessing and optimal control procedures for computer-aided design technologies. The main stages of computational processes are analysed in terms of accordance and transformation of flexible data structures: geometric and functional data, grid and algebraic ones.

1. INTRODUCTION

Mathematical modeling of technical, physical or nature processes and phenomena deals with the numerical solution of boundary value problems (BVPs) for partial diffirential equations (PDEs), or equivalent variational statements, in the complicated computational domains consisted of numerous subdomains with different material properties. Formally, the considered mathematical 3D non-stationary problems can be presented as search of the solution $\vec{u}$ of the operator equation:

$$L(\vec{c})\vec{u} = \vec{f}(\vec{x},t), \vec{x} = (x_1, x_2, x_3) \in \Omega \subset R^3, \quad 0 \le t \le T < \infty, \tag{1}$$

$$l(\vec{b})\vec{u}\big|_{\Gamma} = g(\vec{x}), \ \vec{x} = \Gamma, \ \vec{u}(\vec{x}, t=0) = \vec{u}^{\,0}(\vec{x}), \tag{2}$$

where L and l are differential operator of PDE and operator of boundary conditions respectively, with some piece-wise smooth vector (in general) coefficients $\vec{c}$, $\vec{b}$, which can be depended on the unknown solution, Ω is three-dimensional bounded computational domain with the boundary Γ and closure $\overline{\Omega} = \Omega \cup \Gamma$, $x_1 = x, x_2 = y, x_3 = z$ are Cartesian coordinates, for example, and t is time variable.

Strictly speaking, Ω is open bounded domain, and Γ is piece-wise smooth, in general, multi-connected 2D manifold. The solution $\vec{u}$ and right hand side function $\vec{f}$ can be vector functions, in this case L and l are matrix operators (may be, nonlinear). It is supposed, that the properties of L, l, Ω, and Γ provide the existence of the solution $\vec{u}$, unique or non-unique, with piece-wise smooth properties, necessary for validity of approximate methods to be used.

The system (1)-(2), under given boundary and initial data, as well as for given geometric and functional parameters $\vec{b}$, $\vec{c}$, describes so called direct problem. More general, and ideal for the end user, are inverse problems, in which any input data can be dependent on the parameter vector $\vec{p} = (p_1, p_2, \dots, p_m)$ to be found from the condition of the minimizing some cost (goal) functional:

$$\Phi_0\left(\vec{u}\left(\vec{r}, t, \vec{p}_0\right)\right) = \min_{\vec{p}} \Phi_0\left(\vec{u}\left(\vec{r}, t, \vec{p}\right)\right), \tag{3}$$

under additional linear or non-linear restriction

$$p_k^{\min} \le p_k \le p_k^{\max}, \ k = 1, \dots, m_1, \ \Phi_l\left(\vec{u}\left(\vec{r}, t, \vec{p}\right)\right) \le \delta_l, \ l = 1, \dots, m_2. \tag{4}$$

Here $p_k^{\min}, p_k^{\max}, \delta_l$, and $m_1 + m_2 = m$ are given values, and Φ_l are some functionals on the solution $\vec{u}$. An example of inverse problem is identification of unknown model parameters which can not be defined by the help of direct physical measurements. The search of optimal parameter $\vec{p}_0$ in inverse problem needs usually multi-variant solutions of direct problems with permutations of geometric and functional data. Such typical task is logging problems in electro-geoprospecting, [1], and shape optimization is the aim of research in many other applications, see [2], [3].

If $\vec{u} = \left(u_1, u_2, \dots, u_{M_u}\right)$ is the solution of multi-physics problem, the various fields are described by different PDEs which are defined, in principal, in different non-intersected subdomains. Here, representative example is the problem of complex simulation of technological processes in aluminum electrolizer, including electromagnetic fields and heat transfer, thermo-elasticity and melt circulation [4].

The main approaches for solution of considered problems are finite element and finite volume methods (FEM & FVM, see [5], [6]), based on the adaptive grid generation, element-by-element computational technologies and special data structures [7]. The geometric and algebraic issues of grid generation methods are the topics of numerous papers and books, see [8] for example.

After obtaining the grid solution, some geometric tasks arise in postprocessing the numerical results connected with computing and visualization of the iso-lines, iso-surfaces,vector fields, graphics, etc.

2. GEOMETRICAL OBJECTS AND DATA STRUCTURE

The computational domain Ω is presented as the union of non-intersected computational subdomains Ω_i:

$$\Omega = \bigcup_l \Omega_l, \ l = 1, \dots, \bar{l}, \tag{5}$$

and each of them has the closure $\overline{\Omega}_l = \Omega_l \cup \Gamma_l$. The external domain R^3 / Ω will be noted as subdomain Ω_0, which can be non-connected if the computational domain Ω has one or several holes. The adjacent boundary of the neighbour subdomains Ω_i and Ω_k is denoted as $\Gamma_{i,k} = \overline{\Omega}_i \cap \overline{\Omega}_k$ and is called as internal boundary segment. In each internal subdomain coefficients $\vec{c} = (c_1, c_2, \ldots)$ are supposed to be smooth and present the material properties of the corresponding media.

If the coefficients of PDEs have a jump at the internal boundary between two subdomains, then on the corresponding $\Gamma_{i,k}$ the adjacent condition holds:

$$l_{i,k}^{-} u\Big|_{\Gamma_{i,k}^{-}} = l_{i,k}^{+} u\Big|_{\Gamma_{i,k}^{+}}, \qquad (6)$$

where indexes "+,–" correspond to different sides of $\Gamma_{i,k}$.
The boundary of computational domain is presented as the union of external and internal parts:

$$\Gamma = \Gamma^{ex} \cup \Gamma^{in} = \bigcup_m \Gamma_m,\ m = 1, \ldots, \overline{m},\ \overline{m} = m_{ex} + m_{in},$$

$$\Gamma^{ex} = \bigcup_{m'} \Gamma_{m'}^{ex} = \bigcup_{m'} \Gamma_{m',0} = \bigcup_{m'} \left(\overline{\Omega}_{m'} \cap \overline{\Omega}_0\right),\ m' = 1, \ldots, m_{ex},$$

$$\Gamma^{in} = \bigcup_{m''} \Gamma_{m''}^{in} = \bigcup_{i,k} \Gamma_{i,k}^{in} = \bigcup_{i,k} \left(\overline{\Omega}_i \cap \overline{\Omega}_k\right),\ m'' = 1, \ldots, m_{in},\ i,k \neq 0, \qquad (7)$$

where indexes m, m', and m'' correspond uniquely to some pairs of indexes *i,k***.**

Each particular boundary segment $\Gamma_{i,k}$ (external or internal) can be defined by only smooth geometrical surface and only by one type of boundary condition $l_{i,k}$ which is given on the $\Gamma_{i,k}$. Each pair of intersecting boundary surface segment $\Gamma_m, \Gamma_{m'}$ forms the boundary edge $R_{m,m'}$, linear or curvilinear. The set of such edges can be numbered by one index:

$$R_{m,m'} = R_q,\ q = q(m, m') = 1, \ldots, \overline{q}. \qquad (8)$$

Formally, the edge R_q is open 1D point set and its closure is

$$\overline{R}_q = R_q \cup R_{q,1} \cup P_{q,2}, \qquad (9)$$

where $P_{q,1}$ and $P_{q,2}$ are the beginning and end vertexes of R_q respectively. The set of all vertexes in $\overline{\Omega}$ we denote as $P = \{P_r, r = 1, \ldots, \overline{r}\}$. The closure of surface segment Γ_m is

$$\overline{\Gamma}_m = \Gamma_m \cup \overline{R}_{m,q} = \Gamma_m \cup R_{m,q} \cup P_{m,r},$$
$$q \in \omega_m^{f,e},\ r \in \omega_m^{f,p}. \qquad (10)$$

Here $\omega_m^{f,e}$ and $\omega_m^{f,p}$ note the sets of edges and vertices incident to Γ_m, i.e. they form the boundary of Γ_m.

The total set of subdomains $\Omega_l, l = 1, \ldots, \bar{l}$, , surface segments $\Gamma_m, m = 1, \ldots, \overline{m}$, boundary edges $R_q, q = 1, \ldots, \overline{q}$, and vertexes $P_r, n = 1, \ldots, \overline{r}$, we shall consider as macrogrid, and its object will be called macroelements, macrofaces, macroedges, and macronodes respectively. The topology of the macrogrid is defined uniquely by set of own objects and by connections between them. For describing these connections we can introduce, similar to $\omega_m^{f,e}$ and $\omega_m^{f,p}$, the sets of indexes: $\omega_r^{P,\Omega}, \omega_r^{P,f}$, and $\omega_r^{P,R}$ are the sets of the numbers of macroelements, macrofaces, and macroedges which are incident to the macronode $P_r; \omega_l^{\Omega,f}, \omega_l^{\Omega,R}$ and $\omega_l^{\Omega,P}$ – the subsets of the numbers of macrofaces, macroedges and macronodes which are incident to the macroelement Ω_l.

In addition to topological information, the necessary data for identification of computational domain should include geometric description of boundary surfaces, presented by their algebraic equations. Because systems of such equations can have non-unique solutions, some addition constraints have to be given, for unic definition of surface intersections. The collection of considered information presents the geometrical data structure (GeomDS) for BVP.

The geometric objects have to be provided by the reference to the functional data which define parameters of PDEs and boundary conditions at each Ω_l and Γ_m.

Similar to definition of geometric objects of macro-level, the set of grid objects includes nodes, edges, faces and volume elements, defined by discretization procedure. Also, the grid computational domain and subdomains are constructed:

$$\Omega^h = \bigcup_l \Omega_l^h,\ l = 1, 2, \ldots, \bar{l}^h, \qquad (11)$$

where the value $\bar{l}^h$ can differ from $\bar{l}$, in priniple. We shall consider the adaptive grids only, in the sense, that all intersections of grid edges with external or internal boundary surface are presented as grid nodes. Also, all macrovertexes must be grid nodes and intersections of macroedges with grid faces must be nodes.

So, the grid boundary segments and closures of grid objects are defined similar to (7):

$$\Gamma_h = \Gamma_h^{ex} \cup \Gamma_h^{in} = \bigcup_m \Gamma_m^h,\ m = 1, \ldots, \overline{m} = m_{ex} + m_{in},$$

$$\Gamma_h^{ex} = \bigcup_{m'} \Gamma_{h,m'}^{ex} = \bigcup_{m'} \Gamma_{m',0}^h = \bigcup_{m'} \left(\overline{\Omega}_{m'}^h \cap \overline{\Omega}_0^h\right),\ m' = 1, \ldots, m_{ex},$$

$$\Gamma_h^{in} = \bigcup_{m''} \Gamma_{h,m''}^{in} = \bigcup_{i,k} \Gamma_{i,k}^h = \bigcup_{i,k} \left(\overline{\Omega}_i^h \cap \overline{\Omega}_k^h\right),\ m'' = 1, \ldots, m_{in},$$

$$\overline{\Omega}^h = \Omega^h \cup \Gamma_h = \bigcup_l \overline{\Omega}_l^h = \bigcup_l \left(\Omega_l^h \bigcup_l \Gamma_l^h\right),\ l = 1, \ldots, N_\Omega, \qquad (12)$$

where the values m_{ex}, m_{in} can differ from the ones in (7). The grid approximations of macroedges R_q are presented as

$$\overline{R}^h_{m,m'} = \overline{\Gamma}^h_m \cap \overline{\Gamma}^h_{m'} = \overline{R}^h_q = R^h_q \cup P^h_{q,1} \cup P^h_{q,2}, \quad q = q(m, m'). \tag{13}$$

The sets of grid nodes, edges, faces, and elements we shall denote as

$$P^h = \left\{P^h_r, r = 1, \ldots, N_P\right\}, R^h = \left\{R^h_q, q = 1, \ldots, N_R\right\}, \quad F^h = \left\{F^h_m, m = 1, \ldots, N_F\right\}, E^h = \left\{E^h_l, l = 1, \ldots, N_E\right\}. \tag{14}$$

Total information about topology connections between different types of grid objects presents grid data structure (GridDS):

$\omega^{P,R}_{h,r}, \omega^{P,F}_{h,r}, \omega^{P,E}_{h,r}$ – the sets of the numbers of grid edges, faces, and elements, incident to the node P^h_r;

$\omega^{E,P}_{h,l}, \omega^{E,R}_{h,l}, \omega^{E,F}_{h,l}$ – the sets of the numbers of the grid nodes,edges, and faces, incident to the element E^h_l.

GridDS must includes also information between topologic data of the macro- and micro-levels: to which subdomain $\Omega_{l'}$ the grid element E^h_l belongs and to which boundary segment $\Gamma_{m'}$ the grid face F^h_m belongs.

3. GEOMETRIC TASKS AND ALGORITHMS

The geometric tasks in mathematical modeling can be classified in a following way:

- elementary operations: intersections of the surfaces and curves, localization of point, computation of the distances between different objects;
- modifications of geometry and shape optimization including shifts, rotations, and scaling of the objects;
- element-by-element geometric constructions for FVM or FEM approximations of original mathematical statement;
- computing the iso-curves and iso-surfaces of solution as well as constructing various graphis in the postprocessing stage for visualization of the resulting grid functions.

The special problem is grid generation, i.e. constructing the Voronoi-Dirichlet cells or triangulazion of computational domain. It can use conform or quasi-conform mapping, differential geometry or special empiric approaches. The universal mesh construction is based on the using quasi-structured grids with grid subdomains which can include own different types of elements: parallelepipeds, tetrahedras, etc. In each grid subdomain respective mesh generator can be used.

An implementation of these and other algorithms of computational geometry depends on the methods of presentation of the objects, for example, see [9]–[11] and references citied therein. In different Computer Aided Design systems the various objects and approaches are used: Bezier and Coons surfaces, nonuniform *B*-splines (NURBS), triangular patches, transfinite interpolation (TFI), alpha shapes, multiresolution methods, etc. The perspective description of complex topology is based on set-theoretical formulas and operations proposed by V.L.Rvachev [9].

An implementation of these approaches is made efficiently by object-oriented programming, with the definition of geometric primitives and figures provided by their properties, communications, and possible transformations.

Automatical construction of the above algorithms for various computational domains, boundary conditions and PDEs is supported by internal geometric and functional data structures, which are provided by the wrapper for communication with some GUI or CAD system. Implementation of different computational stages is made by the libraries of grid generators, FVM or FEM approximators and algebraic solvers. The last ones are problem independent, because they are supported by abstract algebraic data structures which include an information about original mathematical problem in a very indirect form.

Let us remark in conclusion that modifications of computational domain and shape optimization problems needs definition of geometric objects in parametrized form to provide complicated transformations during multi-variant successive solutions of the direct problems.

4. REFERENCES

[1] Il'in V.P. On the numerical solution of direct and inverse problems of geo-electromagnetic exploration (in Russian).-–Sib.J.Num. Math., v. 6, N 4, 2003, 381-394.

[2] Il'in V.P., et al. Emission-Imaging Electron-Optical system Design.–Advances in Electronics and Electron Physics, vol. 78, Acad.Press, 1990, 156-278.

[3] Hoppe R.H. Shape and topology optimization in aterials sciense// Proceeding of ICCM, Novosibirsk: NCC Publ., 2002, 17-31.

[4] Golosov I.S., Gorbenko N.I., Gurieva Y.L., Il'in V.P. and others. Program package BASIS-A for simulation of technological processes in an aluminum electrolyser.–Krasnoyarsk: NTZ ``Light metals''. proc. of the 8-th International Conference ``Aluminum of Siberia-2002'', 2002, 187-192.

[5] Axelsson O., Barker V.A. Finite element solution of boundary value problems: Theory and computations. New York: Acad. Press, 1984.

[6] Il'in V.P. Finite Difference and Finite Volume Methods for Elliptic Equations.–Novosibirsk: NCC Publ., 2001 (in Russian).

[7] Il'in V.P. Computational-informational technologies of mathematic modeling.–Optoelectronics, nstrumentation and Data Processing (Avtometriya), N 1, 2000, 3-13.

[8] Liseikin V.D. Grid generation methods.–Berlin, pringer, 1999.

[9] Rvachev V.L. The Theory of R-Functions with applications (in Russian).–Naukova Dumka, Kiev, 982.

[10] Kozlov V.I., Yudin A.N. Set-theoretic geometric

escription of three-dimensional regions with internal structure for CAD problems.–Optoelectronics, instrumentation and Data Processing (Avtometriya), Novosibirsk, N 2, 1999, 88-98.
[11] Farin G., Hamann B. Current trends in geometric modeling and selected computational applications.– J.Comp. Phys., v. 138, 1997, 1-15.

About the author

Valery P. Il'in is a Head of Department of Math. Problems in Physics and Chemistry, ICM&MG, SBRAS.
His contact email is ilin@sscc.ru.