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NUMERIC CALCULATION IN CONTEXT OF RELATIONAL ARCHITECTURE

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Abstract

In this paper a basic points of numeric methods for solving a problems of mathematical physics by means of tools of relational architecture are described.
Instruments of relational Database Management Systems (RDBMS) for achievement a general stages of numeric modeling, such as mesh generation, discretization of equations of initial model, solving a system of linear algebraic equations (SLAE), interpretation and analysis resulting data, are described.
Strategies for building algorithms and formats of data storage in relational architecture are described for each stage of numeric experiment.
In paper meshing algorithms for finite elements method (FEM) and finite differences method (FDM) are considered. And data structures for structured and nonuniform unstructured mesh representation are described. The algorithms for discretization of initial model and building SLAE matrix by means of storage procedures on SQL are offered. There are offered algorithms for SLAE solving with discharged matrix by means of Krilov's iterative method in relational architecture. The calculation algorithms on SQL of integral characteristics of discrete field of required value are offered.
There are described strategies in RDBMS for export and manufacturing data that was obtained during numeric experiment.

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Additional Key Words and Phrases: finite elements method (FEM), finite differences method (FDM), algorithms for discretization, relational architecture

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1. INTRODUCTION

The decision of the majority nonlinear problems of mathematical physics by analytical methods is possible only for a narrow circle of problems. The usage of modern firmware in aggregate with the advanced mathematical methods allows expanding a circle of nonlinear problems of mathematical physics for which is possible to receive the numeric decision.

In the given work realization of the basic stages of numerical modeling with use of methods of finite differences (MFD) and finite elements (MFE) in view of features of relational architecture is considered.

2. NUMERIC CALCULATION STAGES IN RELATIONAL ARCHITECTURE

At practical realization of the given methods the basic stages are following:

1. Construction (generation) of a grid in the problem space. There is a plenty of the algorithms, allows covering with a grid area of the decision of a problem. Thus algorithms of generation of a grid for MFD are easier in realization (the regular grid is more often applied), but irregular adaptive grids for MFE allow to consider geometry of investigated model more effectively. Process of construction of a grid of final elements (FE) in MFE demands greater computational burden and we should use special algorithms of smoothing.

2. Digitization of the equations of initial model and construction of the linear algebraic equations system (SLAE). When we use MFD the given stage is carried out by replacement of initial equations by difference analogues. In MFE is made digitization of the integrated equations expressing conservation laws but not the equations in private derivative. For an initial problem is construct functional which extremum is delivered with the function, being the decision of an initial problem. Thus, MFE is a variation-grid method. At practical realization with use of the computer final differences easier to present, than integrated correlations of MFE.

3. Decision SLAE. Matrixes SLAE in MFE and MFD essentially differ. If in MFD the matrix is unloaded, mainly tape, with width of a tape depending of a problem dimension and sample approximation, then in MFE demands special algorithms for renumbering units FE with the purpose of reception of a matrix with the minimal width of a tape. Also essentially differ methods of decision SLAE. For MFE traditionally use iterative-gradient methods, biadjoint gradients. Also apply iterative methods for MFD, but their convergence essentially below in comparison with matrixes for MFE.

4. The analysis and interpretation of results. As a result of decision SLAE receive a set of discrete numerical values of required sizes in units of a grid. In practice yielded results are often intermediate and demand the further processing: calculation of integrated characteristics of a discrete field of settlement size, construction and analysis of schedules of decisions. The given stage demands greater computing expenses, considering great volumes of processable data.

As we see from the description of separate stages, at the decision of problems of mathematical physics by numerical methods the greater share of operations is matrix-vector. At practical realization of methods as structures of data are optimal a vector, a matrix, lists, sets. The relational architecture allows submitting data mathematical objects in the form of relational attitudes. Thus, relational control systems of databases (RCSDB) represent the developed means of data processing of great volumes.

Let's consider realization of each of stages of numerical modelling with use of toolkit of relational databases.

2.1. Mesh generation in solution domain by means of DBMS

Generation calculation grids for numerical methods within the limits of relational architecture are carried out with use of language SQL. Process of construction of a grid for MFD is reduced to consecutive performance by the operator INSERT of new record which fields except the service information contains the field for storage of coordinate of a net level. Thus, irrespective of dimension of a solved problem, the one-dimensional grid in one coordinate direction (for example on axis Ox) is under construction. Then the received sequence of units is copied by operator INSERT ... SELECT on other coordinate axes. If it is necessary, SQL-operator UPDATE carries out change of values of coordinates of net levels. As a result we receive set one-dimensional grids in separate coordinate directions.

To receive final covering of area of the decision of demanded dimension, it is necessary to execute full external association by operator SELECT ... FULL JOIN ... all one-dimensional grids.

After reception final sets of units, it is necessary for each unit to appropriate the unique identifier. For this purpose operator UPDATE makes updating a key field. Process of construction of a three-dimensional regular grid for MFD with use of inquiries SQL is schematically represented on figure 1

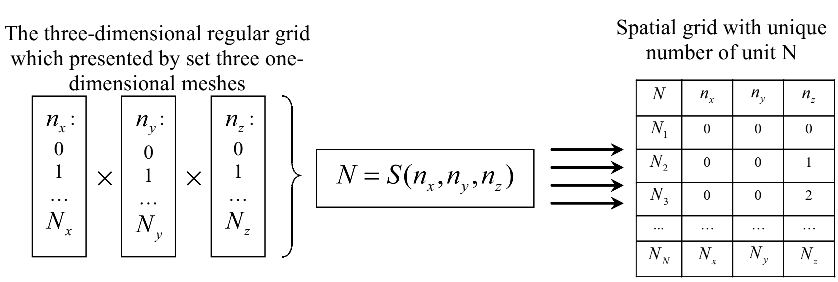

Figure 1 - The scheme of construction of a spatial grid with unique number of unit from three one-dimensional

At generation of a grid for MFE are used complex iterative algorithms: advanced front method, quadric algorithm, and immediate assembly method. The given algorithms are intended for construction of a primary grid. For reception of the net final partitioning we should execute procedure of smoothing. This stage is the most labour-consuming at construction of a grid, and demands application of special methods: like Laplace smoothing.

In MFE method uses triangle based data structures. With each triangle are associated its three edge neighbors (in two dimensional case). The neighborhood relationship are encoded such that $k = Neight\ (i, j)$, which means that the triangle of index k is adjacent to the triangle of index i and that the edge j of triangle i is common edge ($k=0$ means that the edge j of triangle i is a boundary edge). Vertex j of triangle i is opposite to edge j of this triangle. A pair of triples vertices-neighbors is the way of representing a triangulation. A representation is based upon the triples of vertices and the connection matrices. Each triangle K is endowed with a 3x3 matrix defined as follows (Figure 2):

- the diagonal coefficient i, c_{ii} indicates the local index of the triangle vertex opposite to triangle K by the edge i,

- another coefficient c_{ij} gives the index of the j-th vertex of K in its i-th neighbor.

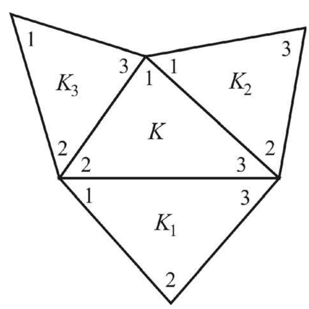

Figure 2 - The Definition of a triangle K and of its three neighbors K_i.

According to its definition, the adjacency matrix of triangle K in Figure 2 is:

$$C^K = \begin{pmatrix} 2 & 1 & 3 \\ 1 & 3 & 2 \\ 3 & 2 & 1 \end{pmatrix}$$

Matrix C^K are associates with each triangle. We need a data storage to store all matrices and methods to manipulate and update data structure (when adding, deleting triangles). Relational Database Management Systems give us data manipulating language and database to store matrices. All matrices a stored in one relational table, and triangles are stored in another one. Tables are related by one-to-many link. Matrices are selected from database by means SQL language.

2.2. Model Discretization

Digitization of model in MFD and reception of matrix SLAE is reached by performance of sequence of SQL-inquiries: by one inquiry about each type of assembly (for different types of assembly various patterns of approximation are defined).

Construction SLAE for MFE demands a preliminary choice of form functions for finite elements. As well as in MFD reception of matrix SLAE is reached by sequence of SQL-operators. Matrixes SLAE at realization of net numerical methods are unloaded and for the further calculations it is expedient to store only nonzero elements. Therefore only the elements consider a portrait of a matrix are stored in the table of a database. It saves time of construction of a matrix and computing resources at decision SLAE.

2.3. Solution of SLAE

At the decision of greater SLAE iterative methods are most effective. Thus methods are applied to reduction of time of calculation without change of initial matrix SLAE.

Methods of Krylov type satisfy to these conditions. For increase of speed of convergence of iterative algorithms expediently introduction in the sheme of the procedure of the factorization method (for example ILU-factorization).

Iterative process of decision SLAE in RDB is reduced to performance in a cycle of SQL-inquiries. Each SQL-inquiry allows receiving new approximation to decision SLAE on the basis of an initial matrix not changeable during the decision, and the approach received at the previous stage.

At decision SLAE with use of toolkit RDBMS there is an opportunity of preservation of all intermediate decisions, and not just the result received on final iteration. It allows to spend supervision over character of convergence of iterative process and to reveal the factors as much as possible influenced for speed of the decision.

It is possible to stop process of the decision, we can analyze the received decision, and if we need, we can specify the decision carrying out of additional iterations of algorithm of Krylov.

2.4. Calculation of integral properties of numerical field

After decision SLAE we receive a set of discrete values of required size. In the majority of the problems, the given result is intermediate. It is necessary to use these data for reception of values of energy, force, the moments of forces. The given sizes are integral on volume (or surfaces) in some subarea of the decision of a problem. At use of numerical grid methods, integration is replaced with summation. Summation on settlement values in the set grid units with use of toolkit of a SQL-server is made with use aggregating functions of language SQL. Thus, use of one command SQL it is possible to receive value of force or the moment of force concerning some point, and also to count energy of a field of discrete size in the set volume.

2.5. Analyze and visualization of calculation result

Modern RDBMS possess the developed integration tools with programming systems and visualization of data. Therefore carrying out of calculations within the limits of relational architecture allows exporting results of the decision for the further analysis to the formats accessible to the majority of systems of scientific calculations.

Not all relational DBMS possess the built in means of visualization of the information, but ample opportunities on export of data allow deducing the received decision of a problem practically in the form of multivariate schedules, diagrams in specialized appendices.

3. DBMS PROGRAM COMPLEX ARCHITECTURE

At programming program complexes for calculations with use of numerical grid methods it is expedient to adhere to client-server architecture with technology "the thin client". It will allow minimizing the dataflow between the program-client appendix and a server of databases.

The client appendix is intended only for input of parameters of initial model, monitoring of process of the decision and visualization of results. All computing load concentrates on party RDBMS.

The given approach allows:

1. To develop procedures for realization of stages of numerical modelling only in language SQL. Thus there is no necessity to realize separate modules in other programming languages.
2. To organize uniform base intermediate and final data. It allows using earlier received decision as initial approach a new problem.
3. To carry out paralleling decisions of a problem means RDBMS, thus creation of special procedures or applications of the special software for the organization paralleling is not required.

4. SUMMARY

Using RDBMS can do the process of creation of parallel program complexes for numeric mesh calculation more simple.

Vector and matrix operations, which are prevalent in FDM and FEM methods, are realized in one only SQL-query. It isn't necessary to realize nested cycles, such as in high language programming.

DBMS features, such as triggers, stored procedures, user functions, along with mathematical iteration methods, provides to create complicated algorithms, which consider high task parallelism in FDM or FEM.

DBMS gives an opportunity to long time storage data, but not only means for data manipulations. This feature of relational architecture speeds up the program debug process, manage calculation process and calculation results analyses.

Relational architecture along with FDM or FEM methods, provides for acceptable time to get numerical solution nonlinear PDE problem in complex geometrical areas and heterogeneous physical areas. Diagram, which present a rate of convergence of numeric calculation process, are presented in Figure 3.

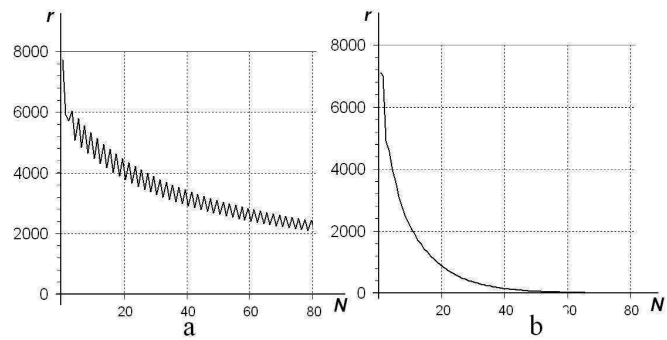

Figure 3 - The rate of convergence of iteration calculation process: a – using full ortogonalization modified method (FOM(m)); b - using FOM(m) with ILU-factorization. *N* – iteration number, *r* - solution error.

As a result of using a program complex is a diagram (Figure 4), which presented a distribution of scalar magnetic potential in calculation area with permanent magnet immersed in magnetic liquid (testing problem).

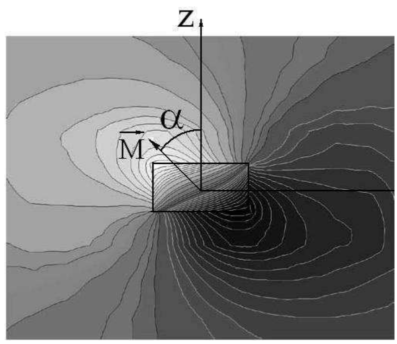

Figure 4 - The diagram of distribution of scalar magnetic potential in calculation area: permanent magnet immersed in a vessel with magnetic liquid ($\vec{M}$ - magnetization vector, $\alpha = 45^\circ$).

Also it provides an great opportunity to data analyze, export data and RDB program complex update.

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