

Methods and parallel code "FREGAT" for distribution of substances in mixed cells of computational meshes

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Abstract. *To solve a task of substances distribution and physical values computation in mixed cells of arbitrary hexagonal meshes developed was parallel program FREGAT as a part of computer codes of 3D preprocessor in RFNC VNIITF. The results of intersects of mesh cells with arbitrary CAD model geometry domains, where domains characterize substance, are the basis for calculating mass and volume concentrations of substances in mixed cells and other physical values. In result generated is the initial profile of mesh fields of physical values, which are transferred to be calculated to applied programs in HDF format. The paper presents results of numerical investigations at different models. Calculations were conducted in different modes with various numbers of processes.*

1 Introduction

Definition and calculation of initial data (CID) is the first step in technological chain of applied numerical modeling. In connection with active development of principally different 3D complexes of numerical modeling, the task of updating the techniques and software of 3D CID is very actual. In order to obtain reliable results of applied numerical modeling it is necessary to have tested physical and mathematical models, algorithms, codes of programs and smoothly running system of verification. As practice shows, for effective resolving CID problems for selected classes of physical processes, one needs thematic orientation.

For applied program complexes (PC) of mathematical modeling for continuum mechanics (CM), in CID it is necessary to calculate substance distribution in mixed cells of computational meshes. At the initial instant it is necessary to form mesh field of substance concentration in the cells and scalar and vector fields of substances average by masses, densities, energies, velocities and other physical values. For solving this problem on big meshes the there were developed methods and parallel code FREGAT as a part of PC 3D CID [1, 2].

The main stages of definition and calculation of initial data in CM are:

- Building a structure and geometrical description of physical system under modeling.
- Topological splitting the system into computational regions.
- Definition of physical properties of computational regions.
- Building computational meshes in regions.
- **Calculation of physical values in the cells.**
- **Presenting CID result in the form of description of physical system initial state and recording initial data in required structures and formats.**

Code FREGAT solves selected problems: calculation of physical values in mesh cells; presenting CID result in the form of description of initial state of physical system.

2 Problem set-up

Input data are regular computational mesh, geometry of mathematical regions for the model and a set of physical characteristics specified in geometrical regions of the model. The prepared mesh model with a set of physical characteristics at the initial instant mathematically describes physical model. Let us call this set of data the initial profile of the problem.

For FREGAT, the mesh is specified in various codes, for example, in software platform SALOME [3], and it is provided in consistent form in formats based on HDF library [4], in MED format [3] and internal RFNC-VNIITF format. Input geometry of a model is accepted in two variants: from CAD packages in BREP format in the form of combinatoric set-theoretical description in text format DAT (such method is used in Monte-Carlo). Figure 1 shows two models in the GEOM subsystem of SALOME platform: to the right, the model is in BREP format, and to the left it is imported from combinatoric DAT format. BREP format is the format of geometric kernel in open codes OpenCascade [5], into which it is possible to convert the geometry from CAD-formats STEP, IGES, STL.

Physical properties of geometric regions are described in XML format, and governing parameters for calculation are described in text format. Figure 2 shows the same two models, but in the frames of VNIITF visualization system "ViziGeom" [6] for combinatoric models.

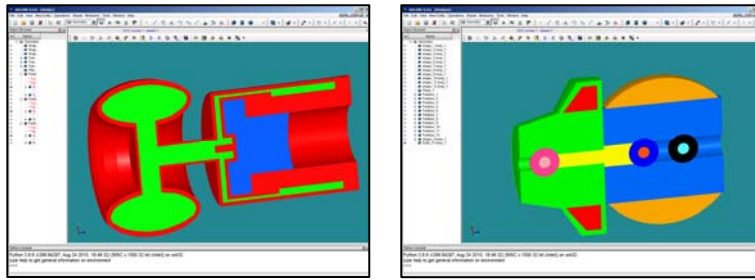


Fig.1. Two geometrical CAD models in SALOME

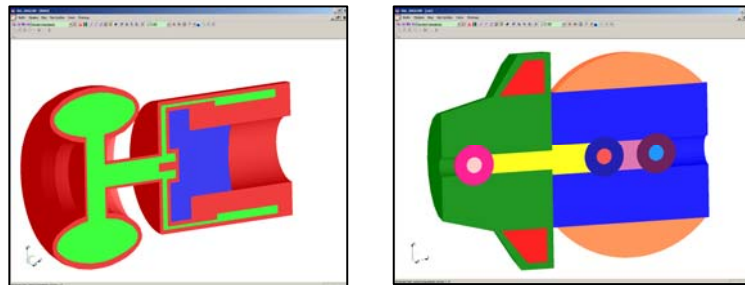


Fig.2. Two geometrical combinatoric models in ViziGeom code

Input physical data are described in editor or directly in text of XML file. Figure 3 shows an example of editor and XML form.

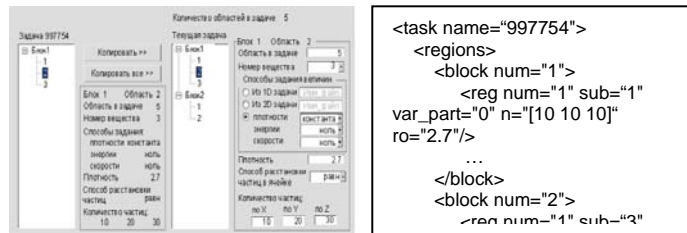


Fig.3. Creation and editing physical data

Figure 4 shows examples of two types of input meshes in HDF format in VNIITF visualization system "Vizi3D" [7], and figure 5 shows the same meshes in MED format in subsystem SMESH of SALOME platform.

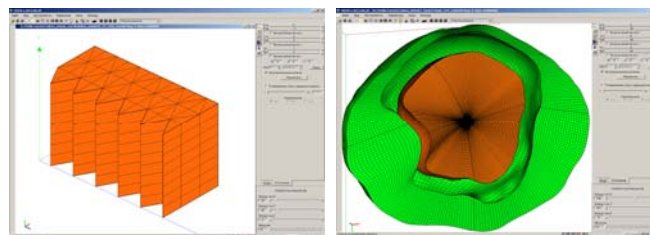


Fig.4. Meshes in HDF format in visualization system Vizi3D

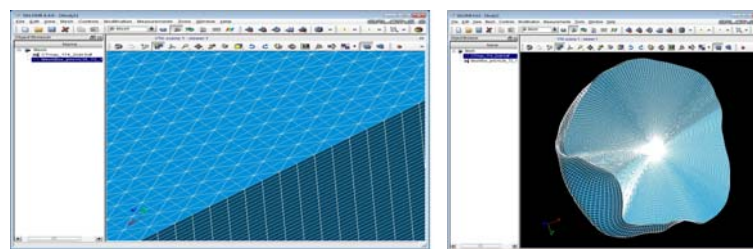


Fig.5. Meshes in MED format in SALOME

Basis of technique – finding of volumes of mesh cells crossing with the model geometrical regions, i.e. the cells are described in the form of solid body and cross over solid geometry of regions. This volume is used for determining the substance concentrations in mixed cells and other physical characteristics.

The volume of crossing is calculated in two ways: approximate and accurate. For combinatoric method of describing geometry crossing is calculated only in approximate way with the help of approximation of the cell volume by the population of the particles. For this purpose, operation of particle localization relatively to the solid body is used. For CAD format, both methods of calculation of crossing volumes work.

FREGAT is oriented to the account of various types of nonsingular and singular hexagonal cells: parallelepiped, curvilinear cell with lined facets, prism and pyramid. Figure 6 shows various types of cells.

Flexible algorithm of automated selection of crossing calculation method was realized. This is targeted on resolving two problems:

- reducing the time of crossing volumes calculation;
- minimizing the losses of data under emergency stops if one of the methods gives an error.

Examples with such problems solution.

1. Account for cell geometry in concrete mesh, while building solid-body cell and methods of searching the crossing.
2. Selectivity of crossing volumes calculation method: building by stretching is used, if there is an error building by surfaces is used, if there is an error again, approximate method of crossing is used.

Methods of crossing calculation for BREP format are performed by the functions of OpenCascade library, and with approximating tetrahedrons crossing VNITF program is used.



Fig.6. Types of cells

Building a cell in the form of solid body is performed by various methods. For example, a cell with lined facets is built using operation of stretching, as it is shown in figure 7 in the left part or cell decomposition is performed into tetrahedrons – figure 7 in the right part.

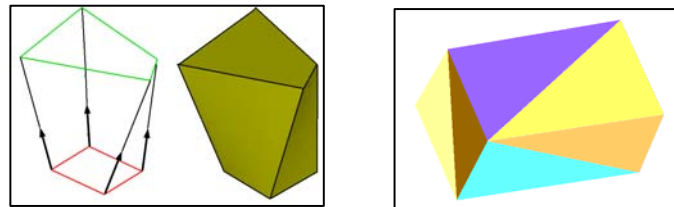


Fig.7. Approximation of cells with lined facets

Calculation of accurate volume V_T for hexagonal lined cell is made by volume approximation into two decompositions by 5 tetrahedrons. Figure 8 shows 2 decompositions. V_1 – the sum of tetrahedrons volumes under the first decomposition, V_2 – the sum of tetrahedrons volumes under the second decomposition. Accurate volume V_T – average of two volumes V_1 and V_2 .

$$V_1 = \sum_{i=1}^5 V_i, \quad V_2 = \sum_{j=1}^5 V_j, \quad V_T = \frac{V_1 + V_2}{2}$$

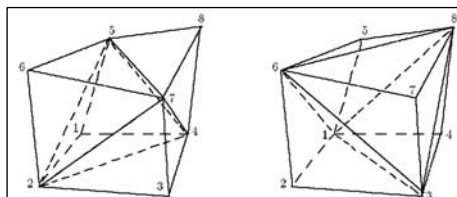


Fig.8. Two variants of decomposition of lined cell into tetrahedrons

Calculation of approximate volumes of the mesh cells crossing with the model regions is realized with the help of approximation of the cell volume by particle population. For this purpose, operation of particle localization relatively

to the volume is used. Two ways of particle arrangement in the cell were realized – regular and random, as it is shown in figure 9.

Volume of elementary particle neighborhood is calculated by the formula:

$$V_p = \frac{V_T}{N_p}, \quad \text{where } N_p - \text{the number of particles.}$$

Volume of region:

$$V_{reg} = \sum V_p$$

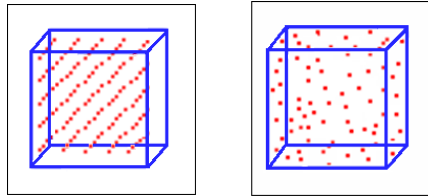


Fig.9. Two ways of volume approximation by particles

3 Calculation of physical characteristics in the mesh cells

For calculating volume concentration of substances in the cell, the following is calculated:

- Cell volume.
- Volume of cell crossing with physical region of the model.
- Volume concentration of the substance α in the cell V_{ijk}^α - is ratio of volumes: of crossing volume to the cell volume, as it is shown in figure 10.

$$V_{ijk}^\alpha = \frac{\text{Volume of substance in cell}}{\text{Cell volume}}$$

Fig.10. Calculation of substance volume concentration.

After that, other values are calculated: mass, density, components of velocities, mass concentration, and specific internal energy. As the result, the initial state of the problem on defined computational mesh is formed, it is transferred to calculation in applications in HDF format. The examples of cell volumes calculation are presented in figure 11.

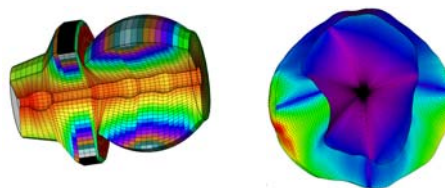


Fig.11. Visualization of lined cells volumes.

Calculations in PC FREGAT in one-processor and parallel modes [8].

4 Parallel program implementation

For parallel mode of calculations, decomposition by mesh regions is performed (Fig. 12) or by mesh fragments (Fig. 13), which are computationally distributed by the processes.

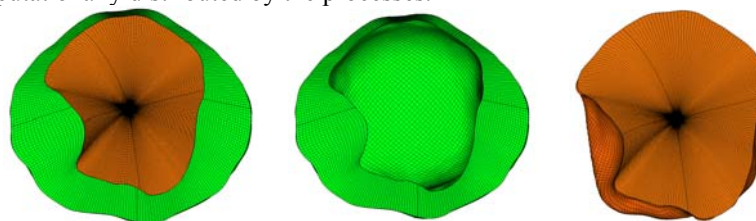


Fig.12. Decomposition of computational mesh by mesh regions.

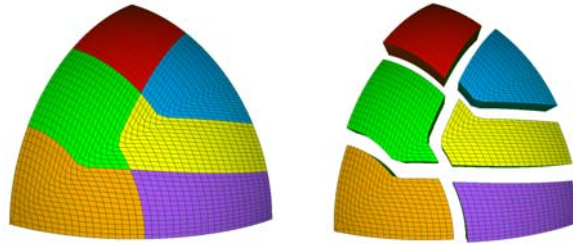


Fig.13. Decomposition of computational mesh by the mesh fragments.

Each process records its part of resulted mesh with physical filling into HDF file (left part of Fig. 14), and if it is necessary, one full profile of the mesh model is compiled into one file (right part of Fig. 14).

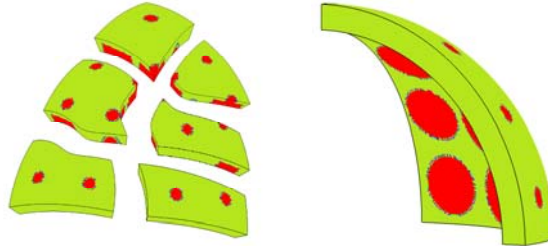


Fig.14. Final mesh model by fragments and full profile after CID.

There are functions to diagnose the results of CID in mixed cells:

- Controlling conservation of mass and volume.
- Controlling the ratio of volume of substance transported from part of regions into the cells to accurate volumes. It is necessary for localization and processing empty and semi-empty cells.
- Fixing the mesh fragments and cells with potential errors for their subsequent processing.
- Issuing calculation statistics.

For analyzing the profiles on big meshes, visualization in parallel mode is used.

5 Numerical study

Let us consider the examples, with which verification of technique and FREGAT program realization were performed. Calculations were made in various modes using parallel calculations.

Problem 1. We have a model defined combinatorially consisting of 12 regions, densities of materials are defined in regions (right part of Fig. 2), and rectangular mesh with mesh guidelines parallel to coordinate axes with the size 88x88x108. Left part of figure 15 shows mesh model by the substances and the right part of the figure shows iso-surfaces of regions.

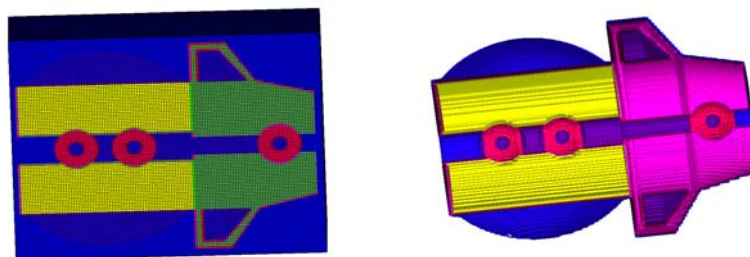


Fig15. Mesh model and iso-surfaces obtained from combinatoric geometrical model.

While assessing the efficiency of parallel calculations, acceleration and efficiency of paralleling by the formulas $S = \frac{T_1}{T_n}$, $E = \frac{T_1}{nT_n} \cdot 100\%$, where T_1 - astronomic time of the problem calculation on one process, T_n - astronomic time of the problem calculation on n processes. Table 1 gives the data on the efficiency of paralleling and acceleration for the problem 1.

Table 1. Numerical characteristics of paralleling

n	time, hr	S	$E, \%$
1	4,72	-	-
4	1,61	2,9	73
8	0,84	5,6	70

Size of resulting profile – 308,4 Mb.

Problem 2. We have CAD-model of pellets geometry and specified density of pellet material (left part of fig. 16), as well as regular mesh 30x180x180 with densities in the cells (right part of fig. 16). The cells with lined facets. It is necessary to put pellets into the mesh with account for substance concentration.

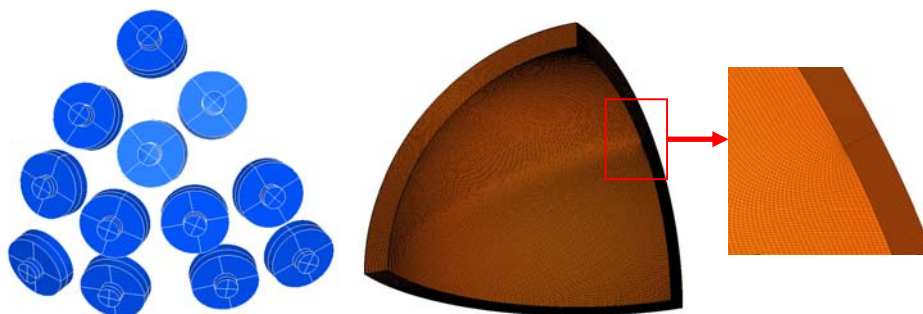


Fig.16. CAD geometry pellets and initial mesh

As the result, the following vector is calculated of the values in the cells: mass and volume concentrations of substances, substances densities, average masses, densities and volumes. Figure 17 shows the results of CID performance, i.e. mixed cells in the form of mass concentration field. Figure 18 (left picture) presents density field, and right picture shows iso-surface shows the shape of pellets in mesh model.

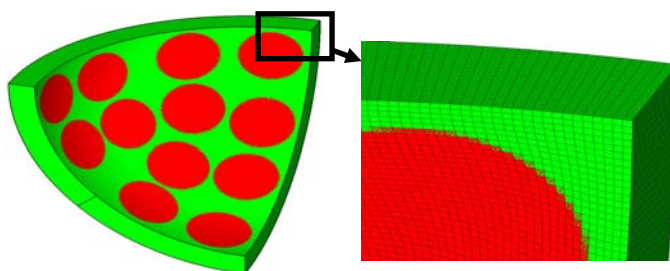


Fig.17. Field of mass concentrations

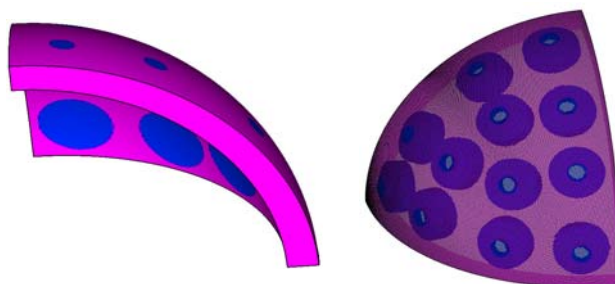


Fig.18. Filed of density with iso-surfaces

The problem was calculated on 1 (89hr.) and 81 (1,5hr.) processes. The efficiency of paralleling is 73%. Acceleration makes 59,3. The size of resulting profile is 102,2 Mb.

Problem 3. We have a test CAD-model of empiric flying vehicle from 5 regions and specified density of materials in regions (Fig. 19). There were also 4 types of meshes with various cells, in which it is necessary to put CAD-model and to describe it in the form of substances in mixed cells. As the result, the following vector is calculated of the values in the cells: mass and volume concentrations and densities of substances, average masses, densities and volumes.

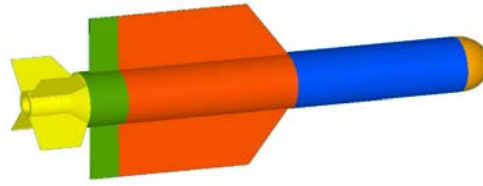


Fig.19. CAD-model of empiric flying vehicle from 5 regions

Variant 1. We have a rectangular non-uniform mesh with mesh guidelines parallel to coordinate axes with the size 30x70x110. Figure 20 (left picture) presents the results of CID performance, i.e. mesh model in the form of density field in the cells, and right picture shows the regions of the substances, which are marked with the help of iso-surfaces by the density of the regions.

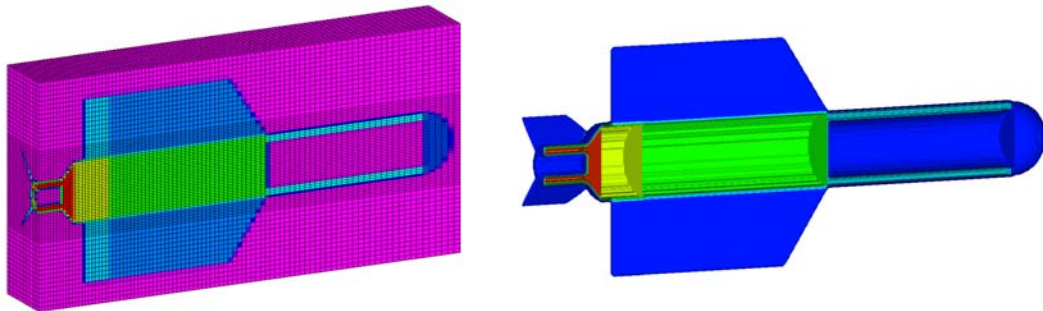


Fig. 20. Mesh model of flying vehicle on rectangular mesh

Time of calculation in one-processor mode was 24 minutes. The size of resulting profile was 46,5 Mb.

Variant 2. We have rectangular mesh with rotation around axis X and size 60x100x220. Figure 21 (left picture) presented mesh model in the form of density field, and right picture shows regions of substances, which are marked with the help of iso-surfaces by the density of the regions.

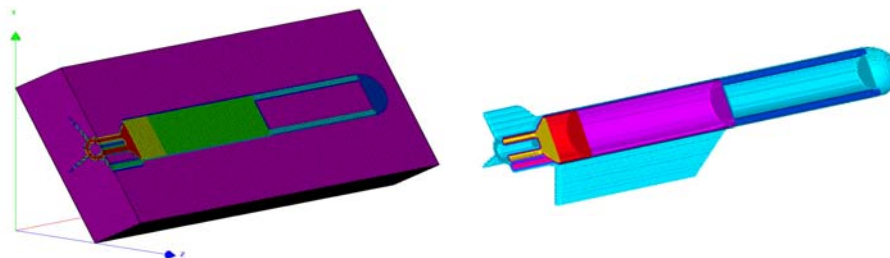


Fig.21. Mesh model of flying vehicle on rectangular mesh with rotation

Time of calculation in one-processor mode was 45 minutes. The size of resulting profile was 46,5 Mb.

Variant 3. We have curvilinear mesh with the sizes 60x60x83 and 59x59x20. Figure 22 presents mesh model in the form of density field in the cells.

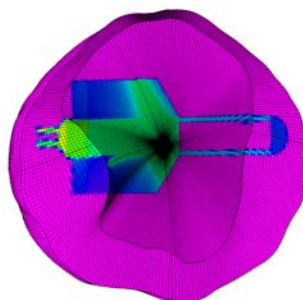


Fig.22. Mesh model of flying vehicle on curvilinear mesh

The problem was calculated on 1 (54,8m.), 4 (16,2m.) and 8 (8,1m.) processes. The efficiency of paralleling is 84%. Accelerations are 3,4 and 6,8. The size of resulting profile was 65,5 Mb.

Variant 4. We have a mesh, where the cells are rectangular prisms. Figure 23 (left picture) presents density field, and the right picture shows the field of mass concentrations.

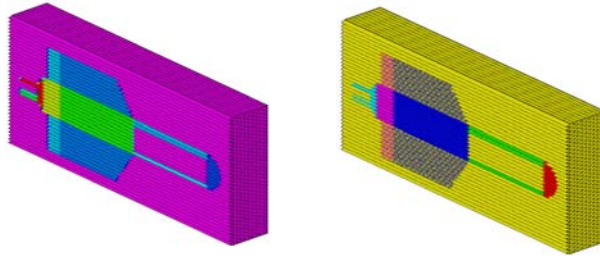


Fig. 23. Mesh model of flying vehicle on a mesh with the cells in the form of rectangular prisms.

Time of calculation in one-processor mode was 1 hour 20 minutes. The size of resulting profile was 75,1 Mb.

Problem 3. We have a model, specified combinatorially from 3 regions, specified densities of materials in the regions (left part of figure2, as well as rectangular mesh with mesh guidelines parallel to coordinate axes with the size 68x68x110. Figure 24 presents mesh model by substances and in the right picture shows iso-surfaces of the regions.

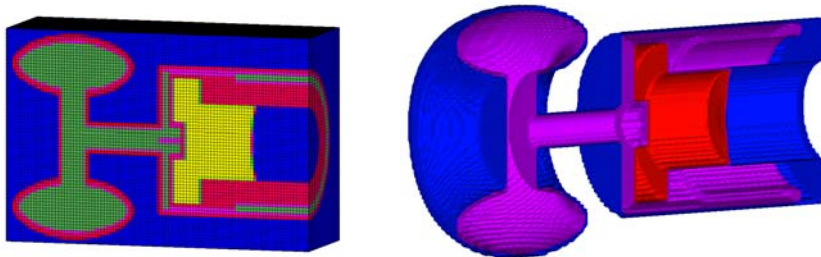


Fig. 24. Mesh model on rectangular mesh obtained from combinatoric geometrical model.

Table 2 gives the data on the efficiency of paralleling and acceleration for problem 3.

Table.2. Numerical characteristics of paralleling.

n	time, m	S	$E, \%$
1	314,92	-	-
8	48,41	6,5	81
80	4,95	63,6	79

The size of resulting profile is 77,8 Mb.

6 Conclusion

1. A technique and code FREGAT were developed for distribution of substances in mixed cells on arbitrary hexagonal meshes.
2. Parametrization of calculation with wide possibilities was realized.
3. Numerical study of algorithms and program realization of interpolation was developed.
4. The program was verified on the profiles with complicated mesh geometry.
5. Interpolation accuracy was assessed by criterion of mass conservation and transported volumes of the cells.
6. The influence of calculation parameters and methods of crossing on approximation accuracy was investigated.
7. FREGAT was transferred to operation for applied program packages of RFNC-VNIITF.

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