Numerical analysis of the effects of intense energy flows on a cylindrical target in a magnetic field

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Abstract. In this paper, a new version of the method for numerically solving the equations of radiation magneto-plasma dynamics is presented. The developed numerical technique was verified by solving a number of test (model) problems. The one-dimensional calculations of the plasma-dynamic parameters of a cylindrical target for the combined scheme of the effects of magnetic inertial fusion take into account a wide range of physical effects. A method is proposed for the transition from a tetrahedral to a hexagonal irregular computational grid. A variant of the elliptic “regularizer” of the grid is developed, which is based on the “mechanical analogy” and is based on the solution of linear equations of the theory of elasticity. The paper presents the initial results of the reconstruction and “regularization” of the computational grid, as well as the distribution of the “angular” criterion for assessing its quality.

1. Introduction

One of the important points in the numerical modeling of the Reynolds equations is the construction of a computational grid $\Omega_h$ (in complex two-dimensional and three-dimensional regions $\Omega$), which represents the computational domain $\Omega$ in the form of separate finite elements (cells). As applied to the discretization problem, “computational” areas are called computational domains, on which the mathematical features of the problem being solved or the numerical method impose some additional restrictions. Typically, these restrictions are in the form of lines or surfaces that should not be crossed by the edges of the computational grid $\Omega_h$.

At the same time, certain requirements are also imposed on the spatial dimensions and shape of the finite elements, since they significantly affect the approximation error and the convergence rate of the numerical methods used. A certain problem is the import of the geometry of the boundaries of the computational domain $\Omega$, the verification of the correctness of the computational grid $\Omega_h$, the problem of its visualization and quality assessment [1-3]. Such technique can be applied for experimental and theoretical investigations of laser-plasma interactions, including magneto-inertial fusion [4-7].

In principle, several methods for obtaining a hexagonal irregular computational grid can be considered, for example:
1. Method based on the rebuilding (to hexagonal) of simplicial finite elements — triangles in the two-dimensional case and tetrahedrons in the three-dimensional (Figure 1);  
2. The use of hybrid unstructured block-tetrahedral computational grids. To do this, as the initial approximation, a uniform partition of the region into rectangular cells of size $D_s$ is used, and the boundary of the computational domain $\Omega$ is represented as a piecewise-smooth contour $\partial\Omega$ consisting of curved segments approximated by Bezier curves.

It should be noted here that the quality of the initial grid directly affects the quality of the resulting computational grid $\Omega_h$, and in some cases even the very possibility of constructing it. Therefore, it is necessary to check the initial mesh for self-intersections, remove “double” nodes, determine a list of faces for grinding (faces on narrow sections of the mesh, faces of a large area, etc.) and fragmentation of such faces into quadrangles, transition to flat faces.

In the first case, the construction of an irregular hexagonal grid takes place in several stages: construction of a geometric model, allocation of boundary nodes (or triangulation of the surface bounding the computational domain $\Omega$), initialization of the tetrahedral bulk computational grid and its transformation into the hexahedral, and subsequent correction (“Regularization”) of the hexahedral network. In order to rebuild the grid, additional nodes are introduced into the "center of mass" of each face and into the tetrahedral finite element itself. The connection diagram of these nodes, leading to the construction of a hexahedral finite element, is shown in Figure 1.

However, with this method of rebuilding the computational grid, an additional stage of its optimization (improvement - “regularization”) with an assessment of its quality is required. For this reason, the stage of improving the grid using an elliptical generator was introduced into the grid construction process.

![Figure 1. Transition in a computational grid from tetrahedral computational cells to hexahedral calculated cells.](image)

2. Problem statement and mathematical model
It is important to note here that the proposed approach to the “regularization” of the hexagonal computational grid $\Omega_h$ allows, in the case of modeling on an unstructured grid, gas or plasma flows taking into account the motion of hard boundaries $\partial\Omega$ (this boundary can be represented as a piecewise-smooth contour or surfaces, approximated respectively by Bezier curves or NURBS
surfaces) of the calculated volume \( \Omega \) or flows with free boundaries, adjust the computational grid \( \Omega_h \) to the position of the boundaries that change over time. Obviously, this method of mesh deformation is based on the use of the existing (before deformation) connectivity of nodes of the computational mesh \( \Omega_h \). At the same time, the main difficulty in implementing computational algorithms on moving unstructured grids is to maintain the quality of the deformed mesh within the computational domain \( \Omega \) (in particular, it is necessary to ensure the positive volumes of the finite elements of the deformed mesh).

In this paper, a variant of the elliptic “regularizer” of the grid is based on a “mechanical analogy” and is based on solving linear equations of the theory of elasticity, which describe the deformation of an unbounded elastic medium with a force \( F \) applied to a small area (W. Thomson problem) \([8]\).

\[
\Delta \bar{u} + \frac{1}{1-2\sigma} \nabla \left( \text{div} \bar{u} \right) = -\frac{2(1+\sigma)}{E} F \delta(\bar{r}),
\]

where \( \delta(\bar{r}) = \delta(x)\delta(y)\delta(z) \), and the origin of the coordinate system is chosen at the point of application of force \( F \), \( \bar{u} = \bar{r}^* - \bar{r} \) is the strain vector (or displacement vector), \( \bar{r}^*, \bar{r} \) are the radii of the nodes of the computational grid \( \Omega_h \) after and before its deformation, \( \sigma \) is the Poisson's ratio, \( E = 2(1+\sigma)\mu \) is the tensile modulus (Young's modulus), \( \mu \) is the shear modulus (can be put \( \mu \approx 1 \)).

Note that the Poisson's ratio, which characterizes the ratio of lateral to longitudinal deformation, in the physical region of the change of parameters for various substances can only vary from -1 to 1/2. Thus, the physical domain (recall that here the equations of the theory of elasticity are applied to solve the problem that does not have physical meaning: “regularization” of the hexagonal computational grid \( \Omega_h \)) of changes in the Poisson's ratio is located \(-1 \leq \sigma \leq 1/2\). Poisson's ratio significantly affects the shape of the computational grid \( \Omega_h \). A larger value of the coefficient leads to deformations similar to the deformation of rubber (\( \sigma \approx 0.9 \)) and, therefore, the Poisson's ratio for these purposes can take a range of values \( \sigma \in [1/2, \infty) \). The equations of elasticity theory at \( \sigma \to \infty \) will take on a simpler form:

\[
\Delta \bar{u} = -F \delta(\bar{r}).
\]

An analytical solution to this problem is given in \([8]\) and is determined by the expression:

\[
\bar{u} = \Phi \left\| \bar{r} \right\|, \Phi = \frac{(1+\sigma)}{8\pi E(1-\sigma)} \left( 3 - 4\sigma \right) \bar{F} + \bar{n} \left( \bar{n} \bar{F} \right),
\]

where \( \bar{n} \) is the unit vector directed along the radius vector \( \bar{r} \), \( \left( \bar{n} \bar{F} \right) \) is the scalar product of the unit vector \( \bar{n} \) and the force \( \bar{F} \).

Further, to simplify the description, additional notations are introduced: the edge connecting the nodes \( i \) and \( j \), denote by \( (i, j) \), and the face of the computational grid \( \Omega_h \) formed by the nodes \( i, j \) and \( k \) denote by \( (i, j, k) \).

The relation \( \bar{u} = \Phi / \left\| \bar{r} \right\| \) allows (if the value of the force \( \bar{F}_i \) in the node \( i \) is known) to determine the displacement vector \( \bar{u}_j \) at all nodes \( j \) connected to the node \( i \) through edges \( (i, j) \) or the offset \( \bar{u}_i \) in the node \( i \). Those, find the displacement \( \bar{u} \) from the action of the forces \( \bar{F}_j \) the application point (nodes \( j \)) of which is located on the surface \( S_i \) located from the node \( i \) at a distance of the length of the
rib $|\vec{r}|_{ij}$ associated with the node $i$. Hence the following expression is derived: 
$$\langle \vec{u} \rangle = \sum_{j=1}^N \frac{\Phi_j}{|\vec{r}|_{ij}} \approx \int \frac{\Phi}{|\vec{r}|} ds .$$
Then the approximate offset $\vec{u}_i$ value can be determined as follows: 
$$\vec{u}_i = \sum_{j=1}^N \frac{\Phi_j}{|\vec{r}|_{ij}} \approx \int \frac{\Phi}{|\vec{r}|} ds \langle 1/|\vec{r}| \rangle ,$$
where $\langle 1/|\vec{r}| \rangle = \int \frac{1}{|\vec{r}|} ds$, $N_i$ is the number of edges associated with the node $i$. This method of finding
the displacement values $\vec{u}_i$ is a rationalized version of the multidimensional interpolation method
known as the Shepard method [9] (IDW Inverse Distance Weighted), in which the values of the
function at arbitrary points are the sum of the weighted values of the function at the starting points.

The approach used in the work is universal from the point of view of the form (type) of forces used
in the method $\vec{F}$. For example, to determine the forces $\vec{F}$ acting on the nodes of the computational grid $\Omega_h$, you can use the work [10]. In this case, the main idea of the method is based on the "electrostatic analogy"
and consists in the fact that the nodes of the future grid are the same charged particles, with charges $q_i$ having mass $m_i$. Charged particles interact with each other. The interaction forces are of an
electrical nature and repulsive force $F_{ij}$ acting on the $i$th particle (node $i$) from the $j$th particle (node $i$
proportional to the distance between charges. The resultant of the forces of interparticle interaction can
be represented as: 
$$\vec{F}_i = \sum_{j=1}^N \vec{F}_{ij} , \quad \vec{F}_{ij} = -C \frac{q_i q_j}{|\vec{r}_{ij}|^2} \frac{\vec{r}_{ij}}{|\vec{r}_{ij}|} , \quad k \geq 1 , \quad |\vec{r}_{ij}| = \ell ,$$
where $\ell$ is the radius vector length or distance between charges; $C$ is the constant normalization. For the proposed method, it is
important that, in addition to the Coulomb interaction force $\vec{F}_i$, resistance forces $\vec{F}_{r,i}$ act on the
particles, which are determined by their speed and have a direction opposite to the velocity vector:
$$\vec{F}_{r,i} = -K \frac{|\vec{v}_i|^m}{|\vec{v}_i|} \vec{v}_i , \ m \geq 2 .$$

In addition, one can also use the results of [11]. In this paper, a method for generating a tetrahedral
computational grid, in which grid nodes are considered as interacting atomic particles ("molecular dynamics analogy") is proposed. This approach to grid generation begins with determining the
function of the potential energy of the system $\phi$. Usually the most important part of the potential is
the pair potential. $\phi\left(|\vec{r}|_{ij}\right)$, which depends only on the distance between the two particles $|\vec{r}|_{ij}$. Given
only the pair potential, the potential energy of the system can be represented as: 
$$\phi = \sum_{i} \sum_{j \neq i} \phi\left(|\vec{r}|_{ij}\right) ,$$
where $\phi\left(|\vec{r}|_{ij}\right)$ is the pair potential, which can be written through the Lennard-Jones potential
$$\phi\left(|\vec{r}|_{ij}\right) = 4\epsilon \left[ \left( \frac{\sigma}{|\vec{r}|_{ij}} \right)^{12} - \left( \frac{\sigma}{|\vec{r}|_{ij}} \right)^{6} \right]$$ (Figure 2), where $\sigma , \epsilon$ are the selected parameters during
the "regularization" of the grid. Then the paired force \( \vec{F} \) resulting from the Lennard-Jones potential will have the form:

\[
\vec{F}_{ij} = -\nabla \phi \left( \frac{r_{ij}}{\sigma} \right) = -24 \varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} \left( \frac{\sigma}{r_{ij}} \right)^{6} \frac{\vec{r}_{ij}}{r_{ij}}.
\]

\[\text{Figure 2. Schematic representation of the Lennard-Jones potential.}\]

In this paper, to determine the forces \( \vec{F} \) acting on the nodes of the computational grid \( \Omega_h \), a "mechanical analogy" is used. In this case, the tensile or compressive force acting on the rib \((i, j)\) is represented as the "Hook force":

\[
\vec{F}_{i} = -\frac{\alpha \left( \ell_i - h_i \right) \vec{r}_{ij}}{\max(\ell_i, h_i) |\vec{r}_{ij}|}, \quad h_i = (V_i)^{1/3}, \quad V_i \text{ is the local volume of the hexagonal finite element attributed to the node } i, \quad \alpha \sim S_i. \]

And to take into account the "torsion" of the edges of the hexagonal finite element relative to the node, additional forces are introduced, attached to each node of the computational grid and taking into account the possible "torsion" of the edges of the finite element. These forces can be written as follows:

\[
\vec{F}_{i} = -\frac{\beta \left( \ell_j - L_i \right) \vec{r}_{ij}}{\max(\ell_j, L_i) |\vec{r}_{ij}|},
\]

where \( L_i = (\ell_{in} + \ell_{im}) \cos(\pi/4) \), \( \ell_j = |\vec{r}_{ij}| \), \( \beta = S_i \), where \( \ell_{in}, \ell_{im} \) are the lengths of the ribs \((i, n)\) and \((i, m)\), starting from the node \(i\) and located on the verge \((i, n, j, m)\) of the hexahedral finite element, \( \ell_j = |\vec{r}_{ij}| \) is the distance between opposite nodes \(i\) and \(j\) lying on the verge \((i, n, j, m)\).

The adaptation of the computational grid to the physical features of the problem under consideration is taken into account by introducing additional control functions into the Hooke force \( P^i \). So, for example, to adapt the computational grid \( \Omega_h \) in the vicinity of the node \(i\), the force \( \vec{F}_i \) can be written in the following form [12-13]:
\[ \bar{F}_i = \alpha \bar{P}_j \frac{\bar{r}_j - \bar{r}_i}{|\bar{r}_j - \bar{r}_i|}, \quad p^i = b \cdot \text{sign}(\bar{r} - \bar{r}_i) \exp[-d|\bar{r} - \bar{r}_i|], \quad \alpha - S_i, \quad b > 0, \quad d > 0. \]

In this formula, the constant \( b > 0 \) controls the intensity of the thickening, and \( d > 0 \) the size of the thickening area. In the case when the constant \( b < 0 \) is negative, the grid is rarefied near the node \( i \).

Since each arbitrary curve \( L \) or surface \( S \) forms a set of points in space \( \mathbb{R}^3 \) (\( L \subset \mathbb{R}^3 \) or \( S \subset \mathbb{R}^3 \)), applying this formula to this set of points (\( L \) or \( S \)) allows you to adapt the computational grid to the corresponding curve \( L \) or surface \( S \).

In Table, for reference, some criteria for assessing the quality of a computational grid \( \Omega_h \) consisting of tetrahedral elements are given.

| Criterion | Formula | Range of possible values | Optimal value |
|-----------|---------|--------------------------|---------------|
| The ratio of the radius of the described sphere to the inscribed radius | \( \beta = \frac{R_s}{R_i} \) | \([1, +\infty)\) | 3.0 |
| The ratio of the length of the largest edge to the radius of the inscribed sphere | \( \sigma = \frac{L_{\text{max}}}{R_i} \) | \([1, +\infty)\) | 4.898979... |
| The ratio of the radius of the described sphere to the length of the largest rib | \( \omega = \frac{R_s}{L_{\text{max}}} \) | \(\left[ \frac{1}{2}, +\infty \right)\) | 0.612375... |
| The ratio of the cube of the arithmetic mean length of the edges to the volume of the tetrahedron | \( \alpha = \frac{L}{V} \) | \([1, +\infty)\) | 8.4852816... |
| Minimum solid angle | \( \theta \) | \((0, \pi/2)\) | \(\pi/2\) |
| The ratio of the volume of the tetrahedron to the largest of the products of the lengths of the triple edges coming from one vertex | \( \eta = \frac{V}{\max_i \prod_{j=1}^{4} l_{ij}} \) | \((0, \sqrt{2}/12)\) | \(\sqrt{2}/12\) |

3. The Numerical Analysis

The paper considers the result of the “regularization” of the grid consisting of hexahedral finite elements. Therefore, in order to assess the quality of the computational grid \( \Omega_h \), the following criterion was used: "the ratio of the arithmetic mean of the angles between the edges containing the node under consideration, to the angle \( \pi/2 \)." This value varies within the interval \([0, 1]\) so that the closer it is to 1, the closer the quality of the final element to the ideal.

The approach, based on the “mechanical analogy” of tension and torsion, has good performance indicators, including on three-dimensional grids. In this case, gesahedral cells with a close aspect ratio are obtained. Figures 3-4 show the results of numerical construction on the surface and in volume for a geometric model of a hypersonic aircraft (HA) [14-16] tetrahedral grid (Figure 3) and its conversion to a hexahedral computational grid (Figure 4).
Figure 3. Tetrahedral surface mesh of HA geometric model.

Figure 4. Hexagonal rebuilt surface mesh geometric patterns.

Figure 5 shows the hexagonal “regularized” computational grid, as well as the distribution of the “angular” criterion (Figure 6) for assessing its quality for the geometric model of HA.
Figure 5. Hexagonal “regularized” computational grid of a HA geometric model.

From the calculation results shown in Figures 5 and 6 it follows that the "regularized" grid $\Omega_h$ fills almost the entire volume of the computational domain $\Omega$, and the criterion for assessing the quality of the hexagonal "regularized" computational grid is more than 0.7. Moreover, to achieve this result, ~20 iterations were required only.

Figure 6. Distribution of the “angular” criterion for assessing the quality of hexagonal “Regularized” computational grid of a HA geometric model.

4. Conclusion
A new mathematical model of the dynamics of processes in those parts of a three-dimensional target where the laser radiation power density is most intense or relatively low. This paper has described getting and regularizing a hexagonal irregular grid. A tetrahedral computational grid is generated, in which grid nodes are considered as interacting atomic particles (“molecular dynamics analogy”). A new method of transition from a tetrahedral to a hexagonal irregular computational grid is indicated in the paper, a method of its “regularization” is developed. This method of “re-regularization” is based on “mechanical analogy” and is based on solving linear equations of the theory of elasticity. The initial results of the reconstruction and “regularization” of the computational grid, as well as the distribution of the “corner” criterion for assessing its quality are presented.

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