Application of 3D basic operators method extension to astrophysical problems

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Abstract. Basic (support) operators method (Samarskii’s method, operator-difference method) has proven itself well in 2D numerical simulations of the astrophysical problems. An idea of the operator approach consists of the inclusion of boundary conditions in a finite difference form into the grid analogue of solving problem and formulation of the finite difference problem as an operator equation. The finite difference operators are constructed in the way to fulfill corresponding relations between continuous operators (for instance, div(rot)=0, div is conjugated to -grad; -div(grad) is self-conjugated etc.). The approach allows obtaining completely conservative finite difference schemes. The matrix which corresponds to the self-conjugated operator is symmetrical and can be inversed efficiently by modern iteration methods. In the paper a 3D generalization of 2D grid analogues for continuous differential operators using a cell-node approximation on triangular grid was realized for tetrahedral mesh. For testing we calculated a 3D Newtonian gravitational potential, and a stationary heat transfer equation in spherical layer with the first type boundary condition on the inner surface and the third type boundary condition on the outer one was calculated. The method was applied to simulation of anisotropic heat transfer in magnetized neutron star crust.

1. Introduction
Numerical simulations of physical problems become more and more important nowadays. The operator approach in numerical methods [1] was proposed by Soviet and Russian mathematician Alexander Andreyevich Samarskii. His idea consists of the inclusion of boundary conditions into a finite-difference form and formulation a finite-difference problem as an operator equation. It allows to study operators properties and use corresponding efficient methods for the solution of the numerical problem. The idea of the basic (support) operator method consists of the grid analogue construction of one of the continuous operator (e.g. div), which approximates corresponding continuous operator. The grid analogue of the relative conjugate operator (e.g. -grad) is constructed using a corresponding integral relation. In this way operator-difference equations will have the same properties as the differential problem. For example, self-conjugated continuous operator remains symmetrical in the grid form, and sparse and symmetrical matrix corresponds to it. Also basic operators method allows to obtain completely conservative finite-difference schemes. After obtaining the grid formulation of the solving problem, the sparse and symmetrical matrixes can be inversed efficiently by modern iterative or direct methods. Two dimensional operator-difference completely conservative Lagrangian method for
the magnetohydrodynamical equations was built by Ardeljan et al. in the series of papers [2, 3, 4, 5] for triangular grid of a variable structure. The method was successfully applied for the different astrophysical problems [6, 7, 8]. The mesh remapping procedure was developed in [2], the criteria for a mesh rarefaction and contraction were suggested in [8]. In astrophysical simulations we often have huge gradients or many orders variations of physical values and the mesh remapping procedure allows to refine the mesh in regions with strongly changing parameters and rarefy the grid in the regions with smooth flow. In this paper the 3D grid analogues for the differential operators in Cartesian coordinates were described. Following the operator formalism from [2, 3, 4, 5], the 3D grid analogues of basic differential operators were suggested and the operator formulations of some boundary problems were written.

2. Grid analogue of the gradient operator (nodes to cells)

We use the grid which consists of the tetrahedra. So-called cell-node approximation is used: node grid functions are defined in the grid nodes, and cell grid functions are defined to be constant in the grid cells and the boundary nodes. Following [2, 3, 4], let's introduce linear spaces of cell grid functions, node functions and boundary node functions. This formal approach allows to study the approximation and stability of the numerical schemes using efficient modern methods.

First we introduce the grid gradient operator, which converts the scalar node function into the cell vector function. For definition of the grid analogue of the differential gradient we have used the following invariant definition of the $\nabla$ operator:

$$\nabla p = \lim_{V \to 0} \frac{1}{V} \int_S p \cdot dS.$$  \hspace{1cm} (1)

Let $p$ is a scalar node grid function. Inside each cell we additionally define it as a linear interpolation of node values of the cell's nodes. After integration of this linear interpolation, taking into account mean value theorem, we get the definition of operator $\nabla$ grid analogue of:

$$\nabla \Delta p)_i = \frac{1}{V_i} \sum_{k=1}^{4} (\bar{p}_k S_k \vec{n}_k)_i.$$  \hspace{1cm} (2)

Here $\bar{p}_k = \frac{(p_1+p_2+p_3)}{3}$ - is an average interpolated value of $p$ in the $k$-th tetrahedron face, indexes 1,2 and 3 correspond to $p$ node values on the $k$-th face; $\vec{n}_k$ is a unit external normal to the $k$-th face, $S_k$ is a square of the $k$-th face and $V_i$ is a volume of the cell with the index $i$. Expression (2) is the first order approximation for the differential operator $\nabla$. The grid analogues of other (nodes to cells) operators (such as $\text{div}$(vector), $\text{grad}$(vector), $\text{rot}$(vector) etc.) can be derived in a similar way.

3. Grid analogue of the divergence operator (cells to nodes)

Let us introduce the scalar product in the linear grid spaces $(p,g)_{\alpha} = \sum_s U_s p_s g_s$, $\alpha$ corresponds to node and cell spaces. For the cells $U_s = V_i$, for nodes $U_s = W_j$, here $W_j = \frac{1}{4} \sum_{k=1}^{K_j} V_k$ is a "node volume" (see [2] and references in it).

The grid analogue for divergence operator is constructed to be conjugated to the $-\nabla$ grid operator from (2). The Green formula and its grid analogue was used (for the case when all functions vanish on the domain boundary or the domain is infinite):

$$\int p \nabla \cdot \vec{v} dV + \int \vec{v} \cdot \nabla pdV = 0$$  \hspace{1cm} (3)
\[ (\vec{v}, \nabla \Delta p) + (\nabla \cdot \vec{v}, p) = 0; \quad \sum_{l=1}^{N_l} \nabla \times \cdot \vec{v}_l p_l W_l = - \sum_{k=1}^{K_j} \vec{v}_k \nabla \Delta p_k V_k. \]  

(4)

Grid analogue of the Green formula (4) is written in terms of a scalar product in grid spaces. After substitution the $\nabla \Delta$ from (2) and rearrangement of terms for the $j$-th node the expression for the grid operator $\text{div}$ can be written in the form:

\[ (\nabla \times \cdot \vec{v})_j = - \frac{1}{3W_j} \sum_{k=1}^{K_j} \tilde{v}_k \cdot (\vec{n}_1 S_1 + \vec{n}_2 S_2 + \vec{n}_3 S_3)_k, \]

(5)

here $K_j$ is a number of adjacent cells for $j$ node, $\tilde{v}_k$ - value of the cell function $\vec{v}$ in the $k$-th cell. Indexes 1, 2 and 3 correspond only to those cell faces that contain the $j$-th node. Summation is done over all cells adjacent to the $j$-th node.

4. Boundary grid operators

For the numerical simulation of boundary value problems we need to formulate grid analogues for the different boundary conditions. Following [2], a boundary operator $\Phi$ is introduced on the tetrahedral grid. The $\Phi$ operator acts on elements from boundary nodes space and results into boundary nodes space. It is constructed in the way to fulfill the Green grid analogue formula including boundary:

\[ (p, \nabla \cdot \vec{v}) + (\nabla p, \vec{v}) = \oint p \vec{v} d\vec{S}; \quad \sum_{l=1}^{N_l} \nabla \times \cdot \vec{v}_l p_l W_l + \sum_{k=1}^{K_j} p_k \nabla \Delta \cdot \vec{v}_k V_k = \sum_{q=1}^{K_\gamma} \Phi \cdot \vec{v}_q p_q W_q, \]

(6)

here $K_\gamma$ is a number of nodes neighboring to the boundary node $\gamma$, $W_q$ - is a "volume" of the boundary node [2].

The boundary operator $\Phi$ can be introduced in 3 ways. The first one is a simple numerical integration by the cell surfaces near the corresponding boundary node

\[ (\Phi \cdot \vec{v})_\gamma = \frac{\tilde{v}_\gamma}{3W_\gamma} \cdot \sum_{q=1}^{K_\gamma} \vec{n}_q S_q. \]

(7)

The second way is the integration with taking into account linear interpolation of boundary function

\[ (\Phi \cdot \vec{v})_\gamma = \frac{1}{9W_\gamma} \sum_{q=1}^{K_\gamma} (\vec{v}_1 + \vec{v}_2 + \vec{v}_\gamma)_q \cdot \vec{n}_q S_q. \]

(8)

In (8) $\vec{v}_1$ and $\vec{v}_2$ are the values of function $\vec{v}$ in the boundary nodes of the $q$-th boundary cell face, adjacent to the node $\gamma$.

To obtain the third formula, fictitious cells introduced outside the computational domain were used, following [5].

Finally we get the expression for the boundary operator $\Phi$:

\[ (\Phi \cdot \vec{v})_\gamma = \frac{1}{12W_\gamma} \left( \sum_{q=1}^{K_\gamma} (\vec{v}_1 + \vec{v}_2 + \vec{v}_\gamma)_q \cdot \vec{n}_q S_q + \vec{v}_\gamma \cdot \sum_{q=1}^{K_\gamma} \vec{n}_q S_q \right). \]

(9)

Grid approximation of the $\text{div}$ operator including the boundary can be written in the form $(\nabla \cdot \vec{v})_\gamma = \nabla \times \vec{v} + \Phi \cdot \vec{v} + O(h)$, $h$ is a characteristic cell size. 3D boundary operators for other grid analogues of cell to node operators can be constructed in a similar way.
5. Test calculations
To test the described operators we solved several 3D problems numerically. The first one is a Dirichlet problem for Poisson equation. The physical interpretation of the solution is a Newtonian gravitational potential generated by the spatial distribution of the matter. Differential formulation is (gravitational constant $G = 1$)

$$\begin{cases}
\Delta \Psi = 4\pi \rho, \\
\Psi |_{\Gamma} = \Psi_{\gamma}.
\end{cases} \tag{10}$$

We consider $\rho = \frac{z}{4\pi \sqrt{x^2 + y^2 + z^2}}$ further.

The general solution of the (10) is given by the volume potentials formula

$$\Psi(\vec{r}) = -\int\int\int_V \frac{d\vec{r}^* \rho(\vec{r}^*)}{|\vec{r}^* - \vec{r}|}. \tag{11}$$

For the numerical solution of the problem (10) we need to know the boundary values of the gravitational potential. The approximation of the formula (11) on the tetrahedral grid gives the expression for the calculation of the boundary values $\Psi_{\gamma}$.

$$\Psi_{\gamma}(\vec{r}_{q}) = -\sum_{k=1}^{K_j} V_k \rho(\vec{r}_{\Delta}) \frac{|\vec{r}_{\Delta} - \vec{r}_q|}{|\vec{r}_{\Delta} - \vec{r}_q|}. \tag{12}$$

where $\vec{r}_{\Delta}$ is an average cell value of $\vec{r}$, $K_j$ is a total number of grid nodes.

Similarly to the approach developed in [2] we include the grid boundary conditions into the grid operator form of the problem. We write the Poisson equation in the boundary knots: $\delta \nabla \cdot \nabla \triangle \Psi_{\gamma} = 4\pi \rho$, and distinguish the boundary in that equation: $\nabla \cdot \nabla \delta \Psi = 4\pi \rho$. Further, we subtract one from another and get:

$$(I - \delta) \nabla \cdot \nabla \triangle (I - \delta) \Psi = 4\pi (I - \delta) \rho - (I - \delta) \nabla \cdot \nabla \triangle \Psi_{\gamma} \tag{13}$$

operator $\delta$ works as follows: it equals to 0 in the internal nodes and 1 on the boundary, $I$ is a unit operator.

It can be seen that grid formulation of the problem gives us one operator equation which includes the boundary condition. $(I - \delta) \nabla \cdot \nabla \triangle (I - \delta)$ is a grid Laplace operator, which is self conjugate as a continuous Laplace operator.

The solution of the operator-difference equation (13) and analytical gravitational potential are represented on the fig. 1. The maximal relative numerical error on the 3D grid of 2000 knots was $\leq 5\%$.

The second test problem is stationary heat transfer equation in the spherical layer with the Dirichlet boundary condition on the inner bound and the 3rd type boundary condition on the outer bound. In the general form the problem can be written as:

$$\begin{cases}
\nabla \cdot A(T, \vec{r}) \nabla T = f(\vec{r}), \\
T |_{inn} = T_0, \\
(\vec{n}, A(T, \vec{r}) \nabla T) + g(T, \vec{r}) |_{out} = 0.
\end{cases} \tag{14}$$

here $A(T, \vec{r})$ is a thermal conductivity, it can be scalar or tensor function, $g(T, \vec{r})$ in the boundary condition corresponds to physical processes on the boundary surface (convection, radiation, etc.).
We represent the problem (14) as one grid equation including boundary conditions following the approach from [2].

\[(I - \delta_1) \nabla \times A(P_\Delta T) \nabla \triangle (I - \delta_1) T + (I - \delta_1) \nabla \times A(P_\Delta T) \nabla \triangle T_0 - \delta_2 \Phi \cdot \vec{n} g(T) = (I - \delta_1) f. \quad (15)\]

\(P_\Delta T\) is an interpolation of the node function \(T\) into the cells (heat fluxes are defined in the cells and boundary nodes), indexes 1 and 2 in the \(\delta\) operators correspond to inner and outer boundary respectively.

6. Heat transfer simulation in neutron star crust

Neutron star (NS) is a final stage of stellar evolution of massive stars with masses more than \(\sim 8 M_\odot\) and less than \(25 - 30 M_\odot\) (upper limit depends on particular theoretical model; \(M_\odot\) is a solar mass). It is a product of core-collapse supernova explosion, bright and high-energy astrophysical phenomenon. NS is a very compact object with linear sizes approximately 10-20 kilometres. The density in the central parts of the NS can reach \(10^{14-15} g/cm^3\), the magnetic fields are \(\sim 10^{12} G\) on the NS surface. The aim of this work is to calculate the temperature distribution on the surface of the neutron star by the solution of the heat transfer equation for crust in the presence of the strong magnetic field. The anisotropy of the temperature distribution is connected with the dependence of nonlinear thermal conductivity tensor function on the magnetic field configuration.

The problem was simulated in 2D (axial symmetry) in [9, 10].

Thermal conductivity tensor was derived in the paper of Bisnovatyi-Kogan and Glushikhina [11] for the plasma with arbitrary degenerate electrons and nondegenerate ions in the presence of magnetic field. It was obtained with the Chapman-Enskog method from the Boltzmann equation. The thermal conductivity tensor takes into account heat fluxes along and across the magnetic field and the Hall effect. It is written for the strongly degenerate electrons as follows

\[
\begin{align*}
A_{ij} &= \frac{k^2 T n_e}{m_e} \tau_d \left( \lambda^{(1)} \delta_{ij} + \lambda^{(2)} \epsilon_{ijk} \frac{B_k}{B^2} + \lambda^{(3)} \frac{B_i B_j}{B^2} \right), \\
\lambda^{(1)} &= \frac{5 n_e^2}{6} \left( \frac{1}{1 + \omega \tau_d} - \frac{6}{5} \left( \frac{\omega \tau_d}{1 + \omega \tau_d} \right)^2 \right), \\
\lambda^{(2)} &= -\omega \tau_d \frac{4 \pi n_e}{6} \left( \frac{1}{1 + \omega \tau_d} - \frac{3}{4} \left( \frac{\omega \tau_d}{1 + \omega \tau_d} \right)^2 \right), \\
\lambda^{(3)} &= \left( \omega \tau_d \right)^2 \frac{5 n_e^2}{6} \left( \frac{1}{1 + \omega \tau_d} - \frac{6}{5} \left( \frac{1}{1 + \omega \tau_d} \right)^2 \right),
\end{align*}
\]

(16)

where \(k\) is a Boltzmann constant, \(n_e\) is a concentration of electrons, \(m_e\) is an electron mass, \(\omega\) is a cyclotron frequency, \(\tau_d\) is an average time between electron-ion collisions in the absence of
Figure 2. Temperature distribution in the neutron star crust (in units $10^5 K$), $r_{inn} = 4 km, r_{out} = 10 km$

magnetic field. $\omega r_d$ is a magnetization parameter, which corresponds to the dependence of a spatial temperature anisotropy on the magnetic field.

On the inner boundary of the crust in our simulations we assume constant temperature $T_0$, on the outer boundary we assume radiation with the Stephan-Boltzmann law, $g(T, \vec{r}) = \sigma T^4$ in (14). Also we assume the absence of heat sources in the interior of the crust ($f = 0$).

After the approximation of the continuous problem (14) using the developed 3D operators and the inclusion of the boundary conditions into the operator equation we get nonlinear set of algebraic equations which is solved using the Newton method.

On the fig. 2 some preliminary numerical results for octant are shown for the constant magnetic field, $B_z = 5 \cdot 10^{11} G, n_e = 10^{29} \div 10^{31} cm^{-3}$. The temperature distribution on the outer crust surface is anisotropic: at the magnetic pole it is hotter ($T = 6.5 \cdot 10^4 K$), than at the equator ($T = 3.5 \cdot 10^4 K$).

We plan to simulate this problem in the full 3D formulation with various magnetic field configurations and more realistic physical parameters. Results will be published elsewhere.

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References

[1] Samarskii A A 1989 *Finite difference schemes theory* Moscow: Nauka
[2] Ardeljan N V and Kosmachevskii K V 1995 *Comput. Math. Modelling* 6 209
[3] Ardeljan N V and Kosmachevskii K V 1987 *Problems of Construction and Research of Conservative Difference Schemes for Magneto-gas-dynamics* MSU, Moscow
[4] Ardelyan N V and Gushin I S 1982 *Vestnik MSU* 15, 3 3
[5] Ardelyan N V 1983 *Comp. Math. Math. Phys.* 23 1168
[6] Ardeljan N V, Bisnovatyi-Kogan G S and Moiseenko S G 2000 *Astron. Arstophys.* 355 1181
[7] Ardeljan N V, Bisnovatyi-Kogan G S and Moiseenko S G 2005 *Mon. Not. R. Astron. Soc.* 359 333
[8] Ardeljan N V, Bisnovatyi-Kogan G S, Kosmachevskii K V and Moiseenko S G 1996 *Astronomy and Astrophysics Supplement* 115 573
[9] Geppert U, Kuker D and Page D 2004 *Astron. Astrophys.* 426 267
[10] Perez-Azorin J F, Miralles J A and Pons J A 2006 *Astron. Astrophys.* 451 1009
[11] Bisnovatyi-Kogan G S and Glushikhina M V 2018 *Plasma Physics Reports* 44 4 355