An iterative method for solving difference problems of gas dynamics in the mixed Euler-Lagrangian variables

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Abstract. The method proposed is intended to solve implicit conservative operator difference schemes for a grid initial-boundary value problems on a simplex grid for a system of equations of gas dynamics in the mixed Euler-Lagrangian variables. To find a solution to such a scheme at a time step, it is represented as a single equation for a nonlinear function of two arguments from space – the direct product of the grid spaces of gas-dynamic quantities. To solve such an equation, a combination of the generalized Gauss-Seidel iterative method (external iterations) and an implicit two-layer iteration scheme (internal iterations at each external iteration) is used. The feature of the method is that, the equation, which is solved by internal iterations, is obtained from the equation of the difference scheme using symmetrization – such a non-degenerate linear transformation that the function in this equation has a self-adjoint positive Frechet derivative.

1. Introduction
In accordance with the operator approach of the theory of difference schemes [1], in order to find a solution to the initial-boundary value problem of gas dynamics on a certain time interval, it is necessary to split this time interval to time steps, and at each time step to find a solution to the difference scheme that would approximate the original problem at the time instant corresponding to this step. This difference scheme is, in the general case, a nonlinear operator equation for an argument from a direct product of the Euclidean spaces, in which the gas-dynamic quantities are determined:

\[ F(\bar{y}) = 0. \]  (1)

This representation makes it possible to study the properties of the difference scheme and to find its solution using the general theory of operator equations.

This paper describes an iterative method for solving equation (1), which corresponds to an implicit difference scheme constructed by the method of consistent operators for the gas dynamics problem in the mixed Euler-Lagrangian variables. Due to the fact that the scheme is constructed in accordance with the operator approach, sufficient conditions for the solvability of the grid problem at a time step and a constructive description of finding its solution can be formulated in terms of the general theory of iterative methods [2],[3].

The method of consistent operators for constructing difference schemes was developed and proved to be effective in solving the gas dynamics problems and the MHD problems in the
boundary \partial \Omega \subset \Omega:

\begin{cases}
\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{v} + \mathbf{w} \cdot \nabla \rho = 0; \quad \mathbf{w} = \mathbf{v} - \mathbf{u}, \\
\rho \frac{D\mathbf{v}}{Dt} + \mathbf{E}_\nu \mathbf{v} + \nabla \mathbf{p} = 0; \quad \mathbf{E}_\nu \mathbf{v} = -\nabla \nu \nabla \cdot \mathbf{v}, \\
\rho \frac{DT}{Dt} + E_\theta T + \beta \nabla \cdot \mathbf{v} = 0; \quad E_\theta T = -\nabla \cdot c_v^{-1} \theta \nabla T, \\
\beta = c_v^{-1} g, \quad g = p - \nu \nabla \cdot \mathbf{v}, \quad p = R\rho T.
\end{cases}

(2)

Here \mathbf{u} is the speed of a moving coordinate system relative to the reference (stationary) coordinate system (assume that this speed is known at any moment of time), \(D/ Dt\) – the full time derivative, \(c_v \equiv \text{const}\) – the specific heat, \(\nabla\) – the invariant differential operator ”nabla”, the square brackets denote the terms that remain in the equations in the Lagrangian variables.

Assume that the following boundary conditions are specified on \(\partial \Omega\):

\begin{align*}
\partial \Omega_\gamma &= \partial \Omega_0 + \partial \Omega_{v1} + \partial \Omega_{v2}; \quad \delta_0 \rho = y_0, \quad \delta_1 \rho = y_2; \quad (\mathbf{n} \cdot \mathbf{v})|_{\partial \Omega_{v2}} = y_2, \\
\partial \Omega_\gamma &= \partial \Omega_0 + \partial \Omega_{v1}; \quad \delta_0 T = y_0; \quad (\mathbf{n} \cdot c_v^{-1} \theta \nabla T)|_{\partial \Omega_{v1}} = y_1.
\end{align*}

(3)

The operator difference scheme is constructed using analogs of the differential operators that act in the Euclidean spaces of functions defined on a grid that approximates the computational domain \(\bar{\Omega} = \Omega \cup \partial \Omega\). In the method of consistent operators, the simplex grids are used and the grid operators and scalar product formulas are determined from the grid analogue of the integral formula

\[
\int_\Omega \left( \frac{\partial f}{\partial x_\alpha} \right) \eta \, dV = - \int_\Omega f \left( \frac{\partial \eta}{\partial x_\alpha} \right) \, dV + \int_{\partial \Omega} (f \eta) \nu_\alpha \, ds \quad \forall f, \eta \in C^1 (\bar{\Omega}).
\]

(4)

Here \(dV\) is the volume element, \(\nu_\alpha\) – the direction cosine for the coordinate \(x_\alpha\). The specific form of this analogue depends on the grid elements in which the grid functions are defined. These can be barycenters and cell vertices [8], only vertices [9], vertices and barycenters of cell faces [10]. For example, in the case when all grid functions are given on the set \(\omega_x = \{x_j\}\) of the vertices (nodes) of the cells of the simplex grid, to construct a grid analogue of formula (4) it suffices to substitute in this formula for the interpolation of nodal grid functions by the piecewise linear continuous coordinate functions \(\{\theta_j^x\}\) [9] and consider the result of the substitution as a
sumption identity for elements of the Euclidean space:

$$\sum_{x_j \in \omega_x} \eta_j f \left( \frac{\partial (\Pi \eta)}{\partial x_\alpha} \right) \partial_j^x dV = \sum_{x_j \in \omega_x} f_j \left\{ - \int_\Omega \left( \frac{\partial (\Pi \eta)}{\partial x_\alpha} \right) \partial_j^x dV + \int_\partial \left( \Pi \eta \right) \partial_j^x \nu_\alpha ds \right\}$$

with

$$[\eta, \partial_\alpha f]_x = [f, (-\partial_\alpha + \Phi_\alpha) \eta]_x.$$  

Here $\Pi f = \sum_{x_j \in \omega_x} f_j \partial_j^x$ is the interpolation of the grid function $f = \{f_j, \, x_j \in \omega_x\}$, $[\cdot, \cdot]_x$ - the scalar product in the Euclidean space. As a result, we obtain the definition of the grid analogue of the operator “nabla” $\nabla_x = \{\partial_\alpha\}$ and the boundary (that is, with a pattern and nonzero values only at boundary nodes) operator $\Phi = \{\Phi_\alpha\}$, which has no analog in point functions. The operator $\Phi$ is used for constructing grid analogs of the natural boundary condition. The operator interpretation of boundary conditions allows one to determine the difference analogs of the second-order differential operators $E_v$ and $E_\theta$ as self-adjoint positive operators in the Euclidean spaces [4].

2. An iterative method for solving a nonlinear operator equation

An implicit operator difference scheme constructed by the method of consistent operators for the system of equations (2) with boundary values (3) has the form:

$$F(\bar{y}) = \begin{pmatrix} F_\rho (\rho, v) \\ F_v (\rho, v, T) \\ F_T (\rho, v, T) \end{pmatrix} = \begin{pmatrix} E_{\rho \rho} \rho + \rho A_{12} v + A_\rho (w, \rho) + f_\rho \\ E_{vv} v + A_{21} p + A_v (\rho, w, v) + f_v \\ E_{TT} T + \beta A_{12} v + A_T (\rho, w, T) + f_T \end{pmatrix} = 0,$$

(5)

where the Frechet derivative of the operator $F$ at any point $\bar{y}^*$ from the neighborhood $S(\bar{y})$ solutions from the lower time layer $\bar{y}$ is representable in the form:

$$F' (\bar{y}^*) = E + A + B.$$  

Here

$$E = E^* = \begin{pmatrix} E_{\rho \rho} & 0 & 0 \\ 0 & E_{vv} & 0 \\ 0 & 0 & E_{TT} \end{pmatrix} = \begin{pmatrix} \frac{2}{\tau} I + A^\gamma_\rho & 0 & 0 \\ 0 & \frac{2\rho}{\tau} I + E_\nu + A^\gamma_v & 0 \\ 0 & 0 & \frac{2\rho}{\tau} I + E_\theta + A^\gamma_T \end{pmatrix},$$

$$A = \begin{pmatrix} A_{\rho \rho} & \rho^* A_{12} & 0 \\ A_{21} P^*_\rho & A_v & A_{21} P^*_T \\ 0 & \beta^* A_{12} & A_{TT} \end{pmatrix}, \quad A^* = - \begin{pmatrix} A_{\rho \rho} & P^*_\rho A_{12} & 0 \\ A_{21} \rho^* & A_v & A_{21} \beta^* \\ 0 & P^*_T A_{12} & A_{TT} \end{pmatrix},$$

the operator $B$ has a limited norm and the boundary operators $A^\gamma_\rho, A^\gamma_v, A^\gamma_T$ vanish if at the boundary of the computational domain the normal component of the velocity of the coordinate system is equal to the normal component of the velocity of the medium.

Suppose the operators $E$ and $A$ satisfy the conditions:

$$\exists m > 0: \quad E + A > m I,$$

$$\exists c > 0: \quad E \geq \tilde{E} = \frac{\tau}{\tau} I > 0 \implies E^{-1} \leq \tilde{E}^{-1} = \frac{\tau}{\tau} I.$$  

(6)
Then equation (5) can be solved by the generalized iterative Gauss-Seidel method [2]:

\[
\begin{cases}
F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right) = 0, \\
\tilde{y}^{k+1}_1 = \tilde{y}^{k+1}_2,
\end{cases}
\]  

(7)

where \( F \) is defined in such a way that

\[
F \left( \bar{y}, \bar{y} \right) = F \left( \bar{y} \right), \; \partial_1 F \left( \bar{y}, \bar{y} \right) = E + A, \; \partial_2 F \left( \bar{y}, \bar{y} \right) = B.
\]

The required definition \( F \) is obtained from the notation of the difference scheme (5) in the form:

\[
F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right) =
\begin{pmatrix}
E_{pp} \left( \rho^{k+1} - \rho^k \right) + A_{pp} \left( w^k, \rho^{k+1} - \rho^k \right) + \rho^k A_{12} \left( v^{k+1} - v^k \right) + F_1 \left( \bar{y}^k \right) \\
E_{vv} \left( v^{k+1} - v^k \right) + A_{vv} \left( \rho^k, w^k, v^{k+1} - v^k \right) + A_{12} \left( p^{k+1} - p^k \right) + F_v \left( \bar{y}^k \right) \\
E_{TT} \left( T^{k+1} - T^k \right) + A_{TT} \left( \rho^k, w^k, v^{k+1} - v^k \right) + \beta k A_{12} \left( v^{k+1} - v^k \right) + F_T \left( \bar{y}^k \right)
\end{pmatrix}
\]

(8)

It is known [6] that \( k \)-iterations converge, if

\[
\exists \gamma > 0 : \left\| (\partial_1 F \left( \bar{y}, \bar{y} \right))^{-1} \left( -\partial_2 F \left( \bar{y}, \bar{y} \right) \right) \right\| < \gamma < 1 \; \forall \bar{y}, \bar{y} \in S \left( \bar{y} \right).
\]

Due to the boundedness of the operator \( B \) and the operator properties of \( E \), we can always choose a time step at which this condition is satisfied.

To find \( \tilde{y}^{k+1}_1 \) on every \( k \)-iteration, we use the fact that due to (6) a linear operator \( (E + A^*)^{-1} \) is non-degenerate. Therefore, instead of solving the first equation of system (7) we can solve the equivalent equation

\[
\left\{ (E + A^*)^{-1} \left( \bar{y}^k \right) \right\} F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right) = 0.
\]

(9)

The derivative of the operator on the left-hand side of this identity with respect to \( \tilde{y}^{k+1}_1 \) is a symmetric positive operator

\[
(E + A^*)^{-1} \left( E + A \right) = E + A + A^* + A^* E^{-1} A.
\]

(10)

To solve equation (8), use the classical implicit two-layer iteration scheme [3]:

\[
\begin{cases}
\bar{y}^{k+1} - \bar{y}^k / \zeta + \left\{ (E + A^*)^{-1} \right\} F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right) = 0 \\
\bar{y}^{k+1} = \left\{ (E^{-1}) \right\} F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right), \\
D \left( \bar{y}^{k+1} - \bar{y}^k \right) / \zeta + F \left( \tilde{y}^{k+1}_1, \tilde{y}^{k+1}_2 \right) + A^* \bar{y}^k = 0.
\end{cases}
\]

(11)

If the energy inequality

\[
\exists \gamma_2 \geq \gamma_1 > 0 : \; \gamma_1 D \leq (E + A^*)^{-1} (E + A) \leq \gamma_2 D
\]

(12)

is satisfied, then at \( \zeta = 2 / (\gamma_1 + \gamma_2) \) the iterative process (10) converges [3]. If in addition to the conditions (6) the inequality is satisfied

\[
E + A + A^* \geq 0,
\]
then the operator $D$ can be determined by the formula

$$D = \frac{9}{8} E + \tilde{D},$$

(13)

where $\tilde{D}$ is the block-diagonal self-adjoint non-negative operator

$$\tilde{D} = -\frac{1}{\varepsilon} \begin{pmatrix} \tilde{D}_{pp} & 0 & 0 \\ 0 & \tilde{D}_{vv} & 0 \\ 0 & 0 & \tilde{D}_{TT} \end{pmatrix},$$

$\tilde{D}_{pp} = A_{pp}\rho A_{pp} + 2 \left( P_{\rho}^k A_{12} A_{21}^k \right)$,

$\tilde{D}_{vv} = A_{vv} A_{vv} + A_{21} \left( (\rho)^2 + (\beta)^2 \right) A_{12},$

$\tilde{D}_{TT} = A_{TT} A_{TT} + 2 \left( P_{\rho}^k A_{12} A_{21} P_{TT}^k \right)$.

**Theorem.** If the operator $D$ is defined by formula (13), the energy constants in inequality (11) can be determined by the formulas:

$$\gamma_1 = \frac{1}{1 + a}, \quad \gamma_2 = \frac{1 + 2a}{1 + a}, \quad a = 4 \| E^{-1} \| D_0, \quad D_0 = \frac{7}{8} E + \tilde{D}.$$  

(14)

**Proof.** First, we prove the inequalities necessary to obtain the estimate

$$D_0 \leq \| E^{-1} \| D_0 \leq \frac{1}{4} a E, \quad 0 \leq \frac{3}{4} E + A + A^* + A^* E^{-1} A.$$  

(15)

Inequalities (15) follow from assumption (12) and the evaluations

$$ E^{-1/2} \left( \frac{1}{2} E + A \right) y \right)^2 = \frac{1}{4} \| E^{1/2} y \|^2 + \frac{1}{2} \left( (A + A^*) y, y \right) + \| E^{-1/2} Ay \|^2 \Rightarrow$$

$$\Rightarrow \frac{1}{4} E + \frac{1}{2} \left( A + A^* \right) + A^* E^{-1} A \geq 0.$$  

Inequality (16) follows from the assumption

$$A + A^* + A^* E^{-1} A \leq E + 2 \tilde{D},$$

which is obtained from the obvious equalities

$$\frac{1}{2} \left( A + A^* \right) \tilde{y}, \tilde{y} \right] = \left[ (\rho)^k A_{12} \nu, \rho \right] + \left[ (\beta)^k A_{12} \nu, T \right] + \left[ A_{21} \left( P_{\rho}^k \rho + P_{TT}^k T \right), \nu \right] =$$

$$= \left[ E_{pp}^{-1/2} \left( A_{pp} \rho + (\rho)^k A_{12} \nu \right), E_{pp}^{1/2} \rho \right] + \left[ E_{vv}^{-1/2} \left( A_{vv} \nu + A_{21} \left( P_{\rho}^k \rho + P_{TT}^k T \right) \right), E_{vv}^{1/2} \nu \right] +$$

$$+ \left[ E_{TT}^{-1/2} \left( A_{TT} + (\beta)^k A_{12} \nu \right), E_{TT}^{1/2} T \right].$$

$$\left[ A^* E^{-1} A \tilde{y}, \tilde{y} \right] =$$

$$= \left( \begin{pmatrix} E_{pp}^{-1/2} A_{pp} & E_{pp}^{-1/2} P_{\rho}^k A_{12} & 0 \\ E_{vv}^{-1/2} A_{21}^k P_{\rho}^k & E_{vv}^{-1/2} ^{1/2} A_{21}^k P_{TT}^k & E_{vv}^{-1/2} A_{21}^k P_{TT}^k \\ 0 & E_{TT}^{-1/2} (\beta)^k A_{12} & E_{TT}^{-1/2} T \end{pmatrix} \right) \tilde{y} = \left( \begin{pmatrix} E_{pp}^{-1/2} \left( A_{pp} \rho + (\rho)^k A_{12} \nu \right) \\ E_{vv}^{-1/2} \left( A_{vv} \nu + A_{21} \left( P_{\rho}^k \rho + P_{TT}^k T \right) \right) \\ E_{TT}^{-1/2} \left( A_{TT} + (\beta)^k A_{12} \nu \right) \end{pmatrix} \right)^2.$$
Using inequalities (15), we obtain the formula for $\gamma_1$:
\[ E + A + A^* + A^* E^{-1} A - \gamma_1 \left( \frac{9}{8} E + \tilde{D} \right) \geq \frac{1}{4} E - \gamma_1 \left( \frac{1}{4} E + D_0 \right) \geq \frac{1}{4} (1 - \gamma_1 (1 + a)) E = 0. \]

Checking the formula for $\gamma_2$ is carried out as follows
\[ \gamma_2 \left( \frac{2}{3} E + \tilde{D} \right) - (E + A + A^* + A^* E^{-1} A) = \]
\[ = \gamma_2 \left( \frac{1}{4} E + D_0 \right) - \left( \frac{1}{4} E + 2 D_0 \right) + 2 D_0 - \left( \frac{2}{3} E + A + A^* + A^* E^{-1} A \right) \geq \]
\[ \geq \frac{1}{4} (\gamma_2 - 1) E - (2 - \gamma_2) D_0 = \frac{1}{4 a} \left( \frac{1}{4} a E - D_0 \right) \geq 0. \]

It is easy to verify that the parameter $\zeta$ for the energy constants (14) is equal to unity.

3. Conclusion

Thus, the implicit operator-difference scheme (5), that approximates the initial-boundary value problem of the gas dynamics at a time step, can be solved using a combination of the generalized Gauss-Seidel iterative method and the classical two-layer iterative scheme where the iterative parameter is equal to one and the iterative operator is self-adjoint positive. From a practical point of view, it is important that the iteration operator has a block-diagonal structure
\[
D \tilde{y} = \begin{pmatrix}
D_{\rho\rho} & 0 & 0 \\
0 & D_{vv} & 0 \\
0 & 0 & D_{TT}
\end{pmatrix}
\begin{pmatrix}
\rho \\
v \\
T
\end{pmatrix}
= \begin{pmatrix}
D_{\rho\rho} \\
D_{vv} \\
D_{TT}
\end{pmatrix}
\begin{pmatrix}
\rho \\
v \\
T
\end{pmatrix},
D_{ii} = D_{ii}^* \geq \tilde{E}_{ii}, \ i = \rho, v, T.
\]

Therefore, its inversion is reduced to inverting the operators $D_{ii}$ separately.

4. References

[1] Samarskii A A 2001 The Theory of Difference Schemes (New York: CRC Press)
[2] Ortega J M and Rheinboldt W C 1970 Iterative Solution of Nonlinear Equations in Several Variables (New York and London: Academic Press)
[3] Samarskij A A and Nikolaev E S 1989 Numerical Methods for Grid Equations: Volume II Iterative Methods (Basel: Birkhauser)
[4] Ardelyan N V and Kosmachevskii K V 1993 A conservative stable free-Lagrange method for the solution of 2d magnetohydrodynamic flows Preprint Max-Plank-Institut fur Astrophisik N 716
[5] Ardelyan N V and Kosmachevskij K.V. 1995 Implicit free-Lagrange method for computing two-dimensional magnetogas-dynamic flows Computational Mathematics and Modeling 6 209-24
[6] Ardelyan N V 1996 Iterative Methods for Solving of Implicit Difference Schemes of MHD ZAMM Zeitschrift für Angewandte Mathematik und Mechanik 76 123-6
[7] Sablin M N and Ardelyan N V 2003 Operator grid approximation for two-dimensional fluid-dynamic problems in moving coordinates on an irregular triangular grid Computational Mathematics and Modeling 14 217-45
[8] Ardelyan N V and Gushchin I S 1982 One approach to the construction of completely conservative difference schemes Moscow University Computational Mathematics and Cybernetics 3 1-9
[9] Sablin M N, Ardelyan N V and Kosmachevskii K V 2015 Consistent Grid Analogs of Invariant Differential and Boundary Operators on an Irregular Triangular Grid in the Case of a Grid Nodal Approximation Moscow University Computational Mathematics and Cybernetics 39 49-57
[10] Sablin M N 2020 Difference Differential Operators with Values at the Midpoints of the Sides of Cells of a Triangular Grid Moscow University Computational Mathematics and Cybernetics 44 97-108