The time reversibility property in analysis of sound points in balance-characteristic difference methods

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Abstract. A new computational technology of flux-type variables calculation on new time layer is introduced for the balance-difference methods for solving quasilinear hyperbolic systems of PDEs. The proposed method allows to build a scheme, which is locally implicit in the sound points and explicit in all other nodes of the mesh. It also has the second order of approximation in time and space and the property of time reversibility if the flux correction procedure is disabled. Results of test computations for the problem of transonic dam-break are presented.

1. Introduction

High-accuracy numerical solution of quasilinear hyperbolic systems of PDEs has always been an important problem of mathematical modelling. Particular concern is raised by the problem of solving such equations in case of transonic flows. A wide variety of transonic problems includes, for example, the modelling of dam-break using the shallow-water equations or the modelling of gas flow in de Laval nozzle using the Euler’s equations of gas dynamics.

In recent years, the balance-characteristic schemes [1] have become very popular for solving the quasilinear hyperbolic systems of PDEs. There are two types of variables in these methods: conservative-type and flux-type variables. Conservative-type variables are used to formulate the mesh analogues of conservation laws, and flux-type variables are computed with the method of inverse characteristics. This allows to utilize all the properties of hyperbolic systems of PDEs and build such second order schemes as the CABARET scheme [2].

The strengths of this scheme include its flexibility, easy parallelization and high modernization potential. One of its weaknesses is the complications with robust computations in case of transonic flows. There a lot of types of sonic points in these flows, so most of the previously proposed sonic point processing algorithms [2, 3, 4, 5] were either ineffective or too complicated trying to process every type of the point individually. This article presents a description of a new approach to processing of the sonic points, which is based purely on such concepts as approximation and time reversibility.

2. Quasilinear hyperbolic systems of PDEs

Let’s consider a system of \( m \) one-dimensional quasilinear laws of conservation without any sources or sinks:

\[
\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{u})}{\partial x} = 0,
\]  

(1)
here $u$ - $m$-dimensional vector of unknowns, $F(u)$ - $m$-dimensional vector-function of fluxes. Transforming the spatial derivative in (1), another form of the system can be obtained:

$$\frac{\partial u}{\partial t} + A(u) \frac{\partial u}{\partial x} = 0,$$

(2)

here $A(u)$ is Jakobi matrix of $F(u)$. Finally, assuming that the system (2) is of hyperbolic type (i.e. all eigenvalues of matrix $A(u)$ are real and different under all possible values of $u$) and that the analytical expressions for Riemann invariants can be found explicitly, a characteristic form of the system can be obtained:

$$\frac{\partial I}{\partial t} + \Lambda(I) \frac{\partial I}{\partial x} = 0,$$

(3)

here $I = I(u)$ is the $m$-dimensional vector of Riemann invariants, $\Lambda(I)$ - diagonal matrix with the eigenvalues of $A(u)$ on the diagonal. Therefore, the initial system (1) can be reduced to $m$ independent non-linear transport equations. Hence, the considered system must possess the property of time reversibility if the characteristics of the same family do not intersect. It means that if the system turns $u_0 = u(t_0)$ into $u_1 = u(t_0 + \tau)$ over time $\tau$, then it also turns $u_{01}$ into $u_0$ over time $\tau$, where $u_{01}$ is equal to $u_1$ in which all velocities are changed to the opposite ones.

Summarizing these facts about the system of laws of conservation (1), we can state that a good numerical scheme for its solving should capture all or at least some of the properties of the mathematical model, including: conservation of mesh analogues of $u$ (connection with (1)), transfer of Riemann invariants over the characteristics (connection with (3)), time reversibility (corollary of (3)).

3. Balance-characteristic schemes

Many of numerical schemes for solving quasilinear hyperbolic systems of PDEs were derived using different forms of the stated problem. For example, the conservative finite volume schemes are based on the conservation laws (1), characteristic methods - on the characteristic form (3) and do not rely on the laws of conservation. The balance-characteristic methods (like the CABARET scheme) are based both on forms (1) and (3) and use all the information provided by the mathematical model of the problem.

In this work we will only consider the 3-phase balance-characteristic schemes. The family of such method includes the well-known CABARET scheme [2], Sharp scheme [6] and others.

To describe the main principles of this type of methods, we will introduce a space-time mesh and mesh functions on it. Assume that the system (1) is considered in the interval $x \in [a, b]$ during time $t \in [0, T]$. Then let $\omega = \omega_h \times \omega_r$ be the space-time mesh, where $\omega_h = \{x_i | a = x_0 < x_1 < \ldots < x_{N-1} < x_N = b; x_{i+1} - x_i = h_{i+1/2}, i = 0, N - 1\}$ - irregular in general case mesh in space, $\omega_r = \{t_n | 0 = t_0 < t_1 < \ldots < t_{K-1} < t_K = T; t_{n+1} - t_n = \tau_n, n = 0, K - 1\}$ - irregular in general case mesh in time. We also introduce two sets of mesh functions: conservative-type and flux-type functions (see figure 1). The values of conservative-type functions are situated in the centres of space cells on integer and half-integer time layers: $(x_{i+1/2}, t_n) \mapsto \phi_{i+1/2}^{n}$, $(x_{i+1/2}, t_{n+1/2}) \mapsto \phi_{i+1/2}^{n+1/2}$. The values of flux-type functions are situated in the nodes of the mesh $\omega_h$: $(x_i, t_n) \mapsto \psi_{i}^{n}$.

One time step of a 3-phase balance-characteristic scheme consists of three phases. Phases 1 and 3 represent the calculation of conservative-type variables according to the mesh analogues of laws of conservation (1). For example, in second order schemes these phases appear as follows:

**Phase 1:**

$$\frac{u_{i+1/2}^{n+1/2} - u_{i+1/2}^{n}}{\tau_n} + \frac{F(u_{i+1}^{n}) - F(u_{i}^{n})}{h_{i+1/2}} = 0,$$

(4)
Figure 1: Types of mesh functions: conservative (squares) and flux (circles).

\[
\text{Phase 3: } \frac{u_{i+1/2}^{n+1} - u_{i+1/2}^n}{\tau_n/2} + \frac{F(u_{i+1}^{n+1}) - F(u_{i}^{n+1})}{h_{i+1/2}} = 0. \tag{5}
\]

The second phase represents the calculation of flux variables \(u_{i}^{n+1}\) on the new time layer. For that the values of Riemann invariants \(I\) are extrapolated or interpolated and then transferred in the direction of the respective characteristics which slopes are approximated using the values in the centres of space-time cells \(u_{i}^{n+1/2}\). In cases of strictly subsonic or supersonic flows, when all eigenvalues of matrix \(A\) in (2) don’t change signs, every point \((x_i, t_{n+1})\) receives exactly one value for each of \(m\) Riemann invariants, so the flux variables \(u_{i}^{n+1}\) can be uniquely restored. But if at least one of the eigenvalues \(I_k\) changes its sign in two adjacent space-time cells, then the node \((x_i, t_{n+1})\) between these cells will either receive two different values of a corresponding Riemann invariant on the next time layer or receive none of them. Hence, it won’t be possible to uniquely restore the values of the flux variables. In this case we will say that the space-time node \((x_i, t_{n+1})\) is a sonic point along the invariant \(I_k\).

4. Locally implicit sonic point processing algorithm

Several different algorithms were proposed for the processing of sonic points in quasilinear hyperbolic systems of PDEs [2, 4, 5], most of them were tested with the CABARET scheme. Algorithm from [2] based on choosing the right side of transfer according to the sum of eigenvalues beside the sonic point, although being time reversible, can lead to non-physical discontinuities on the rarefaction waves, which is shown in [4]. Explicit [4] and implicit [5] methods also possess the property of time reversibility, but only work for a restricted class of problems.

We will propose a new second order time reversible method of sound point processing based on inverse characteristic method. Assume that the space-time node \((x_i, t_{n+1})\) is a sonic point along the invariant \(I_k\), which means that \((\lambda_k)_i^{n+1/2} \ast (\lambda_k)_i^{n+1/2} \leq 0\). Consider the area of two space-time cells around the sonic point (see figure 2). Let’s trace a straight characteristic with a slope determined by \((\lambda_k)_i^{n} = \lambda_k(u_{i}^{n})\) from the node \((x_i, t_{n})\) and transfer the invariant \((I_k)_i^n\) along the line to the half-integer time layer. Then let’s trace a straight characteristic with a yet unknown slope determined by \((\bar{\lambda}_k)_i^{n+1} = \lambda_k(\bar{u}_{i}^{n+1})\) from the node \((x_i, t_{n+1})\). Next we will introduce a local coordinate system:

\[\xi = x - x_{i-1/2}, \quad x_{i-1/2} = 0.5(x_i + x_{i-1})\]

and construct a second order interpolation \(P_2(\xi)\) of \(I_k\) on the half-integer time layer based on constraints:

\[P_2(0) = (I_k)_{i-1/2}^{n+1/2}, \quad P_2(\bar{\xi}_k) = (I_k)_i^n, \quad P_2(h_i) = (I_k)_{i+1/2}^{n+1/2}\]
\[ \xi_k = 0.5 h_{i-1/2} + 0.5 \tau_n (\lambda_k)^n_i, \quad h_i = x_{i+1/2} - x_{i-1/2}. \]

After that we can find the value of the designated invariant in the point of intersection of \( t = t_{n+1/2} \) and the straight characteristic from \((x_i, t_{n+1})\) and transfer this value to the upper time layer:

\[ \tilde{I}_k^{n+1} = P_2(\xi_k), \quad \xi_k = 0.5 h_{i-1/2} - 0.5 \tau_n (\lambda_k)^{n+1}_i. \]

Hence, returning to the initial coordinate system we get the equation for the invariant \( I_k \):

\[
I_k(\tilde{u}^{n+1}_i) = \frac{\tau_n (I_k)^{n+1/2}_i (h_{i+1/2} + \tau_n \lambda_k (\tilde{u}^{n+1}_i))((\lambda_k)^n_i + \lambda_k (\tilde{u}^{n+1}_i))}{4 h_i \xi_k} - \frac{\tau_n (I_k)^{n+1/2}_i (h_{i-1/2} - \tau_n \lambda_k (\tilde{u}^{n+1}_i))((\lambda_k)^n_i + \lambda_k (\tilde{u}^{n+1}_i))}{4 h_i (h_i - \xi_k)} + (I_k)^{n+1/2}_i \frac{(h_{i-1/2} - \tau_n \lambda_k (\tilde{u}^{n+1}_i))(h_{i+1/2} + \tau_n \lambda_k (\tilde{u}^{n+1}_i))}{4 \xi_k (h_i - \xi_k)}.
\]

Equation (6) is used for invariant \( I_k \) in point \((x_i, t_{n+1})\) only if it is a sonic point along the invariant \( I_k \). In other case the value of \((I_k)^{n+1}_i\) can be found via classic phase 2 algorithms (for example, extrapolation algorithm of the CABARET scheme) and can be considered as a known value. Then a simple functional relationship between the invariants and the initial variables can be used:

\[
I_k(\tilde{u}^{n+1}_i) = (I_k)^{n+1}_i.
\]

Finally, we formulate the whole algorithm for sound points. If a space-time point \((x_i, t_{n+1})\) is a sound point along at least one of the invariants of the system, a system of \( m \) non-linear equations is built. For each invariant with a sign change in its eigenvalue, equation (6) is written. Equation (7) is written for all other invariants. Then the system of \( m \) non-linear equations with \( m \) unknowns \( \tilde{u}^{n+1}_i \) can be solved using, for example, Newton’s method, and a set of new flux variables can be found.

The proposed algorithm has a second order of approximation in time and space and does not violate the property of conservation when used in balance-characteristic methods. Moreover, due to the uniqueness of parabolic function built using values in 3 points and the symmetry of the template (see figure 2), the algorithm possesses a time reversibility property. It is also important to notice, that the method is only locally implicit when used with the CABARET scheme: the system of non-linear equations must only be solved in the sound points, in all other points the values are computed explicitly.
In some problems the monotonicity of the solution is more important than the property of time reversibility. In this case the algorithm (6 - 7) can be extended with a flux correction procedure similar to the one in the CABARET scheme: the value of invariants \( \hat{I}_k^{n+1} = I_k(u_i^{n+1}) \) are changed to stay between the values of \( I_k^{n+1/2}, I_k^{n+1/2} \) and \( I_k^{n} \).

5. Test results
The proposed algorithm, coupled with the CABARET scheme [2], was tested on one-dimensional shallow-water equations for flows above a flat bottom:

\[
\begin{align*}
\frac{\partial H}{\partial t} + \frac{\partial Hu}{\partial x} &= 0, \\
\frac{\partial Hu}{\partial t} + \frac{\partial Hu^2}{\partial x} + \frac{g}{2} \frac{\partial H^2}{\partial x} &= 0,
\end{align*}
\]

(8)

Here \( H \) is height of fluid, \( u \) - velocity of column of fluid, \( g \) - acceleration of free fall.

Although many test have been carried out, we will provide the results for only one of them: the comparison of the proposed algorithm with the explicit method [4] on the problem of transonic dam-break. The initial conditions of the problem have a discontinuity in the middle of the considered interval \( x \in [0, 1] \):

\[
H_{left} = 100.0, \quad H_{right} = 1.0, \quad u_{left} = 0.0, \quad u_{right} = 0.0.
\]

(9)

Figures 3 and 4 show the results for the above-described problem for the moment of time \( t = 0.012 \) computed on a uniform mesh of 200 cells. Figure 3 contains the graphs of results on interval \( x \in [0, 1] \) (the values are shown in every third cell of the mesh), figure 4 - on interval \( x \in [0.7, 0.9] \) (the values are shown in every cell inside the designated interval).

Both algorithms lead to smearing of the shock wave over 3 cells, and they also capture the rarefaction wave very well. However, the locally implicit algorithm deals better with the nonmonotonicity which occurs right after the rarefaction wave (see figure 4). Such nonmonotonicity presumably appears due to the imbalance between the conservative-type and flux-type variables during the first time steps. It is possible to smooth this effect by synchronizing
6. Conclusion
A new locally implicit algorithm of sonic point processing in balance-characteristic schemes was introduced. The resulting conservative method has a second order approximation and property of time reversibility when the flux correction procedure is disabled. Results of test computations for the problem of transonic dam-break were presented. It was shown that the proposed method allowed to get more accurate results as compared with some previously proposed algorithms. The author hopes to generalize the scheme for the case of non-zero right-hand side in the initial equations and the multidimensional case.

Acknowledgments
This work was supported by the Russian Science Foundation, project no. 19-11-00104.

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