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Superconservative Finite Difference Scheme for Gas Dynamics

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ABSTRACT

We present a 4-parameter implicit Lagrangean code which satisfies conservation of mass, linear and angular momenta, energy and entropy simultaneously. The primary advantage of this scheme is possibility to control dissipative properties of the scheme avoiding the effects of numerical viscosity.

Key Words : hydrodynamics – methods: numerical

I. INTRODUCTION

In the numerical simulation of astrophysical gaseous systems it is important to employ numerical schemes satisfying as many conservation laws as possible. This work presents an example of the scheme with better conservative properties against the traditional schemes.

II. BASIC DEFINITIONS

The system of hydrodynamic equations constitutes N scalar hyperbolic equations that can be written in a form of conservation laws. It is significant that such presentation sometimes is non-unique and the number of conservation laws M may be greater than N. For example, for 1D plane-parallel gas flow we have $N = 3$ but $M = 4$ (mass, linear momentum, energy, entropy).

Definition 1 *The numerical scheme is* **conservative** *if it satisfies* $M_{scheme} > 0$ *conservation laws.*

Definition 2 *The numerical scheme is* **completely conservative** *if* $M_{scheme} = N$.

Definition 3 *The numerical scheme is* **superconservative** *if* $M_{scheme} > N$.

In this paper we present an example of a superconservative scheme and sketch briefly its basic properties.

III. SUPERCONSERVATIVE NUMERICAL CODE: ONE-DIMENSIONAL CASE

The Lagrangean form of 1D hydrodynamic equations of a perfect gas with a constant specific heats ratio γ in a plane-parallel geometry is

$$\frac{\partial r}{\partial t} = u, \tag{1}$$

$$\frac{\partial (1/\rho)}{\partial t} = \frac{\partial u}{\partial m}, \tag{2}$$

$$\frac{\partial u}{\partial t} = -\frac{\partial \phi}{\partial r} + \frac{\partial}{\partial m}\Big[-P + \eta\rho\frac{\partial u}{\partial m}\Big], \tag{3}$$

$$\frac{\partial \varepsilon}{\partial t} = -P\frac{\partial u}{\partial m} + \eta\rho\Big(\frac{\partial u}{\partial m}\Big)^2 + \frac{\partial}{\partial m}\Big(\chi\rho\frac{\partial T}{\partial m}\Big), \tag{4}$$

$$P = \frac{\mathcal{R}}{\mu}\rho T, \tag{5}$$

$$\varepsilon = \frac{\mathcal{R}T}{(\gamma-1)\mu}. \tag{6}$$

Here $\phi(r)$ is the external gravitational potential, $\eta = \eta(\rho, T)$ is the coefficient of dynamic viscosity, $\chi = \chi(\rho, T)$ is the coefficient of heat conduction, and the other notations are standard.

The divergent form of equations (2) and (3) reflects conservation of mass and linear momentum, respectively (the momentum is conserved if $\phi = 0$). Two additional conservation laws, for energy and entropy, follow from corresponding deduced equations

$$\frac{\partial}{\partial t}\Big(\varepsilon + \frac{1}{2}u^2 + \phi\Big) = \frac{\partial}{\partial m}\Big[-Pu + \eta\rho u\frac{\partial u}{\partial m} + \chi\rho\frac{\partial T}{\partial m}\Big], \tag{7}$$

and

$$T\frac{\partial S}{\partial t} = \eta\rho\Big(\frac{\partial u}{\partial m}\Big)^2 + \frac{\partial}{\partial m}\Big(\chi\rho\frac{\partial T}{\partial m}\Big), \tag{8}$$

where

$$S = \frac{\mathcal{R}}{(\gamma-1)\mu}\ln\frac{T}{\rho^{\gamma-1}}. \tag{9}$$

We base our scheme on that developed by Samarskij & Popov (1992). We introduce a non-homogeneous grid with a variable mass step $m_{i+1/2}$ and variable time step τ^n. Hereafter subscripts denote the number of a spatial cell whereas superscripts refer to the number of a time step. The superscript n at τ will be further omitted. To abridge notation we use

$$f \equiv f^n, \qquad \check{f} \equiv f^{n-1}, \tag{10}$$

$$f^{(\lambda)} \equiv \lambda f + (1-\lambda)\check{f}, \qquad \lambda \in [0,1]. \tag{11}$$

The fully explicit scheme corresponds to the limiting value $\lambda = 0$, and completely implicit scheme to $\lambda = 1$.

We define kinematic quantities r_i and u_i with integer indices at cell boundaries, while thermodynamic quantities, $P_{i+1/2}$, $\rho_{i+1/2}$, $\varepsilon_{i+1/2}$, $T_{i+1/2}$, with half-integer indices are defined in the centers of cells. In this notation $m_{i+1/2}$ is the mass of the cell between r_i and r_{i+1}. We also introduce a mass step associated with the integer node

$$M_i = \frac{1}{2}\,(m_{i-1/2} + m_{i+1/2}). \tag{12}$$

After all, the finite difference scheme is written as

$$\frac{r_i - \check{r}_i}{\tau} = u_i^{(0.5)}, \tag{13}$$

$$m_{i+1/2} = \rho_{i+1/2}\,(r_{i+1} - r_i), \tag{14}$$

$$M_i\frac{u_i - \check{u}_i}{\tau} = -M_i\frac{\phi(r_i) - \phi(\check{r}_i)}{r_i - \check{r}_i} - (P_{i+1/2}^{[\gamma,\lambda_1]} - P_{i-1/2}^{[\gamma,\lambda_1]}) + (\eta\rho)_{i+1/2}^{(\lambda_2)}\frac{u_{i+1}^{(0.5)} - u_i^{(0.5)}}{m_{i+1/2}} - (\eta\rho)_{i-1/2}^{(\lambda_2)}\frac{u_i^{(0.5)} - u_{i-1}^{(0.5)}}{m_{i-1/2}}, \tag{15}$$

$$m_{i+1/2}\frac{\varepsilon_{i+1/2} - \check{\varepsilon}_{i+1/2}}{\tau} = -P_{i+1/2}^{[\gamma,\lambda_1]}(u_{i+1}^{(0.5)} - u_i^{(0.5)}) + (\eta\rho)_{i+1/2}^{(\lambda_2)}\frac{\left[u_{i+1}^{(0.5)} - u_i^{(0.5)}\right]^2}{m_{i+1/2}} + (\chi\rho)_{i+1/2}^{(\lambda_3)}\frac{T_{i+3/2}^{(\lambda_4)} - T_{i+1/2}^{(\lambda_4)}}{M_{i+1}} - (\chi\rho)_{i-1/2}^{(\lambda_3)}\frac{T_{i+1/2}^{(\lambda_4)} - T_{i-1/2}^{(\lambda_4)}}{M_i}, \tag{16}$$

$$\varepsilon_{i+1/2} = \frac{\mathcal{R}T_{i+1/2}}{(\gamma-1)\mu}. \tag{17}$$

This is a 4-parameter finite difference scheme which can be either explicit or implicit depending on the coefficients λ_j, $j = 1, ..., 4$; here $P_{i+1/2}^{[\gamma,\lambda_1]}$ is an approximation for pressure to be defined later..

It can be easily seen that (13)-(17) satisfy the requirements for a completely conservative scheme irrespective of the specific form for $P_{i+1/2}^{[\gamma,\lambda_1]}$. Indeed, in Lagrangean variables mass is conserved automatically [see (14)]. Equation (15), written in a divergent form, guarantees conservation of linear momentum. Multiplying equation (15) by $u_i^{(0.5)}$, adding this to equation (16) and taking into account equations (13), (14), we obtain the equation of energy conservation

$$m_{i+1/2}\frac{\varepsilon_{i+1/2} - \check{\varepsilon}_{i+1/2}}{\tau} + M_i\frac{u_i^2 - \check{u}_i^2}{2\tau} + M_i\frac{\phi(r_i) - \phi(\check{r}_i)}{\tau} = -P_{i+1/2}^{[\gamma,\lambda_1]}u_{i+1}^{(0.5)} + P_{i-1/2}^{[\gamma,\lambda_1]}u_i^{(0.5)} + (\eta\rho)_{i+1/2}^{(\lambda_2)}\frac{\left[u_{i+1}^{(0.5)} - u_i^{(0.5)}\right]u_{i+1}^{(0.5)}}{m_{i+1/2}} - (\eta\rho)_{i-1/2}^{(\lambda_2)}\frac{\left[u_i^{(0.5)} - u_{i-1}^{(0.5)}\right]u_i^{(0.5)}}{m_{i-1/2}} + (\chi\rho)_{i+1/2}^{(\lambda_3)}\frac{T_{i+3/2}^{(\lambda_4)} - T_{i+1/2}^{(\lambda_4)}}{M_{i+1}} - (\chi\rho)_{i-1/2}^{(\lambda_3)}\frac{T_{i+1/2}^{(\lambda_4)} - T_{i-1/2}^{(\lambda_4)}}{M_i}. \tag{18}$$

In order to make the scheme superconservative we define

$$P^{[\gamma,\lambda_1]} = \frac{\mathcal{R}}{\mu(\gamma-1)}\frac{(\rho^{\gamma-1} - \check{\rho}^{\gamma-1})\rho\check{\rho}[\lambda_1 T + (1-\lambda_1)\check{T}]}{(\rho - \check{\rho})[\lambda_1\rho^{\gamma-1} + (1-\lambda_1)\check{\rho}^{\gamma-1}]}. \tag{19}$$

By using equations (19), (13) and (14) we transform equation (16) into the form of a finite difference analogue of equation (8)

$$\frac{m_{i+1/2}\mathcal{R}\rho_{i+1/2}^{\gamma-1}\check{\rho}_{i+1/2}^{\gamma-1}(T_{i+1/2}\rho_{i+1/2}^{1-\gamma} - \check{T}_{i+1/2}\check{\rho}_{i+1/2}^{1-\gamma})}{(\gamma-1)\mu[\lambda_1\rho_{i+1/2}^{\gamma-1} + (1-\lambda_1)\check{\rho}_{i+1/2}^{\gamma-1}]\tau} = (\eta\rho)_{i+1/2}^{(\lambda_2)}\frac{\left[u_{i+1}^{(0.5)} - u_i^{(0.5)}\right]^2}{m_{i+1/2}} + (\chi\rho)_{i+1/2}^{(\lambda_3)}\frac{T_{i+3/2}^{(\lambda_4)} - T_{i+1/2}^{(\lambda_4)}}{M_{i+1}} - (\chi\rho)_{i-1/2}^{(\lambda_3)}\frac{T_{i+1/2}^{(\lambda_4)} - T_{i-1/2}^{(\lambda_4)}}{M_i}. \tag{20}$$

Thus, in dissipationless case ($\eta = \chi = 0$) entropy of each fluid particle $S_{i+1/2} \propto \ln(T_{i+1/2}\rho_{i+1/2}^{1-\gamma})$ is conserved.

Generally, the scheme (13)-(17), (19) is $\sim O(\tau + h^2)$, except for the case $\lambda_1 = ... = \lambda_4 = 1/2$ when the accuracy in time becomes of the second order.

Let us note that written in the form (16), the energy equation correctly reproduces the balance between thermal and other energies.

IV. TECHNICAL RECIPES

In practical use, to avoid errors arising from small quantities in the denominator of r.h.s. of equation (19) we develop $\rho^{\gamma-1}$ in a series of $\Delta\rho \equiv \rho - \check{\rho}$ at the point $\check{\rho}$ and thus the fraction regularizes

$$\frac{\rho^{\gamma-1} - \check{\rho}^{\gamma-1}}{\rho - \check{\rho}} = (\gamma-1)\Big[\check{\rho}^{\gamma-2} + \frac{(\gamma-2)}{2}\check{\rho}^{\gamma-3}\Delta\rho + ...\Big], \tag{21}$$

with the expansion broken when specified accuracy is reached. If $\gamma = m/n$, where m and n are integer, the expansion breaks off then automatically:

$$\frac{\rho^{\gamma-1} - \check{\rho}^{\gamma-1}}{\rho - \check{\rho}} = \frac{(\rho^{\frac{m-n-1}{n}} + \rho^{\frac{m-n-2}{n}}\check{\rho}^{\frac{1}{n}} + ... + \check{\rho}^{\frac{m-n-1}{n}})}{(\rho^{\frac{n-1}{n}} + \rho^{\frac{n-2}{n}}\check{\rho}^{\frac{1}{n}} + ... + \check{\rho}^{\frac{n-1}{n}})}. \tag{22}$$

In particular, for $\gamma = 5/3$ and $\lambda_1 = 1/2$ we obtain a regularized symmetric second order approximation

$$P^{[5/3,0.5]} = \frac{3\mathcal{R}(\rho^{1/3} + \check{\rho}^{1/3})\rho\check{\rho}(T + \check{T})}{2\mu(\rho^{2/3} + \rho^{1/3}\check{\rho}^{1/3} + \check{\rho}^{2/3})(\rho^{2/3} + \check{\rho}^{2/3})}. \tag{23}$$

Regularized calculation of approximated graviational force in equation (15) is carried out analogously. We expand $\phi(r)$ at the point $r^{(0.5)} = \frac{1}{2}(r + \check{r})$ in $\Delta r = r - r^{(0.5)}$:

$$\frac{\phi(r) - \phi(\check{r})}{r - \check{r}} = \phi'(r^{(0.5)}) + \frac{1}{24}\phi'''(r^{(0.5)})\Delta r^2 + \dots . \quad (24)$$

Here the prime denotes derivative with respect to r.

The functions $\phi'(r)$, $\phi'''(r)$, ... along with $\phi(r)$ should be prescribed in a program analytically as subroutines. Test runs show that one or two terms in expansion (24) are often sufficient for practical use.

If $\phi(r)$ has a polynomial form of rational degree, the fraction (24), similarly to (22), allows exact division.

V. ALGORITHM OF COMPUTATIONS

The scheme is implicit and highly non-linear. In order to solve it numerically, one needs some iterative procedure such as Newtonian iterations. The system (13)-(17), (19) is linearized and is reduced to a tridiagonal system of linear equations which is solved by the direct matrix sweep method. It should be noted that truncation of Newtonian iterations implies an approximate nature of superconservativity in practical computations. However the iterative process converges to computer zero after 4-6 iterations if the time step does not significantly exceed the minimal characteristic time in the problem. Though the superconservative scheme is absolutely stable itself, the Newtonian procedure imposes a time step limitation for convergence.

VI. SUPERCONSERVATIVE NUMERICAL CODE: MULTIDIMENSIONAL CASE

Generalization of the scheme (13)-(17) to multidimensional case is straightforward. However, some new circumstances arise.

First, we have an additional conservation law. In the central field

$$\phi = \phi(r), \qquad r = \sqrt{x^2 + y^2} \quad (25)$$

the angular momentum is conserved. To achieve angular momentum conservation in the scheme we define

$$\frac{\partial \phi}{\partial x} \to (\phi - \check{\phi})\frac{x + \check{x}}{r^2 - \check{r}^2}, \qquad \frac{\partial \phi}{\partial y} \to (\phi - \check{\phi})\frac{y + \check{y}}{r^2 - \check{r}^2}. \quad (26)$$

Secondly, since the system of linearized equations loses its tridiagonal structure, numerical solving of the scheme becomes more expensive. In this case the system can be solved by the conjugate gradient-type iterative method.

Thirdly, in the shear flows the Lagrangean cells have a tendency to overlap so that the grid reconstruction is required. Unfortunately, interpolation disturbs superconservativity. In this case we may either exploit the superconservative scheme in the problems without shear or use the completely conservative version of the scheme by using grid reconstruction.

VII. CONCLUSIONS

The superconservative scheme combines advantages of both the Lagrangean schemes such as high resolution and flexibility, and implicit schemes which lift stability restrictions. However, the primary advantage of the superconservative scheme is that it allows to avoid nonphysical effects of numerical viscosity in hydrodynamic simulation. This property is important in numerical solution of stiff problems in which: i) dissipation is the governing parameter of the model, and ii) the characteristic viscous or heat conductive times are much greater than the dynamical one. Under these circumstances, we can choose a sufficiently large time step of integration being sure that it will not lead to anomalously great numerical dissipation.

1D scheme and its efficiency has been tested in calculations of hydrodynamics with strong heat-conduction and cooling effects (Kovalenko & Shchekinov 1992), and with self-gravity (Kovalenko & Sokolov 1993). 2D scheme has been used for calculation of instability of spherical accretion on to a black hole (Eremin & Kovalenko 2001). Tests show that the superconservative scheme is especially suitable for smooth isentropic flows. At the same time in the flows with discontinuities the effects of numerical dispersion become relatively strong, which is manifested through spurious oscillations across a discontinuity. Thus, a combination of physical or artificial viscosity and artificial dispersion (Samarskij & Popov 1992) are recommended to be added.

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