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Comparison of Various Numerical Techniques in Gas Dynamics

By

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Abstract

In search of reliable numerical methods for gas dynamic flow problems, we apply the MacCormack method algorithm and two new algorithms to two representative problems in gas dynamics. The MacCormack method, which is most commonly employed in aerodynaics, proves to be good for the time developing problem. The explicit Satofuka method, which is claimed to be stable even if the CFL condition is violated, turns out to be rather inaccurate for a problem with a CFL number larger than unity. We find that the New MacCormack implicit method is suitable for the time steady problem.

1. Introduction

It is necessary to solve the equations describing gasdynamic flows in various fields of science and technology. There are two ways to achieve this purpose, i. e. the analytic solution and the numerical solution. If we adopt the analytic method, we can solve only simple problems because of a complexity arising from the non-linear nature of the equations. On the other hand, we can solve complex problems, such as those which flow around a complex shaped wing in the numerical method. The numerical analysis is particularly effective to treat shock waves occurring in transonic and supersonic problems.

In 1940 von Neumann began to investigate the numerical analysis. Following the development of computer architecture, many kinds of numerical methods have been proposed: finite difference methods, spectral methods and finite volume methods etc. (See for example, R. Peyret and T. D. Taylor, 1983.) The most basic and widely used technique is the method of finite difference, whereby differential equations describing a continuous fluid can be discretized. Finite difference procedures are used widely to solve the Navier–Stokes equation subject to arbitrary boundary conditions.

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Until now, many types of the finite-difference scheme for the numerical solution of the compressible Navier-Stokes equation have been presented.   In these, there are various variants such as explicit or implicit, with a different order of accuracy in space and that in time.   The explicit method is easy to understand and straightforward to program, but the time step is severely restricted by the well known Courant-Friedrichs-Lewy condition (CFL condition).   The advantage of an implicit formulation is considerable, particularly as unconditional stability can be achieved and large time steps may consequently be employed.   However, there is a penalty in the programming effort and the computer time per grid point.

The objective of this paper is to supply a comparison of three numerical methods: the MacCormack method (MacCormack, 1969), the Satofuka (RRK) method (Satofuka, 1982) and the New MacCormack implicit method (MacCormack, 1982). Though the Satofuka method permits us to choose an arbitrary order of accuracy in space dimension, we restrict our attention to cases of second order accuracy in space.

The reason for our choice of the Satofuka method is that it is computationally explicit and is unconditionally stable for some class of problems (Satofuka, 1982). By solving a nozzle flow problem, Satofuka claims that his method gives a stable solution with any CFL number up to $O(10^4)$.   If this is the case, the Satofuka method seems to be very attractive.

Viscosity is neglected in the present paper, and we treat the Euler equation rather than the Navier-Stokes equation.   For simplicity, we shall define the algorithms in one space dimension, though they may be easily applied to any number of space dimensions.   These methods are tested for two representative problems in gas dynamics, i. e. the shock tube problem and the nozzle flow.   In these problems, we compare the numerical solution with the exact one.   We also compare computer CPU times to see the effectiveness of these methods.

2. Basic Equations

The unsteady compressible form of the Euler equation in one space dimension may be written in conservation-law form as

$$\boldsymbol{U}_t + \boldsymbol{F}_x = 0 \qquad\qquad (2\cdot1)$$

where the vector of conserved quantities $\boldsymbol{U}$ and the vector of fluxes $\boldsymbol{F}$ are

$$\boldsymbol{U} = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix}, \quad \boldsymbol{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ (e+p)u \end{pmatrix} \qquad\qquad (2\cdot2)$$

where we neglect a source term.   The pressure p is described by the equation of the state of ideal gas as

$$p = (\gamma - 1)\left(e - \frac{1}{2}u^2\right) \tag{2·3}$$

where γ is the ratio of specific heats which is assumed to be 1.4 in the following examples.

3. Numerical Methods

A typical numerical method for the system $(2·1)$ divides the spatial region into N zones centered at the grid points $= i\Delta x$, where $i = 1, 2, \cdots, N$ and Δx is the zone width. It advances the approximate solution from t_n to time t_{n+1}, (where $t_{n+1} = t_n + \Delta t$) by means of a discretized version of the partial differential equation. In the present paper $N = 100$ is used.

3.1. MacCormack Explicit Method

In 1969, a second-order-accurate numerical method was presented by MacCormack (1969), and it has been used widely in aerodynamics. This method uses two steps in calculation. On even time steps it uses a backward predictor step which determines provisional values at t_{n+1}

$$\overline{U}_i^n = U_i^n - (F_i^n - F_{i-1}^n)\Delta t / \Delta x \tag{3·1·1}$$

followed by a forward corrector step which determines the final values at t_{n+1}

$$U_i^{n+1} = \frac{1}{2}\left[U_i^n + \overline{U}_i^n - (\overline{F}_{i+1}^n - \overline{F}_i^n)\Delta t / \Delta x\right] \tag{3·1·2}$$

The corrected value then becomes the current value for the next split-difference operator in the sequence.

3.2. Satofuka Method (RRK Method)

In this method, spatial derivatives are approximated by a weighted sum of the values of an unknown function at properly chosen neighboring points to generate a set of ordinary differential equations in time. Then, the resulting set of ordinary differential equations is solved by using an explicit Rational Runge-Kutta (RRK) time integration scheme proposed by Wambecq (1978). This method has the following charactreristics: it is fully explicit and requires no matrix inversion; it is stable at a very long time-step; and is first- or second-order accurate in time. Although it can have an arbitrary order of accuracy in space, we restrict outselves within the second order of accuracy.

The resultant ordinary differential equation can be written by the matrix form as

$$U' = F(U) \tag{3·2·1}$$

where

$$U = (\rho_1, \cdots, \rho_N, \rho u_1, \cdots, \rho u_N, e_1, \cdots, e_N)^T \tag{3·2·2}$$

$$F(U) = (\rho u_1, \cdots, \rho u_N, (p + \rho u^2)_1, \cdots, (p + \rho u^2)_N,$$
$$(p + e)u_1, \cdots, (p + e)u_N)^T \tag{3·2·3}$$

The prime denotes differentiation with respect to time.

The numerical solution of such a system is obtained in the *RRK* technique as follows:

$$g_1 = \Delta t F(U^n) \tag{3·2·4}$$

$$g_2 = \Delta t F(U^n + c_3 g_1) \tag{3·2·5}$$

$$U^{n+1} = U^n + [2g_1(g_1, g_3) - g_3(g_1, g_1)]/(g_3, g_3) \tag{3·2·6}$$

where $g_3 = b_1 g_1 + b_2 g_2$, b_1, b_2 and c_2 are arbitrary constants satisfying the relation, $b_1 + b_2 = 1$ and (d, e) denote the scalar product of vectors d and e. The accuracy of the Satofuka scheme is generally of order 1 in time, but can be of order 2 if, in addition, $b_2 c_2 = -1/2$ is assumed.

Satofuka insisted in his paper (Satofuka, 1981) that a very long time step can be employed in his method without loss of stability. The reason is that the RRK method of order one is $A(\alpha)$-stable (see Appendix A) by the stability discussion (Hairer 1980). If this is the case, the present method seems to be very attractive since it does not need any complex matrix inversions which are characteristic of all implicit techniques.

3.3. New MacCormack Implicit Method

Use of the implicit algorithm results in a faster convergence to the steady state because of a large allowable time step over the conventional explicit schemes. However, it usually requires a large number of arithmetic operations in order to invert scalar or block tridiagonal matrices. The implicjt method proposed by MacCormack in 1982 eliminates this disadvantage by introducing a predictor-corrector scheme requiring the inversion of only block bidiagonal matrices. This method is second-order accurate in space and time, and contains two stages.

The first stage uses the explicit predictor-corrector finitedifference method discussed in 3.1. The second stage removes the stability conditions by transforming numerically the equations of the second stage into an implicit form. The resulting matrix equations to be solved are either upper or lower block bidiagonal equations.

The predictor step is

$$\Delta U_i^n = -\Delta t \Delta_+ F_i^n / \Delta x \tag{3·3·1}$$

$$(I - \Delta t \Delta_+ |B| \cdot /\Delta x) \delta \overline{U}_i^{n+1} = \Delta U_i^n \tag{3·3·2}$$

$$\overline{U}_i^{n+1} = U_i^n + \delta \overline{U}_i^{n+1} \tag{3·3·3}$$

where $|B|$ is a matrix described later.

The corrector step is

$$\Delta \overline{U}_i^{n+1} = -\Delta t \Delta_- \overline{F}_i^{n+1} / \Delta x \tag{3·3·4}$$

$$(I + \Delta t \Delta_- |B| \cdot /\Delta x) \delta U_i^{n+1} = \Delta \overline{U}_i^{n+1} \tag{3·3·5}$$

$$U_i^{n+1} = \frac{1}{2}(U_i^n + \overline{U}_i^{n+1} + \delta U_i^{n+1}) \tag{3·3·6}$$

where $\Delta_+ Z_i/\Delta x$ and $\Delta_- Z_i/\Delta x$ are difference operators defined by

$$\Delta_+ Z_i/\Delta x = (Z_{i+1} - Z_i)/\Delta x \tag{3·3·7}$$

$$\Delta_- Z_i/\Delta x = (Z_i - Z_{i-1})/\Delta x \tag{3·3·8}$$

The Jacobian $B(\equiv \partial F/\partial U)$ is

$$B = \begin{pmatrix} 0 & 1 & 0 \\ (\gamma-3)u^2/2 & (3-\gamma)u & \gamma-1 \\ -\gamma eu/\rho + (\gamma-1)u^3 & \gamma e/\rho - 3(\gamma-1)u^2/2 & \gamma u \end{pmatrix} \tag{3·3·9}$$

It is possible to diagonalize B as

$$B = S_x^{-1} \Lambda_B S_x \tag{3·3·10}$$

$$S_x = \begin{pmatrix} 1-\alpha\beta/a^2 & \beta u/a^2 & -\beta/a^2 \\ \alpha\beta - au & a-\beta u & \beta \\ \alpha\beta + au & -a-\beta u & \beta \end{pmatrix} \tag{3·3·11}$$

$$\Lambda_B = \begin{pmatrix} u & 0 & 0 \\ 0 & u+a & 0 \\ 0 & 0 & u-a \end{pmatrix} \tag{3·3·12}$$

$$S_x^{-1} = \begin{pmatrix} 1 & 1/2a^2 & 1/2a^2 \\ u & (u+a)/2a^2 & (u-a)/2a^2 \\ \alpha & (\alpha+au)/2a^2 + 1/2\beta & (\alpha-au)/2a^2 + 1/2\beta \end{pmatrix} \tag{3·3·13}$$

where a is sound speed, $\alpha = \frac{1}{2}u^2$ and $\beta = \gamma - 1$. Thus, the eigen-values of B are u, $u+a$, and $u-a$.

The matrix $|B|$ appearing in Eqs. $(3·3·2)$ and $(3·3·5)$ is defined as

$$|B| = S_x^{-1} D_B S_x \tag{3·3·14}$$

$$D_B = \begin{pmatrix} \lambda_{A1} & 0 & 0 \\ 0 & \lambda_{A2} & 0 \\ 0 & 0 & \lambda_{A3} \end{pmatrix} \tag{3·3·15}$$

where

$$\lambda_{A1} = \max(|u| - \Delta x/\Delta t, \ 0) \tag{3·3·16}$$

$$\lambda_{A2} = \max(|u+a| - \Delta x/\Delta t, \ 0) \tag{3·3·17}$$

$$\lambda_{A3} = \max(|u-a| - \Delta x/\Delta t, \ 0) \tag{3·3·18}$$

4. Numerical Examples

We consider two representative examples in gas dynamics.

4.1. Shock Tube

The first example is a shock tube problem. The purpose is to know how precisely the methods can describe the time evolution of flows. Let us consider a tube containing a diaphragm which separates a perfect gas at rest initially with different static pressures, but at a uniform temperature. (See Fig. 1-A.) An expansion wave, a contact discontinuity, and a shock wave propagate with rupture of the diaphragm. The initial pressure ratio across the diaphragm was taken as 1 to 0.1.

High pressure section	Low pressure section

A

Shock

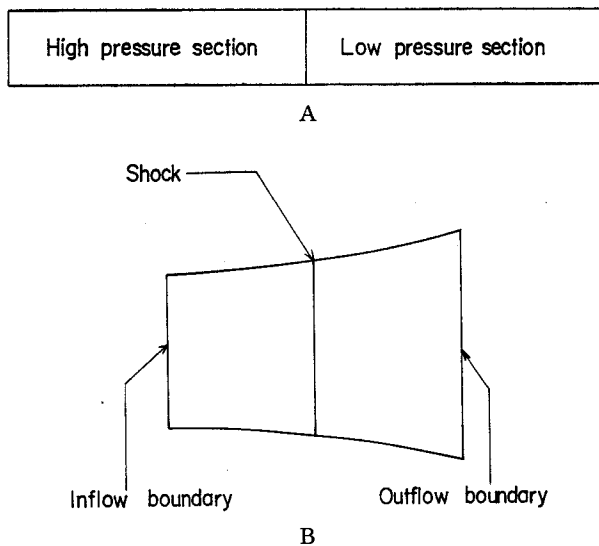Inflow boundary   Outflow boundary

B

Fig. 1.   Geometries for two examples: shock tube problem (A)
and nozzle flow problem (B).

The discontinuity was slightly smeared through five mesh points in order to reduce an unwanted oscillation at the start up.

The initial conditions are:

$$0 \leq x \leq 0.5 \qquad 0.5 \leq x \leq 1.0$$
$$u(x) = 0.0, \qquad u(x) = 0.0$$
$$\rho(x) = 1.0, \qquad \rho(x) = 0.1$$
$$p(x) = 1.0, \qquad p(x) = 0.1$$
$$e(x) = 2.5, \qquad e(x) = 0.25$$

The boundary conditions are:

$$u_1 = 0, \qquad u_N = 0,$$
$$\rho_1 = \rho_2, \qquad \rho_N = \rho_{N-1},$$
$$p_1 = p_2, \qquad p_N = p_{N-1},$$
$$e_1 = e_2, \qquad e_N = e_{N-1}.$$

It is possible to compute analytically the position of the expansion wave, the contact discontinuity and the shock wave, which may be compared with the numerical solutions.

4.2.   Laval Nozzle

The next example is the flow through a Laval nozzle with a prescribed area variation along the axis of the duct. (See Fig. 1-B.) Assuming the variation of the cross-sectional area A to be smooth, we use quasi-one-dimensional approximation here. The quasi-one-dimensional gas dynamic equation is

$$U_t + E_x = A_x H \qquad (4 \cdot 1)$$

where

$$U = \begin{pmatrix} A\rho \\ A\rho u \\ Ae \end{pmatrix}, \quad E = \begin{pmatrix} A\rho u \\ A(\rho u^2 + p) \\ A(e+p)u \end{pmatrix}, \quad H = \begin{pmatrix} 0 \\ p \\ 0 \end{pmatrix} \qquad (4 \cdot 2)$$

The area distribution was chosen to be

$$A(x) = 0.5 + 0.25x^2 \quad 0 \le x \le 1.0 \qquad (4 \cdot 3)$$

This example requires the use of the subsonic outflow boundary condition. The back pressure at $x=1$ is so chosen that a shock is situated at $x=0.5$. The inflow
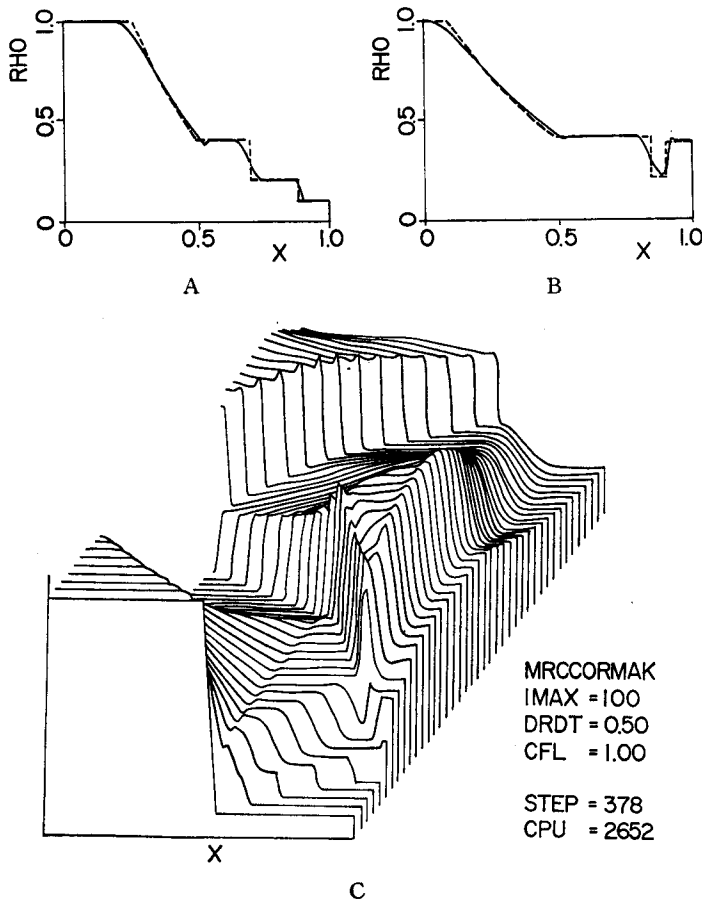

Fig. 2. Results for shock tube problem by the MacCormack method, the upper are the snap shots of density profile at $t=0.2$ and $t=0.35$, and the lower snap shots show the time evolution of the density profile from $t=0.0$ to $t=2.0$. *IMAX* means a number of meshes employed, *DRDT* the allowed maximum variation of density at one time step, *CFL* CFL number, *STEP* a number of steps used, *CPU* a computer processing time consumed.

is prescribed to be supersonic. For an inflow Mach number of 2.0, the numerically obtained pressure distribution is compared with the exact solution.

The initial conditions we employ are:

$$0 \leq x \leq 1.0$$

$$u(x) = 2.0$$

$$\rho(x) = \gamma = 1.4$$

$$p(x) = 1.0 + 3.65x$$

$$e = p/(\gamma - 1) + \frac{1}{2}u^2$$

The inflow boundary conditions are fixed as
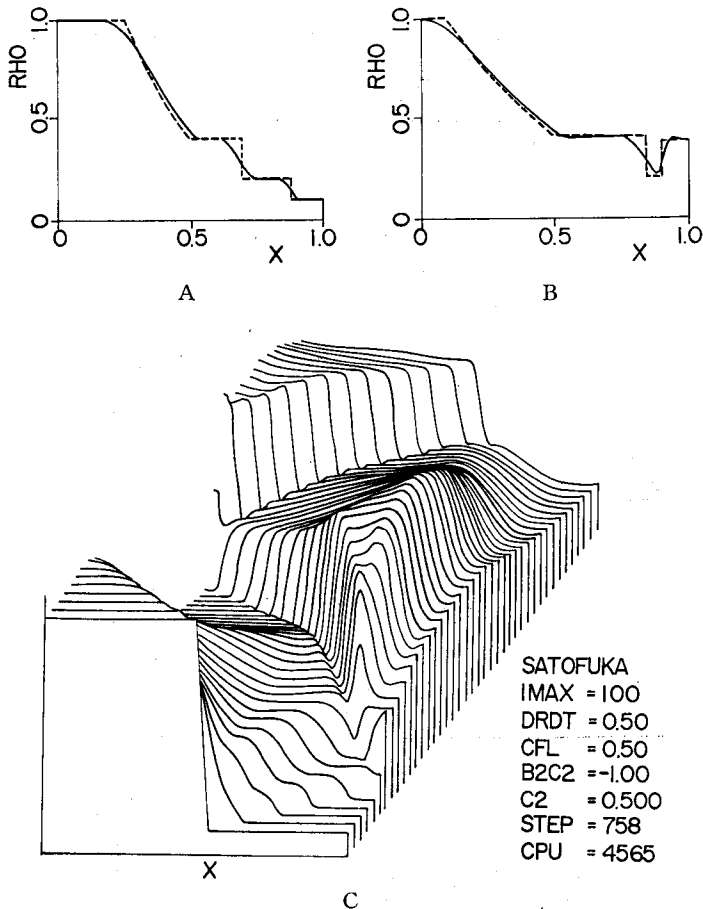
$$p_{in} = 1.0$$

$$u_{in} = 2.0$$

A   B

SATOFUKA
IMAX = 100
DRDT = 0.50
CFL = 0.50
B2C2 = -1.00
C2 = 0.500
STEP = 758
CPU = 4565

C

Fig. 3.   Results by the Satofuka method. The parameter $b_2 c_2$ and c_2 are shown. *CFL* number is 0.5.

$$\rho_{in} = \gamma = 1.4$$
$$e_{in} = 4.5$$

The outflow boundary condition is extrapolated from inner mesh points except the pressure, which is fixed at 4.65.

We introduce fourth order diffusion to avoid small wave length oscillation in our numerical calculation. (See Appendix B.)

5. Results

5.1. Shock tube

In the shock tube problem, we seek the time evolutions of the density distribution and compare them with the analytic solutions.   Figs. 2-A and 2-B are the snapshots of density profile at $t=0.2$ and $t=0.35$ computed by the MacCormack
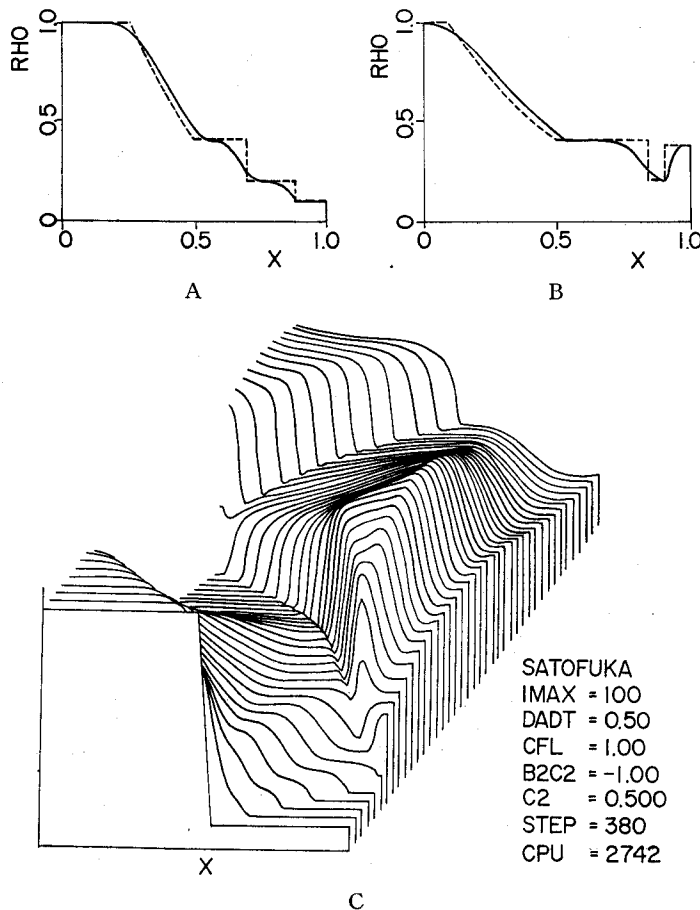
SATOFUKA
IMAX = 100
DADT = 0.50
CFL = 1.00
B2C2 = -1.00
C2 = 0.500
STEP = 380
CPU = 2742

Fig. 4.   Same as Fig. 3 except *CFL* number is 1.

method.   Fig. 2-C shows the time evolution of the density profile from $t=0.0$ to $t=$
2. 0.   We can see the sharp shock profiles, although there exist oscillations called
over shoot behind the shocks.   Although the information of the inside of shocks is
lost, the shock position can be well defined.   Since the conservative form of equa-
tions is adopted, the physical quantities across the shocks are strictly conserved and
the Rankine-Hugoniot relations are satisfied.   The MacCormack method shows good
results in this problem.

Figs. 3-A to 5-C show the results obtained by the Satofuka method.   The Sato-
fuka method shows following features.   When the CFL number is less than 1, the
results agree well with the analytic solution, as can be seen from Figs. 3-A to 3-C.
However, if the CFL number is larger than 1, the time evolution of the density
profile becomes slower than the analytic solution and has a poor profile. (See Figs.
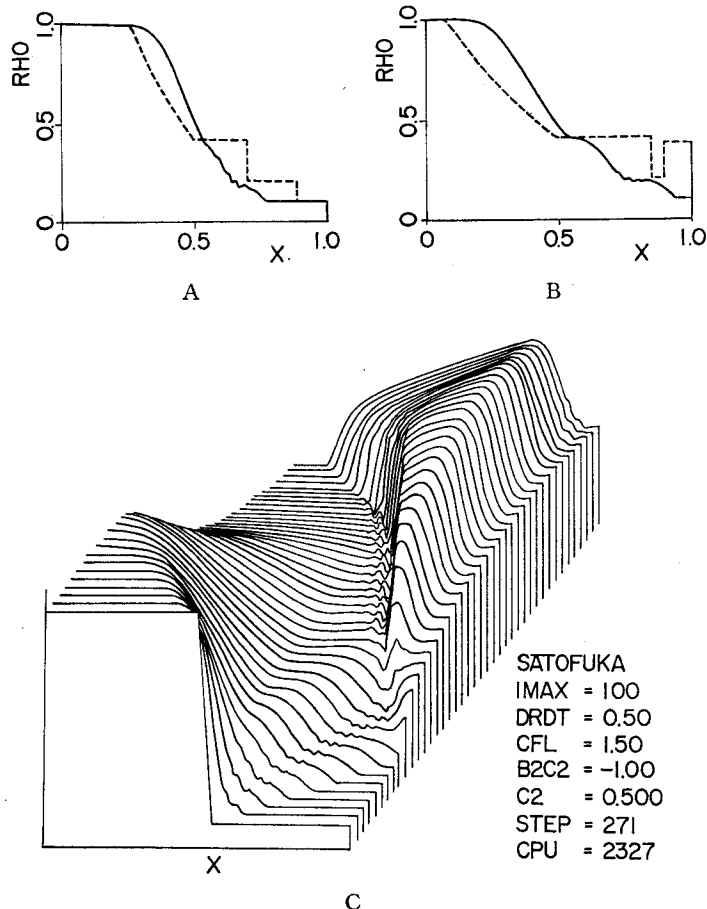

A

B

SATOFUKA
IMAX = 100
DRDT = 0.50
CFL   = 1.50
B2C2 = -1.00
C2   = 0.500
STEP = 271
CPU = 2327

C

Fig. 5.   Same as Fig. 3 except *CFL* number is 1. 5.

5-A to 5-C.) Therefore, we can conclude that in the shock tube problem, the Sato-
fuka method is applicable only if the CFL number is smaller than unity, which is
characteristic of all explicit methods discussed so far.

   Figs. 6-A to 7-C show the results by the New MacCormack method.   In the
New MacCormack method, if the CFL condition is less than 1 the results are iden-
tical to the MacCormack explicit results.   When the CFL number is larger than 1,
the oscillation of profiles grows and the discontinuity profiles become smoother. (See
Figs. 6-A to 6-C.)   Therefore the CFL number should be kept smaller than 1.0 to
obtain precise results.   It is remarkable to see, however, that the New MacCormack
method gives a correct shock position even for such a large CFL number as 5.0.
(See Figs. 7-A to 7-C.)

   In a dynamical problem such as this example, observation of CPU time con-
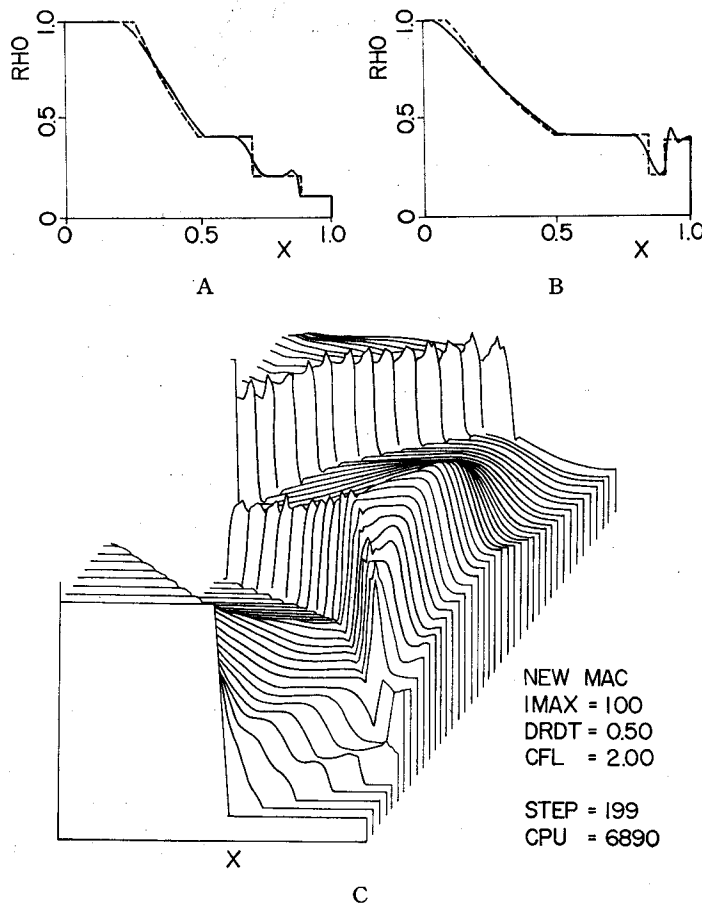

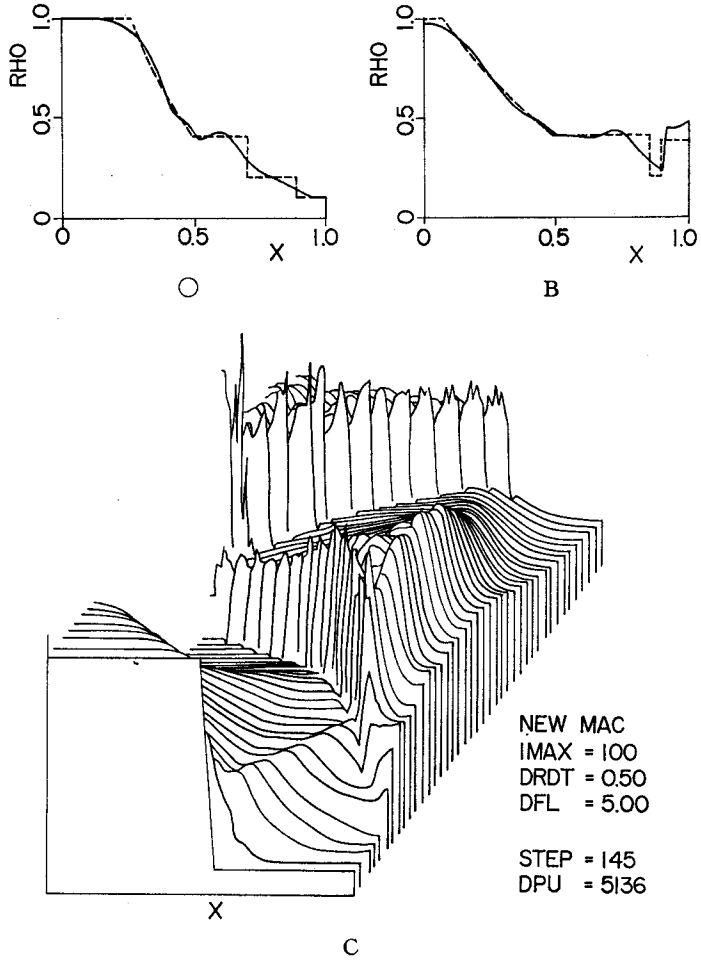Fig. 6.   Results by the New MacCormack method. *CFL* number is 2.

Fig. 7.   Same as Fig. 6 except *CFL* number is 5.

Table 1.   Comparison of CPU time for the shock tube problem.

Method	CFL number	Steps	CPU time (msec)
MacCormack	1.0	378	2,652
Satofuka	0.5	758	4,565
Satofuka	1.0	380	2,742
Satofuka	1.5	271	2,327
New MacCormack	2.0	199	6,890
New MacCormack	5.0	145	5,136

sumed tells us that the explicit second-order method is good. (See Table 1.)

5.2.   Nozzle flow

In the next example we pursue a steady state.   In this case, we wish to obtain

Table 2.   Comparison of CPU time for the nozzle problem.

Method	CFL number	Steps	CPU time (msec)	T
MacCormack	0.5	2,710	13,299	4.20
MacCormack	1.0	1,514	7,246	4.69
Satofuka	0.5	2,432	14,403	3.74
Satofuka	1.0	1,450	8,618	4.50
Satofuka	1.5	—	—	—
New MacCormack	5.0	332	9,452	5.14
New MacCormack	10.0	187	5,445	5.56

In the case of $CFL=1.5$ for the Satofuka method, a steady solution can not be obtained.
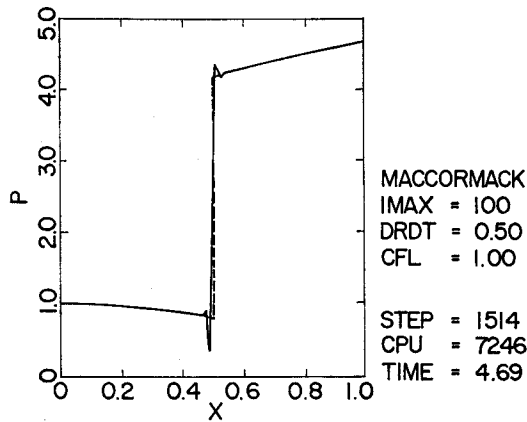
Fig. 8.   Density profile for the nozzle flow at the final steady stare obtained by the MacCormack method. The solid line represents the numerical result and the dotted line the analytical result. *CFL* number is 1.
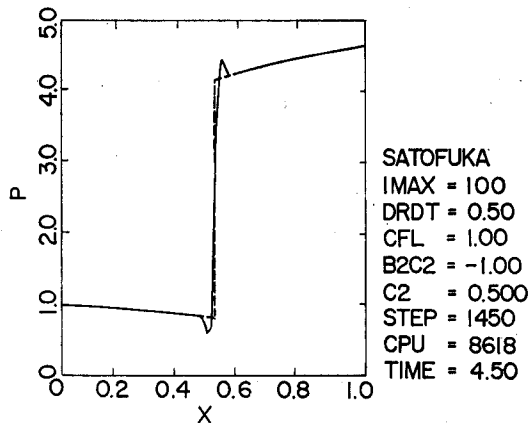

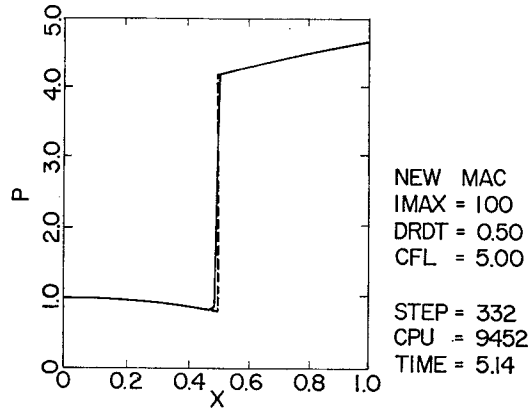Fig. 9.   Result by the Satofuka method. *CFL* number is 1.

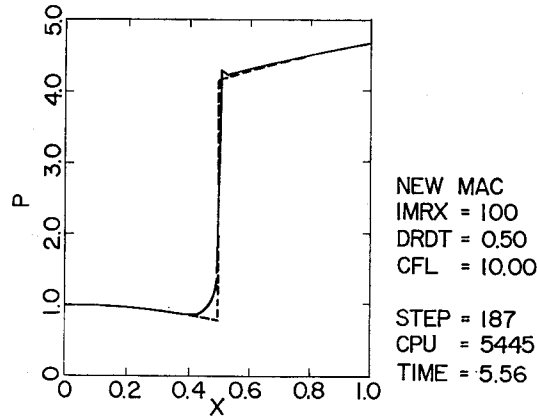Fig. 10.   Result by the New MacCormack method. *CFL* number is 5.

Fig. 11.   Same as Fig. 10 except *CFL* number is 10.

a steady solution in the least CPU time.   We define a solution to be steady when
the density change becomes less than 0. 001 at all mesh points.   From Table 2, it
can be seen that the New MacCormack method requires the least CPU time.   All
methods show a good agreement with the analytic solution except over and under
shoot.   The excellent behavior of the numerical solution near the shock in the pres-
sure distribution in the New MacCormack method is obvious. (See Fig. 10.)   From
Table 2, we can conclude that the New MacCormack method is the most efficient
in the present steady problem.

    We find that the CFL number can be extended only 1. 03 in Satofuka's method
in our experiment, which result is not consistent with Satofuka (1982), who obtained
a CFL number as large as 9600. It seems that a fine tuning of parameters including
artificial viscosity is necessary to reach such a large CFL number.   Therefore, Sato-

fuka's method is not very robust for our Euler equation.

6. Conclusion

From the results of these examples, some conclusions can be drawn about the efficiency of the methods considered.

1. As to the accuracy, we compare the numerical results with the analytic results. The MacCormack method is sufficiently accurate in the propagating shock wave problem. The Satofuka method is accurate if the CFL number is less than unity. If it is larger than unity, the results are different than the analytic results, and can not describe physical quantities properly.

The New MacCormack method gives essentially the same results as the Mac-Cormack results if the CFL number is less then unity. In the second example, the New MacCormack method results give the most accurate shape of shock when the CFL number is equal to 5.0. It is most efficient in such a case.

2. A comparison of the CPU time in such a dynamic problem as the shock tube case tells us that the MacCormack method has good results. If we want to get a steady state solution only, then the New MacCormack method is best, because the CPU time consumed is least.

Acknowledgment

Appendix A   RRK method (Wambecq 1978, Hairer 1980)

Consider the system of differential equations

$$y' = f(y), \quad y(x_0) = y_0$$

where y, y_0, $f(y)$ are elements of R^n (or C^n). The rational Runge-Kutta method of order s for solving the system is defined by

$$y_1 = y_0 + \sum_{i=1}^{s} \sum_{j=1}^{s} w_{ij} g_i g_j / \sum_{k=1}^{s} b_k g_k \qquad (A \cdot 1 \cdot 1)$$

$$g_i = hf\left(y_0 + \sum_{j=1}^{i-1} a_{ij} g_j\right) \quad i = 1, \cdots, s. \qquad (A \cdot 1 \cdot 2)$$

Here, h is the step-size, a_{ij}, w_{ij}, b_k are real parameters and the quotient ab/d is defined in the following way:

$$ab/d = [aRe(b, d) - bRe(d, a) - dRe(a, b)]/(d, d)$$

where (a, b) denotes the scalar product of vectors a and b.

Here, we consider consistent 2-stage rational Runge-Kutta methods:

$$g_1 = hf(y_0) \qquad (A \cdot 2 \cdot 1)$$

$$g_2 = hf(y_0 + c_2 g_1) \qquad\qquad\qquad (A \cdot 2 \cdot 2)$$

$$y_1 = y_0 + g_1 g_1 / (b_1 g_1 + b_2 g_2) \qquad\qquad (A \cdot 2 \cdot 3)$$

$$b_1 + b_2 = 1 \qquad\qquad\qquad\qquad (A \cdot 2 \cdot 4)$$

where b_1, b_2 and c_2 are constants.

The stability region is said to be

A-stable $iff(z \in C \,|\, Re\ z \leq 0)$ is a stability region;

$A(\alpha)$-stable $iff(z \,\|\, \pi - arg\ z \,| \leq \alpha)$ is a stability region;

A_0-stable $iff(x \in R\ x \leq 0)$ is a stability region;

I-stable $iff(iy \,|\, y \in R)$ is a stability region.

Then, the method $(A \cdot 2 \cdot 1)-(A \cdot 2 \cdot 4)$ is

A_0-stable $iff\ b_2 c_2 \leq -1/2$

and

$A(\alpha)$-stable $if\ b_2 c_2 \leq -1/2 \cos(2 - \cos \alpha)$, $(0,\ \pi/2)$

We use $b_2 c_2 = -1.0$ in our calculations, and then our version of the Satofuka method is $A(72.97\ degree)$-stable.

Appendix B Fourth order artificial diffusion

Numerical calculation frequently creates oscillations that remain of finite amplitude, and the computations usually diverge. The normal way to remove these oscillations is to introduce an artificial viscosity or damping factor in the finite difference equations.

The fourth order damping consists of adding a term of a type

$$D = -C \Delta x^4 F_{xxxx}$$

where C is a positive constant. This type of artificial viscosity is easily included in the general scheme in a one-dimensional case, and the stability region of the above scheme is known to be $0 \leq C \leq 1/8$. (See for example R. Peyret T. D. & Taylor, 1983.)

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