APCOM & ISCM

11-14th December, 2013, Singapore

Time-Implicit Gas-Kinetic Scheme

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Abstract

In order to improve the computational efficiency of newly developed gas-kinetic scheme in engineering simulations, the time-implicit GKS is constructed in combination with several common-used time-implicit methods, such as LU-SGS, Point-Relaxation, GMRES and LU-SGS based on the numerical Jacobian matrix. Besides, the Crank-Nicholson method is adopted to achieve second-order accuracy in time. Numerical tests show that implicit schemes based on the numerical Jacobian matrix constructed by gas-kinetic fluxes are better than that based on macroscopic eigen decomposition, due to the distinctive characteristics of GKS, which describes particle movement at the microscopic level. The results also show that the time-implicit technique leads to a significant improvement of computational efficiency.

Keywords: Gas-kinetic scheme, time-implicit, computational efficiency

Introduction

The gas-kinetic scheme (GKS) has shown good performance in various fluid problems, including high speed flows, turbulent flows, etc. When solving engineering problems, besides accuracy, computational efficiency is also an important issue. Therefore in order to improve the computational efficiency, it is worthy to extend GKS to time-implicit.

In researches on time-implicit technique, approximate factorization (AF) has achieved great success. Based on AF, lower-upper symmetric Gauss-Seidel (LU-SGS), point-relaxation (PR), liner-relaxation and etc. have been proposed. In these methods, fluxes are decomposed according to the eigenvalues of Jacobian matrix. Because of simple structure and good stability, these methods, especially LU-SGS, have been widely used in many CFD schemes including GKS (Xu, Mao & Tang, 2005; Li & Fu, 2006). However it is not difficult to notice the shortcomings. First, the approximation decomposition of inviscid fluxes introduces errors, which leads to the spatial accuracy loss of the left side of Eq. (5). Second, the decomposition is based on Euler equations.

When solving viscous problems with Navier-Stokes (NS) equations, the viscous spectral radius is added on diagonal terms directly. This introduces too many approximations to viscosity fluxes. Third, in GKS, the evolution of fluxes is computed by the microscopic distribution function, which is the integral solution of BGK equation,

$$\begin{aligned} f\left(\boldsymbol{x},t,\boldsymbol{u},\xi\right) &= \frac{1}{\tau}\int_0^t g\left(\boldsymbol{x}-\boldsymbol{u}(t-t'),t',\boldsymbol{u},\xi\right)e^{-(t-t')/\tau}dt' \\ &\quad + e^{-t/\tau}\left[\mathrm{H}\left[x-ut\right]f_0^l\left(\boldsymbol{x}-\boldsymbol{u}t\right)+\left(1-\mathrm{H}\left[x-ut\right]\right)f_0^r\left(\boldsymbol{x}-\boldsymbol{u}t\right)\right]. \end{aligned} \tag{1}$$

Here f_0^l and f_0^r are the initial distribution function, g the equilibrium state, H Heaviside function and τ the collision time. Consequently, the mismatch between fluxes and matrix decomposition affects the performances of the implicit methods in GKS. Thus more accurate matrix decomposition is needed. Sun, Wang & Liu (2009) and Zhang & Wang (2004) have proposed implicit method (marked as JA) with the idea of numerical Jacobian matrix, in which the Jacobian is calculated and decomposed from the fluxes only. The method is expected to be more suitable for GKS.

In recent years, generalized minimum residual (GMRES) (Luo, Bauma & Lohner, 2001) has been widely studied. In GMRES, numerical differential is applied in generating the orthogonal basis of Krylov subspace. So the mathematical and physical properties of GKS fluxes can be maintained. It is worth mentioning that the inviscid and viscous fluxes are coupled in GKS. So the numerical Jacobian contains the effect of viscosity naturally. No special treatments on viscosity terms are required. In addition, the numerical Jacobian doesn't lose space accuracy, which keeps the same as the right-side residual items in Eq. (5).

In this paper, the performances of the common-used time-implicit methods are tested in GKS. The second part is an introduction of the numerical schemes. The third part is numerical experiments, which is followed by conclusions.

Time-implicit methods

The time schemes can be written as,

$$\frac{Q^{n+1}-Q^n}{\Delta t} = \varepsilon R\left(Q^n\right)+\left(1-\varepsilon\right)R\left(Q^{n+1}\right). \tag{2}$$

When $\varepsilon = 1$, the scheme is time-explicit. When $\varepsilon = 0$, the scheme is backward-Euler (BE), which is of first-order accuracy in time. When $\varepsilon = 0.5$, the scheme is CN, which is second-order accurate.

The implicit scheme can also be written as,

$$\frac{(1+\phi)\left(Q^{n+1}-Q^{n}\right)-\phi\left(Q^{n}-Q^{n-1}\right)}{\Delta t}=R\left(Q^{n+1}\right). \tag{3}$$

When $\phi = 0.5$, the scheme is second-order accurate, but additional storage for Q^{n-1} is required.

When solving equation (2) or (3), $R\left(Q^{n+1}\right)$ is linearized as,

$$R\left(Q^{n+1}\right)=R\left(Q^{n}\right)+\left(\frac{\partial R}{\partial Q}\right)^{n}\Delta Q^{n},\quad \Delta Q^{n}=Q^{n+1}-Q^{n}. \tag{4}$$

The uniform expression of implicit schemes can be obtained,

$$\left[\frac{I}{\Delta\tau'}-\left(\frac{\partial R}{\partial Q}\right)^{n}\right]\Delta Q=R^{n}+S^{n}. \tag{5}$$

Here S^n is the source term and $\Delta\tau'$ the pseudo-time step. Different implicit schemes focus on different treatments of the left side of Eq. (5). For LU-SGS, the fluxes of the left side are decomposed by maximum eigenvalue. For PR, they are decomposed by positive and negative eigenvalues. For JA, the Jacobian and decomposed fluxes are calculated by numerical differential.

For GMRES, the convergence of solution is related to the condition number of the left-side matrix, which can be reduced by the preconditioner. In the present study, LU-SGS is adopted as the preconditioner.

Among the implicit schemes considered in this paper, LU-SGS is the simplest one, and requires minimal computation and storage cost for a single-step. In PR and JA, the left-side matrix can't be completely diagonalized, so a 5×5 system of equations should be solved at each grid point. Besides, in order to store the numerical Jacobian, JA requires much more storage. In GMRES, the extra storage is little due to the matrix-free approach, and the computational cost for a single-step is determined by the number of orthogonal basis.

Numerical experiments

Case 1: Advection of Density Perturbation

When combined with GKS, the time-implicit schemes are all second-order accurate in time, which can be tested with this one-dimensional case. The computational domain is chosen as $\left[-1,1\right]$. The case is inviscid and the initial condition is set to be (Li, Xu & Fu, 2010),

$$\rho\left(x\right)=1+0.2\sin\left(\pi x\right), U(x)=1, p(x)=1. \tag{6}$$

For this case, the exact solution is,

$$\rho\left(x,t\right)=1+0.2\sin\left(\pi\left(x-t\right)\right),\ U(x,t)=1,\ \ p(x,t)=1. \tag{7}$$

The computed accuracy of different time-implicit schemes is shown in Fig. 1. JA and GMRES show second-order accuracy, while LU-SGS couldn't achieve second-order. As mentioned before, the approximation reduces the accuracy of the matrix in LU-SGS. Although it's nominally second-order accurate in time, the final accuracy couldn't be maintained.

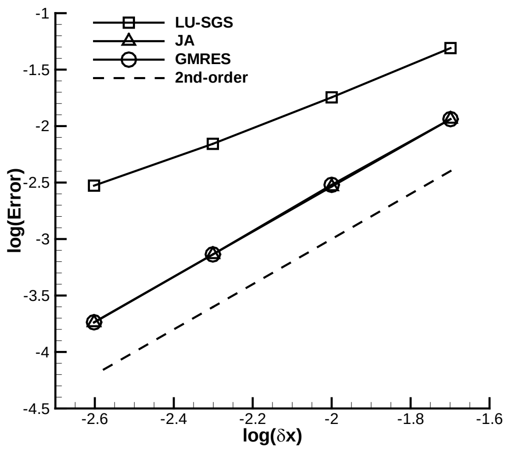

Figure 1 Errors in density vs. cell size of different time-implicit schemes.

Case 2: Sod Shock Tube

The shock tube problem is a typical unsteady case, which can be used to test the performance of the time-implicit scheme in flow field containing shock. The computational domain is chosen as $[-0.5, 0.5]$.The initial condition is set to be (Luo, Bauma & Lohner, 2001),

$$\begin{array}{ll} \rho=1,\ U=0,\ \ p=1.0 & -0.5\le x\le 0 \\ \rho=0.125,\ U=0,\ \ p=0.1 & 0\le x\le 0.5. \end{array} \tag{8}$$

The final computation time is t=0.2. Time steps are set to be 0.004, 0.008 and 0.012. GMRES with BE and CN are used in this case.

Figure 2 shows the distribution of physical quantities computed with different time steps. In the case with shock wave, although the temporal accuracy of CN can't achieve second-order, the solution still shows lower dissipation than the first order. Besides, it can be observed that the time step has little effect on the results, which is important for time-implicit scheme.

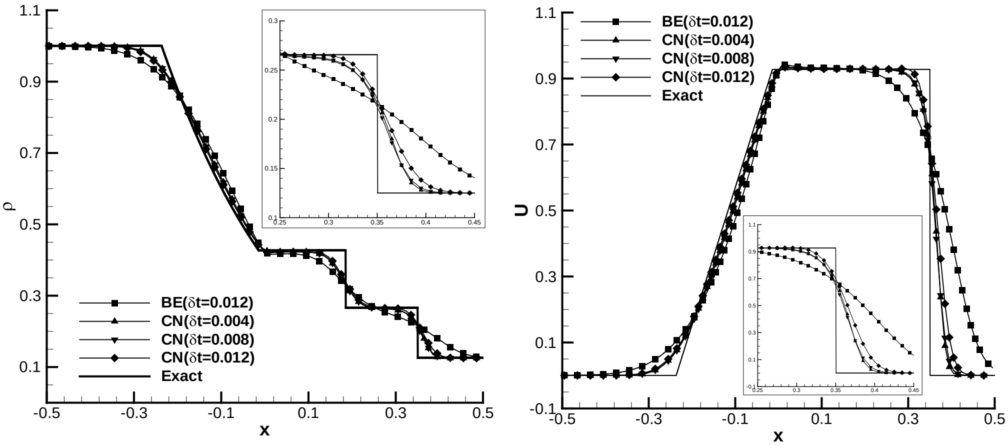

Figure 2 Density and velocity distributions predicted by GMRES.

Case 3: Cavity Flow

This case is chosen to test the computational efficiency of time-implicit schemes when dealing with steady flow problems. A grid with 128×128 cells is used. The computation condition is set to be (Su, Xu & Ghidaoui, 1999),

$$Ma = 0.15, \ \ \mathrm{Re} = 100. \tag{9}$$

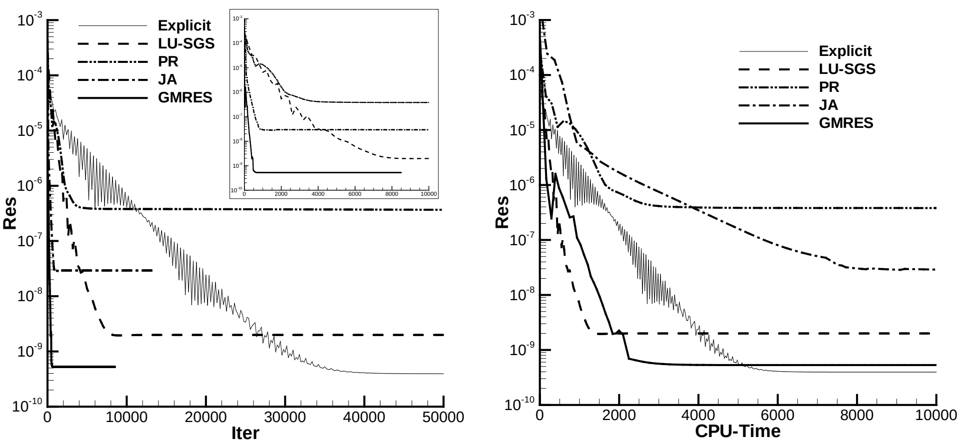

Figure 3 Computational efficiency (Left: iterations, Right: CPU-time).

As shown in Fig. 3, the iteration number for implicit schemes to achieve steady state is dramatically reduced when compared with the explicit method, especially for

GMRES and JA. However, in respect of CPU time, LU-SGS still has superiority, while JA is the most time-consuming one among these schemes.

Figure 4 presents the velocity distributions along the central lines calculated by different time-implicit schemes. The results agree well with each other, which confirm the reliability of the implicit schemes. However it can be found that there is some difference between the present calculations and Ghia's data. This comes from the flux construction, not the time-implicit techniques, where the quasi-one-dimensional extension is adopted for the sake of computational cost, which can introduce large dissipation (Li & Fu, 2006a). In order to illustrate this, the multidimensional flux, where the tangential slopes are included at a cell interface, is tried in the same test case. As shown in Fig. 5, with the help of multidimensional flux, GKS-GMRES, as well as the explicit scheme, yields much better results.

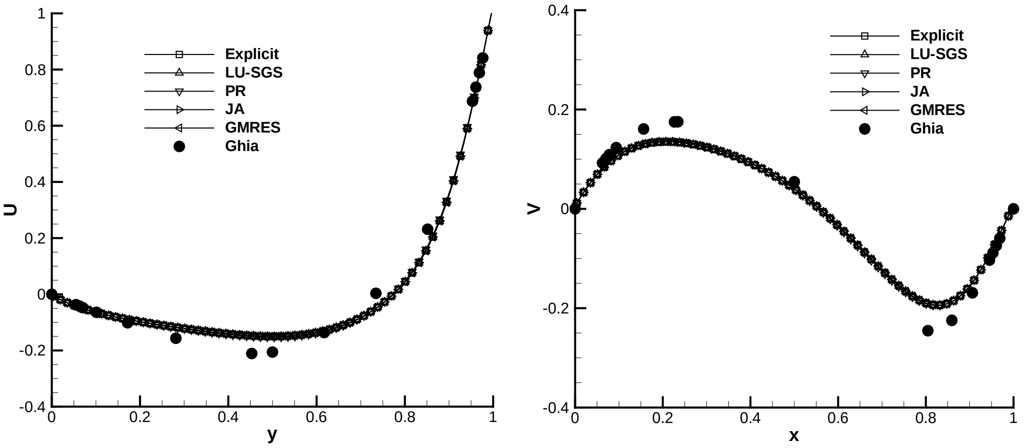

Figure 4 Velocity distributions along vertical and horizontal lines.

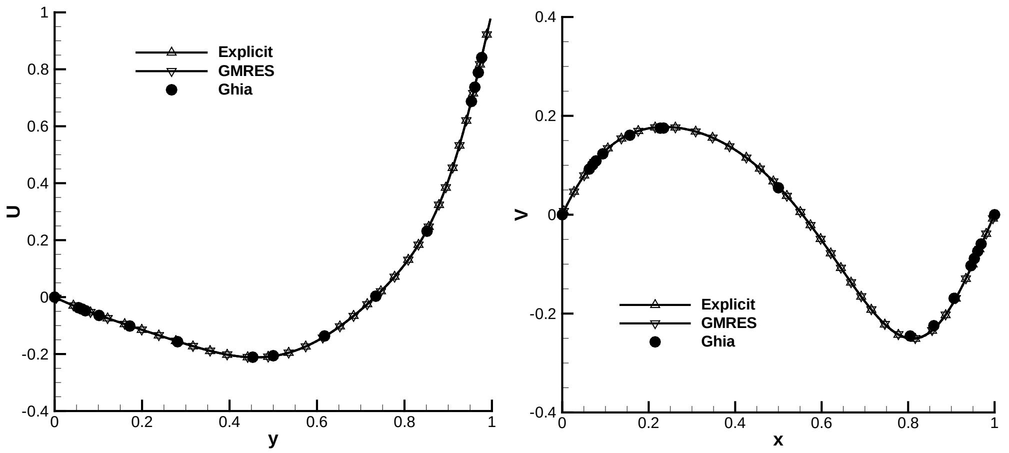

Figure 5 Velocity distributions along vertical and horizontal lines computed with multidimensional schemes.

Case 4: Rotating Flow inside 3D Cavity

A cubic box rotates along an axis in the z-direction and drive the internal fluid. The computational condition is set as (Jin, Xu & Chen, 2010),

$$\begin{aligned} &\omega_z = 1,\ \ Ma = 0.15,\ \ \mathrm{Re} = 1000 \\ &N_x \times N_y \times N_z = 64 \times 64 \times 64. \end{aligned} \qquad (10)$$

In order to keep the rotating speed of the cavity and simplify the boundary conditions, moving mesh technique is applied in this simulation.

Figure 6 shows the velocity profile in the symmetry plane along the vertical centerline after one cycle ($t = 2\pi$). When the explicit scheme is adopted, about 10000 iterations are required in one cycle. With GMRES, 128 iterations are satisfactory, which can give acceptable results compared with the explicit computation. With 1024 iterations, the difference can hardly be observed. So it can be concluded that the time-implicit technique has effectively improved the computational efficiency of GKS in three-dimensional unsteady flow.

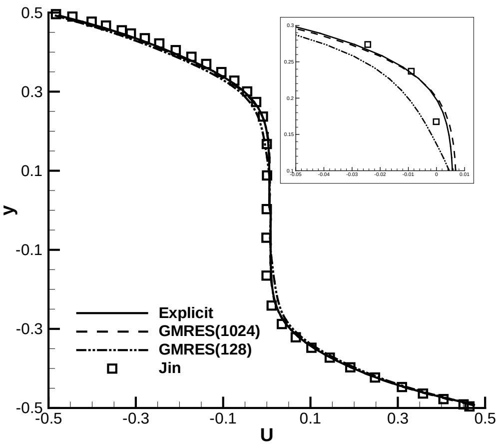

Figure 6 Velocity distributions along vertical central lines in the symmetry plane.

Conclusions

In this paper, the time-implicit GKS is constructed in combination with common-used time-implicit techniques and validated by several typical test cases. The results show a remarkable improvement of the time-implicit GKS in computational efficiency while preserving second-order accuracy. For flow with discontinuities, such as shocks, the scheme can still keep high accuracy.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Project No. 11172154, 10932005).

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