Modified KFVS (m-KFVS) method with velocity dependent dissipation control function

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Abstract. The first order kinetic flux vector split scheme is found to be more dissipative, resulting in smearing of discontinuties. In this paper we have proposed a modified $kfvs$ based on $MCIR$ splitting with a molecular velocity dependent dissipation control function. Different choices for the dissipation control function and the corresponding physical arguments have been presented. The $m-kfvs$ split fluxes are presented. The corresponding split flux Jacobians and the coefficient of numerical dissipation are studied. The scheme is tested on some standard test cases and the results are presented. The $m-kfvs$ scheme is shown to be non-oscillatory at discontinuties and near second order accurate in smooth regions.

Keywords: kfvs, modified-CIR (MCIR), mpde, dissipation.

1 Introduction

The Kinetic Flux Vector Split scheme [4, 7] commonly known as $kfvs$ is an upwind scheme based on the moment method strategy [4] where an upwind scheme is developed at the Boltzmann level and taking moments we arrive at an upwind scheme for the conservation laws of gas dynamics. To capture the discontinuties sharply and for resolving various flow features, a numerical scheme should have less dissipation. The usual first order $kfvs$ scheme is found to be more dissipative, resulting in smearing of discontinuties. However, higher order accurate schemes have been employed for better accuracy and for reducing the numerical dissipation considerably. To control the dissipation in the first order $kfvs$ scheme, Deshpande [8] has proposed a modified way of CIR splitting, namely MCIR splitting of the molecular velocity by introducing a dissipation control function. Using the above idea and with suitable choices for the dissipation control function, low dissipation and single point shock capturing kinetic schemes [5, 6, 8, 1] have been developed recently.

In this paper we pursue yet another version of low dissipative modified $kfvs$ method based on MCIR splitting with molecular velocity dependent dissipation control functions.

2 Basic theory of kinetic schemes

We now explain the basic concepts of $kfvs$ scheme with reference to $1D$ unsteady Euler equations. Consider the $1D$ Boltzmann equation in the Euler limit

$$\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} = 0 \tag{1}$$

Where F is the Maxwellian velocity distribution function given by

$$F = \frac{\rho}{I_0}\sqrt{\frac{\beta}{\pi}}\exp\left[-\beta(v-u)^2 - I/I_0\right] \tag{2}$$

The $1D$ Euler equations can then be obtained as Ψ-moments of the Boltzmann equation (1). That is

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} \;=\; \left\langle \Psi,\; \frac{\partial F}{\partial t} + \frac{\partial (vF)}{\partial x} \right\rangle \;=\; 0 \tag{3}$$

The moment function vector Ψ is defined by

$$\Psi = \left[1 \quad v \quad I + \tfrac{v^2}{2}\right]^T$$

Using CIR splitting of the molecular veolcity and replacing the spatial derivatives with respective finite difference approximations, we get

$$\left(\frac{\partial F}{\partial t}\right)_j + \frac{v+|v|}{2}\frac{F_j - F_{j-1}}{\Delta x} + \frac{v-|v|}{2}\frac{F_{j+1}-F_j}{\Delta x} = 0 \tag{4}$$

Using Taylor series, eq. (4) gives the modified partial differential equation (mpde),

$$\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} = \frac{\Delta x}{2}|v|F_{xx} + O\big(\Delta x^2\big) \tag{5}$$

The leading term in the truncation error shows that the upwind scheme for (1) based on CIR splitting is first order accurate and is dissipative.

3 Modified CIR (MCIR) splitting

The mpde given by eq. (5) shows that $|v|$ contributes to the numerical dissipation. To reduce the dissipation, Deshpande [8] has introduced a dissipation control function ϕ as a multiplying factor for $|v|$. The modified CIR (MCIR) splitting is given by

$$v = v^+ + v^- = \frac{v+|v|\phi}{2} + \frac{v-|v|\phi}{2} \tag{6}$$

It is important to note that $v^+ \neq 0$ for $v < 0$ and $v^- \neq 0$ for $v > 0$. The excessive dissipation in the usual CIR scheme can be reduced because of some downwind effect present in the MCIR scheme. Due to this, v^+ and v^- are never zero regardless of sign of v. Using the above defined MCIR splitting, the mpde analysis for the Boltzmann equation (1) gives

$$\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} = \frac{\Delta x}{2}|v|(\phi F)_{xx} + O\big(\Delta x^2\big) \tag{7}$$

Taking the Ψ - moments, we get the mpde corresponding to $1D$ Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = \frac{\Delta x}{2}\int\limits_{\mathbb{R}^+\times\mathbb{R}} \Psi|v|(\phi F)_{xx}\,dv\,dI + O\big(\Delta x^2\big) \tag{8}$$

It is evident from the above equation that $\phi = 0$ leads to central differencing and $\phi = 1$ gives the usual first order *kfvs* method. Thus, by tuning ϕ such that $0 < \phi \leq 1$ we can control the numerical dissipation and hence order of accuracy. At exactly $\phi = 0$, the numerical scheme is known to be unstable.

4 Choices for the function ϕ

We now present different choices [1] for the dissipation control function ϕ, which is a non linear function of molecular velocity v. Let us consider the mpde obtained in the eq. (8). When $\Psi = 1$, the mpde corresponding to the mass balance equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = \frac{\partial^2}{\partial x^2}\left[\frac{\Delta x}{2}\int\limits_{\mathbb{R}^+\times\mathbb{R}} |v|\phi\frac{\rho}{I_0}\sqrt{\frac{\beta}{\pi}}e^{-\beta(v-u)^2 - I/I_0}dvdI\right] = \frac{\partial^2}{\partial x^2}\Big[\nu_{num}\rho\Big] \tag{9}$$

where ν_{num} is the kinematic numerical viscosity given by

$$\nu_{num} = \frac{\Delta x}{2}\sqrt{\frac{\beta}{\pi}}\int\limits_{\mathbb{R}} |v|\phi e^{-\beta(v-u)^2}dv \tag{10}$$

From the above equation we observe that when $\phi = 1$, maximum contribution to the numerical viscosity comes from particles with velocities close to u, i.e., $c = v - u \approx 0$. Particles with large $|c|$ contribute very little to ν_{num}. If we can suitably weight the particles contributing maximum to ν_{num}, then we can reduce the numerical viscosity in the scheme. The control function ϕ plays this role. Based on these arguments Anil and Deshpande [1] have considered two choices for ϕ, given by

$$\phi = e^{-\frac{\alpha}{|v|}} \qquad \text{and} \qquad \phi = e^{-\alpha|v|} \tag{11}$$

where α could be a mesh dependent function, which we will define later. Note that, for both the choices, we have $\alpha \to 0 \Rightarrow \phi = 1$ and $\alpha \to \infty \Rightarrow \phi = 0$, resulting in first order accurate *kfvs* and central differencing schemes respectively.

When $\phi = e^{-\frac{\alpha}{|v|}}$, for particles with $|v| \ll \alpha$, that is, for low velocity particles the function ϕ is very small and hence contributes very less to ν_{num}. The high velocity particles for which $|v| \gg \alpha \Rightarrow \phi \approx 1$ contribute to the numerical dissipation. In the case of $\phi = e^{-\alpha|v|}$, the low velocity particles, that is, particles for which $\alpha|v| \ll 1$ contribute most to ν_{num}. Obviously, particles for which $\alpha|v| \gg 1$ will contribute very little to kinematic numerical viscosity. Thus, it is possible to weight the velocity space suitably for reducing the dissipation.

Let us understand more about low and high velocity molecules. Consider the steady $1D$ Boltzmann equation with a BGK - model for the collision terms

$$v\frac{\partial f}{\partial x} = A(F - f) \tag{12}$$

Here, f is the velocity distribution function, A^{-1} the relaxation time scale and F the local Maxwellian velocity distribution function. Using the interating factor $e^{Ax/v}$ we can write the solution of (12) as

$$f(x,v) = f(x_0,v)e^{-\frac{A}{v}(x-x_0)} + \int\limits_{x_0}^{x}\frac{A}{v}F(x')e^{\frac{A}{v}(x'-x_0)}dx', \quad v > 0 \tag{13}$$

Assuming $F(x')$ to be a constant over the interval $x_0 \le x' \le x$ (which is $\simeq \Delta x$), we get

$$f(x,v) = f(x_0,v)e^{-\frac{A}{v}(x-x_0)} + F\Big[1 - e^{-\frac{A}{v}(x-x_0)}\Big] \tag{14}$$

It is clear from the above equation that the low velocity molecules are almost always lost (in the sense of loss term in the Boltzmann equation) while high velocity molecules are lost negligibly, that is, they travel

over Δx without any collision. Therefore, it makes sense in using a weight function in velocity space which has the above property. The choice of $\phi = e^{-\frac{\alpha}{|v|}}$ is therefore consistent with the above physical argument. The second choice $\phi = e^{-\alpha|v|}$ leads to much simpler formulae for split fluxes and is shown in the next section.

5 Modified kfvs split fluxes

The $m - kfvs$ split fluxes denoted by $Gm^{\pm}$ are given by

$$Gm^{\pm} = \left\langle \Psi, \frac{v \pm |v|\phi}{2} F \right\rangle = \int\limits_{\mathbb{R}^+ \times \mathbb{R}} \Psi \frac{v \pm |v|\phi}{2} F dv dI \tag{15}$$

For the choice $\phi = e^{-\frac{\alpha}{|v|}}$, closed form expressions for the split fluxes are not available. Also, numerical integration is found to be very expensive. However, some asymptotic and series expansions are available. Anil and Deshpande [1] has observed that the evaluation of the split fluxes using these expressions is computationally expensive and causes some loss in accuracy.

For the second choice, $\phi = e^{-\alpha|v|}$, closed form expressions are available and are given by

$$Gm^{\pm} = \frac{G}{2} \pm \frac{1}{2}\left[e^{\left(\frac{\alpha^2}{4\beta} - \alpha u\right)} G^{+}\left(u - \frac{\alpha}{2\beta}\right) - e^{\left(\frac{\alpha^2}{4\beta} + \alpha u\right)} G^{-}\left(u + \frac{\alpha}{2\beta}\right)\right] \tag{16}$$

where G is the unsplit flux, $G^{\pm}$ are the usual *kfvs* split fluxes for the $1D$ Euler equations. The parameter α can be non-dimensionalised by $\tilde{\alpha} = \frac{\alpha}{\sqrt{\beta}}$. Note that, these expressions are simpler as they are similar to that of *kfvs* split fluxes, except that it involves some exponentials and the arguments of error function are different. Anil et al. [2] have numerically found that for $\tilde{\alpha} \approx 4.0$, $Gm^{\pm} \approx \frac{G}{2}$. Which clearly shows that the upwinding is lost completely. The modified split kinetic flux Jacobians $Am^{\pm}$ are given by

$$Am^{\pm} = \frac{\partial Gm^{\pm}}{\partial U} \tag{17}$$

Since $Gm^{\pm}$ are functions of $\tilde{\alpha}$, and for the case of $\tilde{\alpha} = 0$, we get the Jacobians corresponding to $kfvs$ fluxes. As $\tilde{\alpha}$ increases from zero, the eigenvalues move away from the $kfvs$ case and at $\tilde{\alpha} \approx 4.0$ the eigenvalues become half the eigenvalues of the full flux Jacobian.

To find the numerical dissipation, rewriting (8) as

$$\frac{\partial U}{\partial t} + A\frac{\partial U}{\partial x} = \frac{\partial}{\partial x}\left[\frac{\Delta x}{2}\frac{\partial}{\partial U}\left(Gm^{+} - Gm^{-}\right)\frac{\partial U}{\partial x}\right] + O\left(\Delta x\right)^2 \tag{18}$$

where A is the full flux Jacobian and let us denote $D = \frac{\Delta x}{2}\frac{\partial}{\partial U}\left(Gm^{+} - Gm^{-}\right)$. For the upwind scheme based on $m - kfvs$ to have positive dissipation, the dissipation matrix D should be positive definite. That is, all the eigen values must be real positve and non-zero. Fig. 2 shows that the eigenvalues of D are approaching zero as $\tilde{\alpha}$ increases. A more detailed information on the modified split flux Jacobians and the dissipation analysis are presented in [2]. Thus, by choosing proper $\tilde{\alpha}$ we can reduce the numerical dissipation and can get near second order accuracy in smooth regions although the formal order of accuracy is first order.

6 Results and Discussion

We now illustrate the performance of $m - kfvs$ method by applying it to standard test cases for one-dimensional flows. Based on a sensor[1], near the discontinuity a low value of $\tilde{\alpha}$ is chosen in such a way that the solution is non-oscillatory and discontinuties are not unduly smeared. In smooth regions a high value of $\tilde{\alpha}$ is chosen so that we can obtain near second order accuracy.

6.1 Convergent-divergent nozzle problem:

The *m-kfvs* scheme has been applied to a convergent-divergent nozzle problem. The Maxwellian distribution function and the split fluxes for this quasi-one-dimensional flow are presented in [1]. Numerical simulations are performed on a uniform grid with 61 cells. Fig. 1(a) shows the pressure distribution through the nozzle. Numerical results show that the *m-kfvs* scheme is less dissipative and captures the shock more accurately when compared to *kfvs*. Although the formal order of accuracy is first order, the computed results are in very good agreement with well-known second order accurate MacCormack scheme. Fig. 1(b) shows the corresponding variation in $\tilde{\alpha}$.

6.2 Shock tube problem:

The initial conditions are chosen with a pressure jump of 2 across the shock. Numerical solutions are performed on the computational domain $0 \leq x \leq 1$ with 500 equally spaced cells. Fig. 3 shows the results obtained using *m-kfvs* method with $\phi = e^{-\frac{\alpha}{|v|}}$ and $\phi = e^{-\alpha|v|}$. It has been observed that the *m-kfvs* method captures the discontinuties more crisply compared to usual first order accurate *kfvs* method and very good accuracy is achieved in smooth regions. Fig. 3(c) shows the variation in $\tilde{\alpha}$ after the final solution.

7 Conclusions

The *m-kfvs* method based on MCIR splitting with dissipation control functions $\phi = e^{-\frac{\alpha}{|v|}}$ or $\phi = e^{-\alpha|v|}$ sharply resolves the discontinuties without spurious oscillations and nearly second order accuracy is achieved in smooth regions. The choice $\phi = e^{-\alpha|v|}$ is preferred as the expressions for the modified split fluxes are simpler and computationally the method based on these fluxes is almost as fast as the first order *kfvs* method. Some more mathematical analysis and numerical experiments are required to find the optimal value of $\tilde{\alpha}$.

The potential value addition of the above idea to existing finite volume or grid free codes based on *kfvs* is immense. Just by changing the expressions for the split fluxes in the flux calculation subroutine will yield *m-kfvs* based codes having less numerical disipation, resulting in accurate capture of leading edge suction, crisp shocks, negligible loss of stagnation pressure in isentropic regions and accurate prediction of vortex dominated flows.

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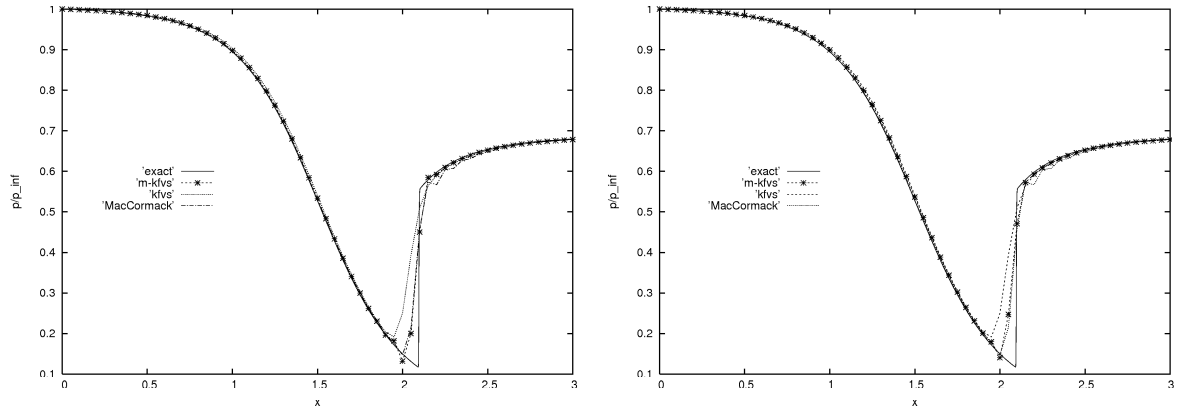
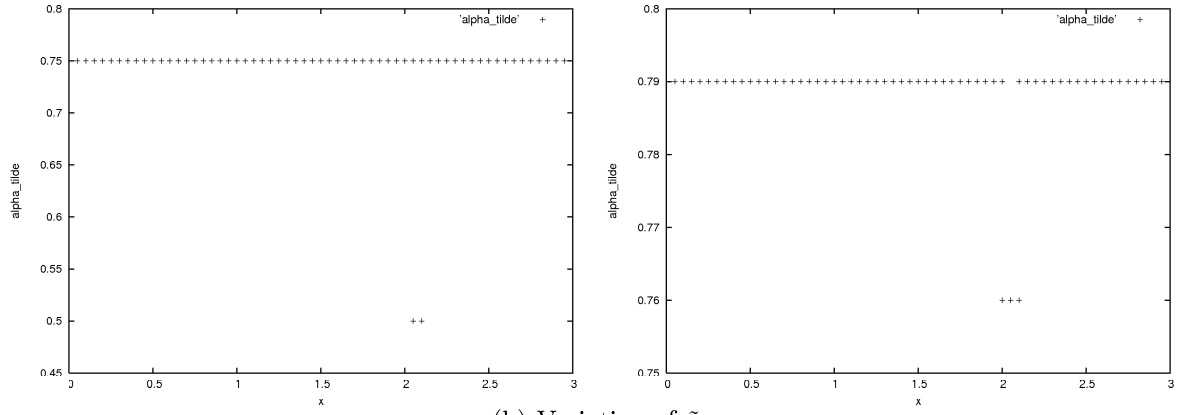
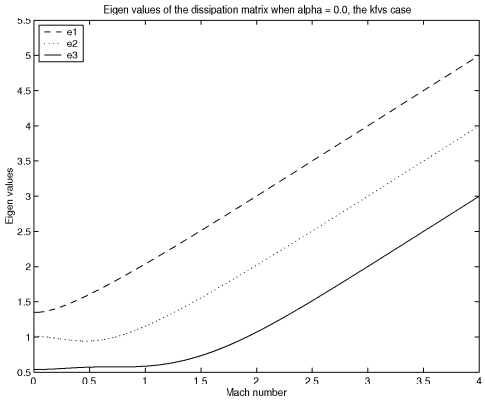


(a) Pressure distribution through the nozzle

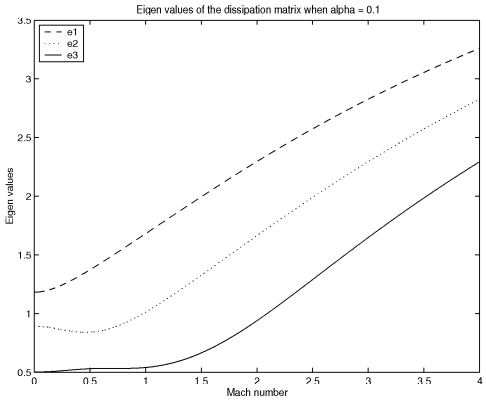


(b) Variation of $\tilde{\alpha}$

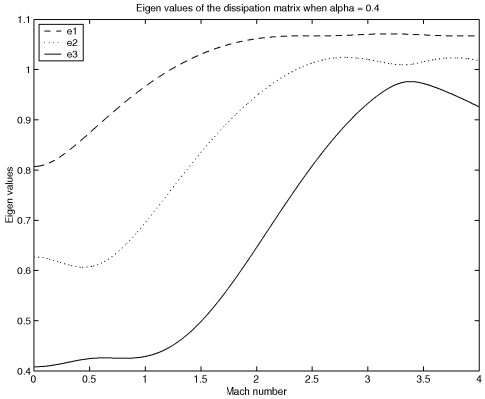
Figure 1: Convergent divergent nozzle problem using the choices $\phi = e^{-\frac{\alpha}{|v|}}$ (left column) and $\phi = e^{-\alpha|v|}$ (right column). Computed results are compared with first order *kfvs*, second order MacCormack scheme and exact solution.



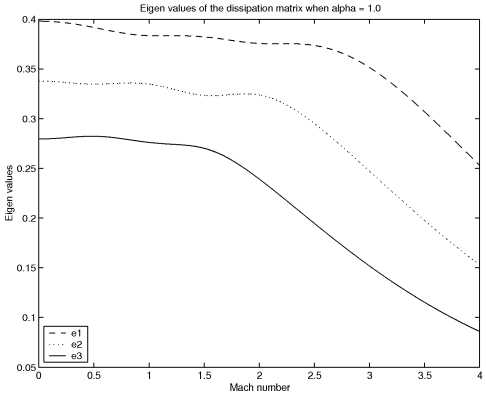
$\tilde{\alpha} = 0.0$



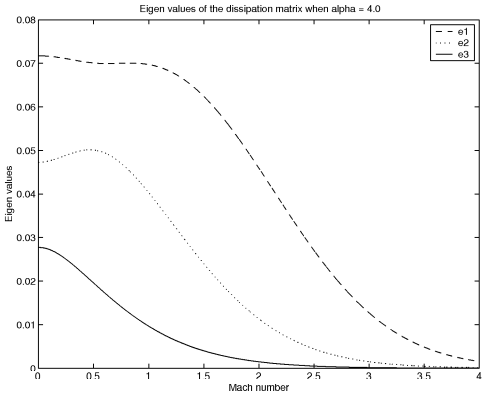
$\tilde{\alpha} = 0.1$



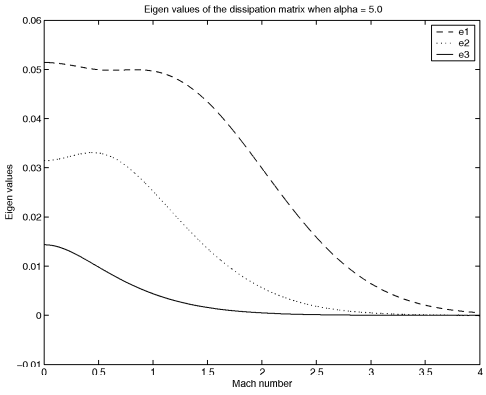
$\tilde{\alpha} = 0.4$



$\tilde{\alpha} = 1.0$

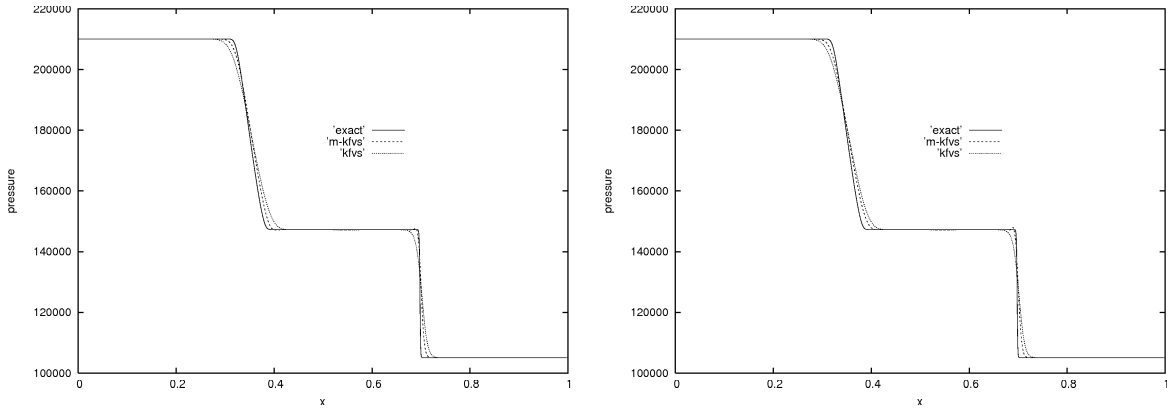


$\tilde{\alpha} = 4.0$

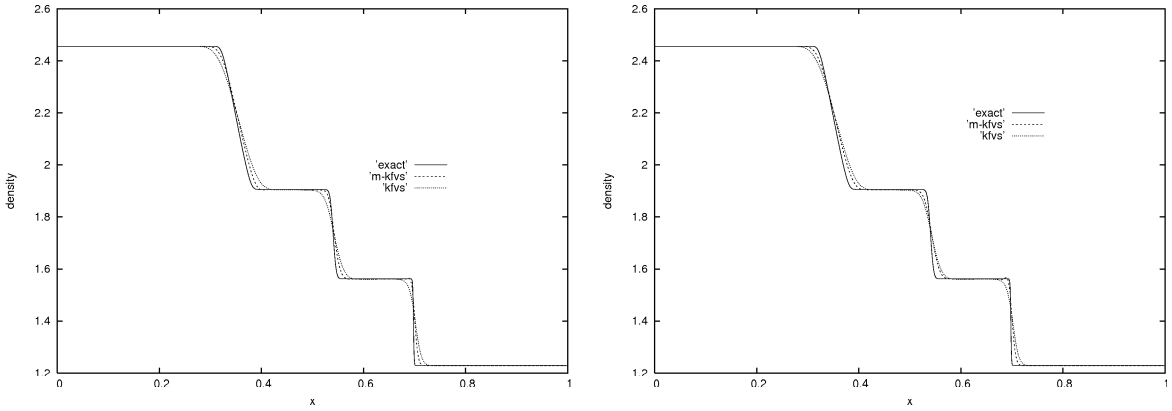


$\tilde{\alpha} = 5.0$

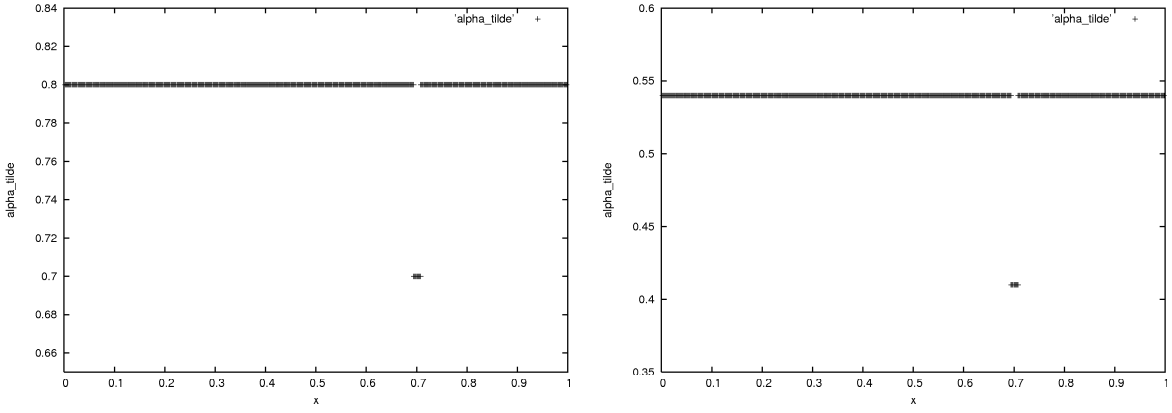
Figure 2: Eigen values of the dissipation matrix based on m-kfvs are plotted with Mach number for different values of $\tilde{\alpha}$.



(a) Pressure plot



(b) Density plot



(c) Variation of $\tilde{\alpha}$

Figure 3: Shock tube problem using *m-kfvs* with $\phi = e^{-\frac{\alpha}{|v|}}$ (left column) and $\phi = e^{-\alpha|v|}$ (right column). Computed results are compared with first order *kfvs* scheme and exact solution.