Modified KFVS (M-KFVS) Method

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1 Introduction

The kinetic flux vector split scheme (*kfvs*) is an upwind scheme which belongs to the family of Boltzmann equation based numerical schemes. It has been demonstrated to be very robust and has been applied to many problems of practical interest [2, 3, 12]. The *kfvs* scheme is based on the moment-method-strategy [7] where an upwind scheme is developed at the Boltzmann level and then taking suitable moments, we arrive at an upwind scheme for the Euler or Navier-Stokes equations.

To capture the discontinuties crisply 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 [13, 14] has suggested 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 functions for the dissipation control function, low dissipation and single point shock capturing kinetic schemes [8, 9, 13, 4] have been developed recently.

In this paper we present a low dissipative modified *kfvs* (*m-kfvs*) method based on MCIR splitting with molecular velocity dependent dissipation control functions.

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2 Basic theory of kinetic schemes

We now explain the basic concepts of *kfvs* scheme with reference to $1D$ unsteady Euler equations given by

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = 0 \tag{1}$$

where U is the vector of conserved variables and G is the flux vector. The above conservation law can be obtained by taking the Ψ - moments of the $1D$ Boltzmann equation in the Euler limit

$$\frac{\partial F}{\partial t} + \frac{\partial (vF)}{\partial x} = 0 \tag{2}$$

where F is the Maxwellian velocity distribution function given by

$$F = \frac{\rho}{I_0}\sqrt{\frac{\beta}{\pi}} \exp\left[-\beta(v-u)^2 - I/I_0\right] \tag{3}$$

where ρ density, v molecular velocity, u fluid velocity, I internal energy variable, $\beta = 1/(2RT)$, R gas constant per unit mass, T absolute temperature and I_0 the internal energy due to nontranslational degrees of freedom, given by $I_0 = (3-\gamma)/(4(\gamma-1)\beta)$. The moment function vector Ψ is defined by

$$\Psi = \begin{bmatrix} 1 \\ v \\ I + \frac{v^2}{2} \end{bmatrix}$$

The Euler equations (1) can then be cast in the form

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} \;=\; \left\langle \Psi,\; \frac{\partial F}{\partial t} + \frac{\partial (vF)}{\partial x} \right\rangle \;=\; 0 \tag{4}$$

and the inner product $\langle \Psi,\; f \rangle$ is defined by

$$\langle \Psi,\; f \rangle \;=\; \int\limits_{\mathbb{R}^+ \times \mathbb{R}} \Psi f(v) dv dI \tag{5}$$

Using CIR splitting [6], eq. (2) gives the semidiscretised upwind scheme for the Boltzmann equation,

$$\left(\frac{\partial F}{\partial t}\right)_j + \frac{v+|v|}{2}\frac{F_j - F_{j-1}}{\Delta x} + \frac{v-|v|}{2}\frac{F_{j+1} - F_j}{\Delta x} = 0 \tag{6}$$

Taking the Ψ - moments with a suitable approximation to the time derivative, we arrive at an upwind scheme for the Euler equations. Using Taylor series, eq. (6) gives the modified partial differential equation (mpde),

$$\frac{\partial F}{\partial t} + \frac{\partial (vF)}{\partial x} = \frac{\Delta x}{2}|v|F_{xx} + O\left(\Delta x^2\right) \tag{7}$$

showing that the upwind scheme for the $1D$ Boltzmann equation using CIR splitting is first order accurate and is dissipative. To control the numerical dissipation, modified way of CIR (MCIR) splitting is presented in the next section.

3 MCIR splitting

The mpde defined by eq. (7) shows that $|v|$ contributes to the numerical dissipation. To reduce the dissipation, Deshpande [14] has introduced a dissipation control function ϕ as a multiplying factor for $|v|$. The modified CIR (MCIR) splitting containing the function ϕ is given by

$$v = v^{+} + v^{-} = \frac{v + |v|\phi}{2} + \frac{v - |v|\phi}{2} \tag{8}$$

Using the above defined MCIR splitting, the corresponding semidiscretised Boltzmann equation is given as

$$\left(\frac{\partial F}{\partial t}\right)_j + \frac{v + |v|\phi}{2}\frac{F_j - F_{j-1}}{\Delta x} + \frac{v - |v|\phi}{2}\frac{F_{j+1} - F_j}{\Delta x} = 0 \tag{9}$$

for which the mpde is given by

$$\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} = \frac{\Delta x}{2}|v|(\phi F)_{xx} + O\big(\Delta x^2\big) \tag{10}$$

Taking the Ψ - moments, we arrive at

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = \frac{\Delta x}{2}\int\limits_{\mathbb{R}^+\times\mathbb{R}} \Psi|v|(\phi F)_{xx}dvdI + O\big(\Delta x^2\big) \tag{11}$$

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.

4 Mathematical models for ϕ

In this section we present different choices 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. (11). When $\Psi = 1$, the mpde corresponding to the mass balance equation is given by

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= \frac{\partial^2}{\partial x^2}\left[\frac{\Delta x}{2}\int\limits_{\mathbb{R}^+\times\mathbb{R}} |v|\phi\frac{\rho}{I_0}\sqrt{\frac{\beta}{\pi}}e^{-\beta(v-u)^2 - I/I_0}dvdI\right] \\ &= \frac{\partial^2}{\partial x^2}\Big[\nu_{num}\rho\Big]\end{aligned} \tag{12}$$

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

$$\nu_{num} = \frac{\Delta x}{2}\sqrt{\frac{\beta}{\pi}}\int_{\mathbb{R}} |v|\phi e^{-\beta(v-u)^2} dv \tag{13}$$

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 [4] have considered two choices for ϕ, given by

$$\phi = e^{-\frac{\alpha}{|v|}} \qquad \text{and} \qquad \phi = e^{-\alpha|v|} \tag{14}$$

where α could be a mesh dependent function, which we will define later. Note that, for both the models, 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. It is possible to weight the velocity space suitably for reducing the dissipation. A detailed analyses of these models is presented in [4].

5 Modified kfvs split fluxes

We now present the closed form expressions for the split fluxes in *m-kfvs* method using the dissipation control functions discussed in the previous section. These split fluxes are denoted by $Gm^{\pm}$ and are given by

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

Note that, when $\phi = 1$ we get $Gm^{\pm} = G^{\pm}_{kfvs}$, the usual first order *kfvs* split fluxes.

5.0.1 For the model $\phi = e^{-\frac{\alpha}{|v|}}$:

The expressions for the *m-kfvs* split fluxes using the first choice $\phi = e^{-\frac{\alpha}{|v|}}$ are given by

$$Gm^{\pm} = \frac{G}{2} \pm \frac{\rho}{2}\sqrt{\frac{\beta}{\pi}} \begin{bmatrix} \frac{1}{\beta}\left(J_1^+ + J_1^-\right) \\ \frac{1}{\beta^{3/2}}\left(J_2^+ - J_2^-\right) \\ \frac{I_0}{\beta}\left(J_1^+ + J_1^-\right) + \frac{1}{\beta^2}\left(J_3^+ + J_3^-\right) \end{bmatrix} \tag{16}$$

where G is the unsplit flux, $J_n^{\pm} = J_n(A, \pm S)$ and the function $J_n(A, S)$ given in [5] is defined by

$$J_n(A, S) = \int_0^{\infty} v^n e^{-(v-S)^2 - \frac{A}{v}} dv \tag{17}$$

where $A = \alpha\sqrt{\beta}$ and $S = u\sqrt{\beta}$. The function $J_n(A, S)$, $\forall A, S \in R$ and $A > 0$ is not in general reducible to any of the standard tabulated definite integrals. Also, numerical integration of the function is difficult and very expensive. However, depending on the value of A and S convergent series [1] and asymptotic expansions [5] of the integral $J_n(A, S)$ are available [4]. Anil and Deshpande [4] has observed that the evaluation of the split fluxes using these expressions is computationally expensive. Also, there will be a loss in accuracy due to these expressions, which are accurate upto two decimal places for some range of values of A and S.

5.0.2 The second model, $\phi = e^{-\alpha|v|}$:

In this case the expressions for the split fluxes are given by

$$Gm^{\pm} = \frac{G}{2} \pm \frac{1}{2}\left[e^{\left(\frac{\alpha^2}{4\beta} - \alpha u\right)} G^+\left(u - \frac{\alpha}{2\beta}\right) - e^{\left(\frac{\alpha^2}{4\beta} + \alpha u\right)} G^-\left(u + \frac{\alpha}{2\beta}\right)\right] \tag{18}$$

where G is the unsplit flux, $G^{\pm}$ are the usual *kfvs* split fluxes for the $1D$ Euler equations. 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. Computationally, the evaluation of these fluxes take the same amount of time as that of *kfvs* split fluxes, except that it involves the evaluation of one more error function. Further, $\alpha = 0$ gives the standard *kfvs* fluxes [11].

6 A finite volume method based on m-kfvs

In this section we derive a numerical scheme based on *m-kfvs* for the $1D$ Euler equations. Consider the $1D$ Boltzmann equation given by (2)

$$\frac{\partial F}{\partial t} + \frac{\partial (vF)}{\partial x} = 0$$

Using MCIR splitting of the molecular velocity v and a finite volume based discretization of the spatial derivative, the above equation reduces to

$$\Delta x \left(\frac{\partial F}{\partial t} \right)_j^n + \Big[(v^+F)_j - (v^+F)_{j-1} \Big]^n + \Big[(v^-F)_{j+1} - (v^-F)_j \Big]^n = 0 \quad (19)$$

Replacing the time derivative by a forward difference approximation and taking the Ψ - moments, we get

$$U_j^{n+1} = U_j^n + \frac{\Delta t}{\Delta x} \Big[\Big\{ Gm_j^+ - Gm_{j-1}^+ \Big\}^n + \Big\{ Gm_{j+1}^- - Gm_j^- \Big\}^n \Big] \qquad (20)$$

which is a numerical scheme for the $1D$ Euler equations based on *m-kfvs* method and and $Gm^\pm$ are the corresponding split fluxes, given by the equations (16) and (18). It can be easily shown that the above scheme is generally first order accurate in space and time. However, the dissipation in the numerical scheme can be controlled by choosing proper value of α. The modified split fluxes $Gm^\pm$ are nonlinear functions of parameter α. We now choose values of α for both the models. Some case is required in choice of α to ensure conservation.

Conservation of scheme (20) is ensured if $G_{j+\frac{1}{2}} = Gm_j^+ + Gm_{j+1}^-$ cancels when two cells C_j and C_{j+1} are considered together. This condition implies that $G_{j+\frac{1}{2}}$ appearing in state update of cell j must be equal to $G_{j+\frac{1}{2}}$ appearing in state update of cell C_{j+1}. Hence there must be only one value of α_j at each j. This is best ensured by specifying

$$\alpha_j = \begin{cases} \tilde{\alpha}_d / \sqrt{\beta}_r, & \text{for } \phi = e^{-\frac{\alpha}{|v|}} \\ \tilde{\alpha}_d \sqrt{\beta}_r, & \text{for } \phi = e^{-\alpha |v|} \end{cases} \qquad (21)$$

where suffix d stands for discontinuous region and β_r is reference value of β. In regions of smooth variation, we specify

$$\alpha_j = \begin{cases} \tilde{\alpha}_s / \sqrt{\beta}_r, & \text{for } \phi = e^{-\frac{\alpha}{|v|}} \\ \tilde{\alpha}_s \sqrt{\beta}_r, & \text{for } \phi = e^{-\alpha |v|} \end{cases} \qquad (22)$$

Obviously, $\tilde{\alpha}_s$ has to be large in smooth regions to ensure low dissipation or low ν_{num}. A sensor is required to decide when $\tilde{\alpha} = \tilde{\alpha}_d$ and $\tilde{\alpha} = \tilde{\alpha}_s$. One possibility is maxmod (opposite of minmod) sensor, that is, define

$$S_j = Max\left\{\frac{|f_j - f_{j-1}|}{\frac{1}{2}|f_j + f_{j+1}|}, \frac{|f_{j+1} - f_j|}{\frac{1}{2}|f_{j+1} + f_j|}\right\} \tag{23}$$

where f could be ρ, p or e. Based on sensor value S_j, we can switch from $\tilde{\alpha}_s$ or $\tilde{\alpha}_d$. Near discontinuity, $\tilde{\alpha}_d$ is specified to ensure non-oscillatory solution.

7 Results and Discussion

We now illustrate the performance of *m-kfvs* method (20) by applying it to standard test cases for one-dimensional flows. Numerical solutions are compared with the results obtained using first order accurate *kfvs* method and exact solution.

7.1 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. Figures 1 and 2 show the results obtained using *m-kfvs* method with $\phi = e^{-\frac{\alpha}{|v|}}$ and $\phi = e^{-\alpha|v|}$ respectively. 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. Figures 1(c) and 2(c) show the variation in $\tilde{\alpha}$ after the final solution.

7.2 Convergent-divergent nozzle problem:

The *m-kfvs* scheme has been applied to a convergent-divergent nozzle problem [10]. This is a steady state test case with flow being quasi one dimensional, inviscid and compressible. Numerical simulations are performed on a uniform grid with 61 cells. Figures 3(a) and 4(b) show 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*. The computed results are in very good agreement with well-known second order accurate MacCormack scheme. Figures 3(b) and 4(b) show the corresponding variation in $\tilde{\alpha}$.

8 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 model $\phi = e^{-\alpha|v|}$ 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. In the case of $\phi = e^{-\frac{\alpha}{|v|}}$, there will be some loss in accuracy due to the expressions for the modified split fluxes and computationally they are more expensive.
The MCIR idea can be easily extended to higher dimensions. Infact, 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. Some more mathematical analysis and numerical experiments are obviously required to find the optimal value of α.

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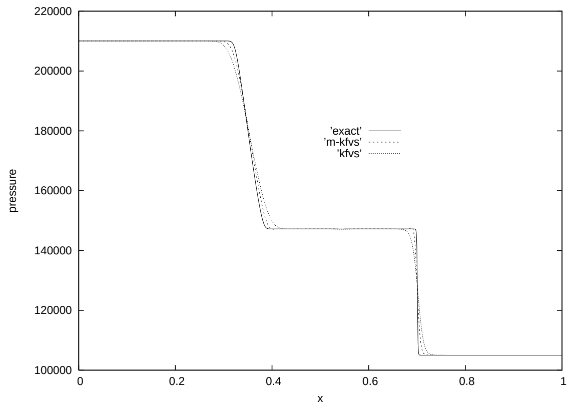
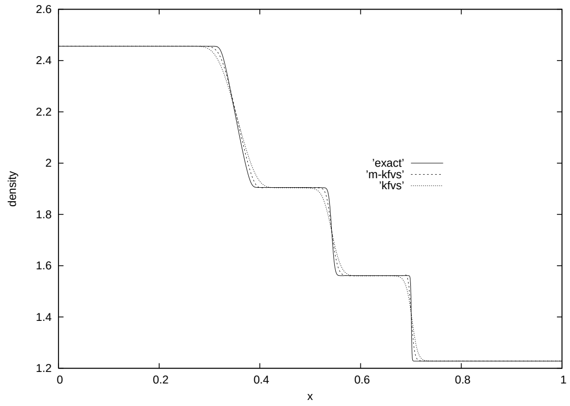
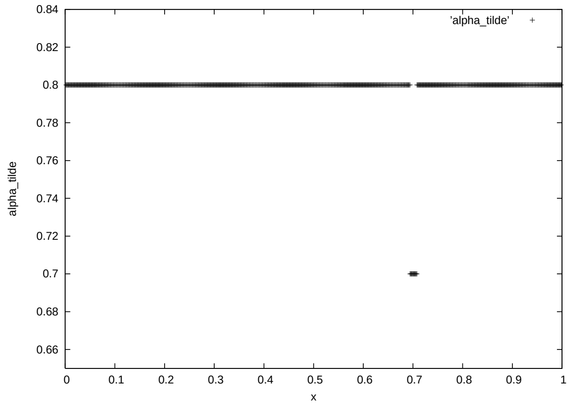


(a) Pressure plot

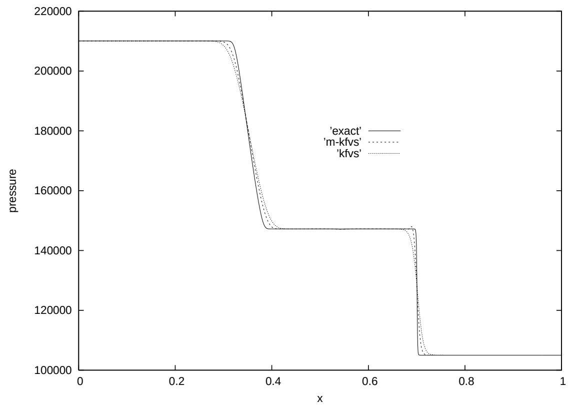


(b) Density plot

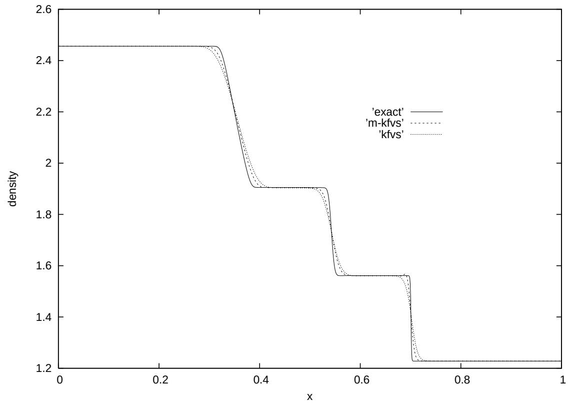


(c) Variation of $\tilde{\alpha}$

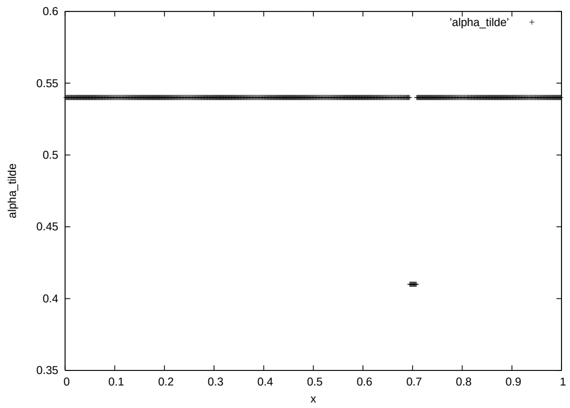
Figure 1: Shock tube problem using *m-kfvs* with $\phi = e^{-\frac{\alpha}{|v|}}$. Computed results are compared with first order *kfvs* scheme and exact solution.



(a) Pressure plot

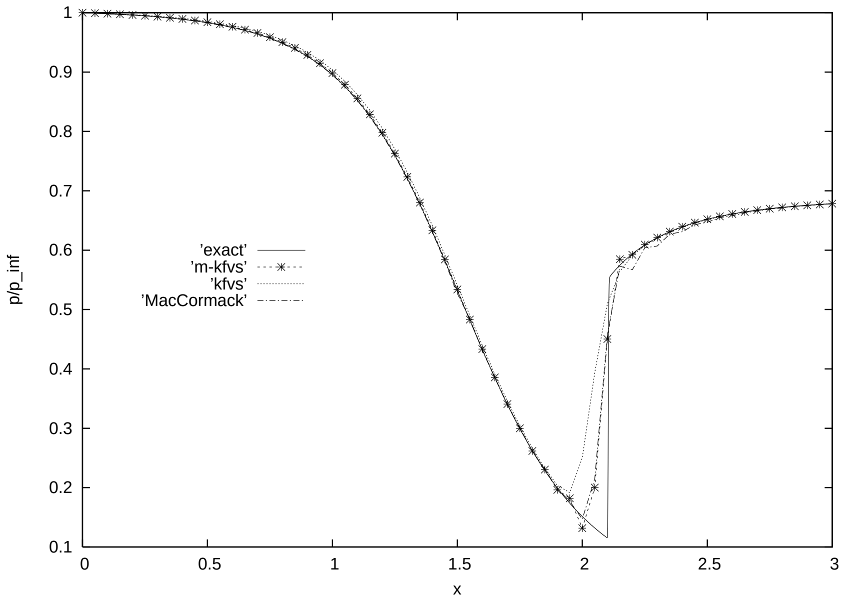


(b) Density plot

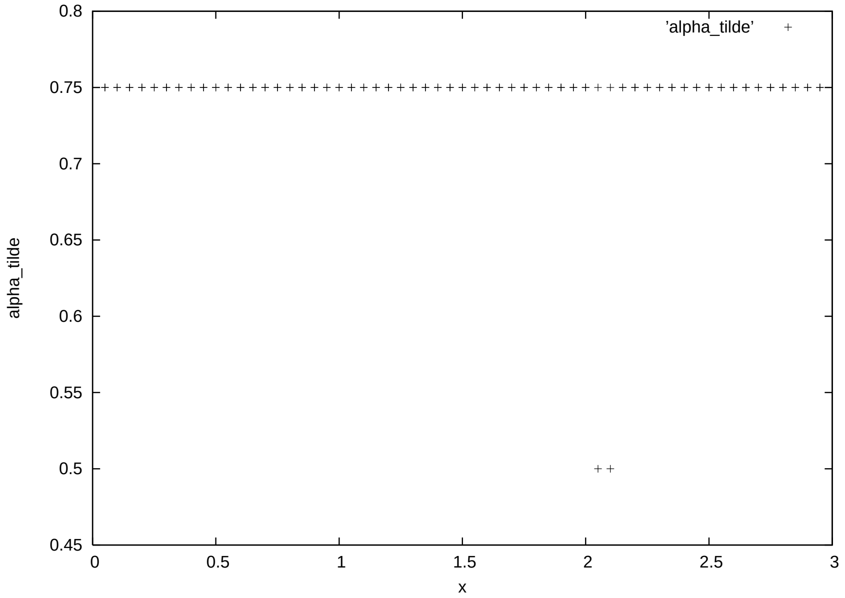


(c) Variation of $\tilde{\alpha}$

Figure 2: Shock tube problem using *m-kfvs* with $\phi = e^{-\alpha|v|}$. Computed results are compared with first order *kfvs* scheme and exact solution.

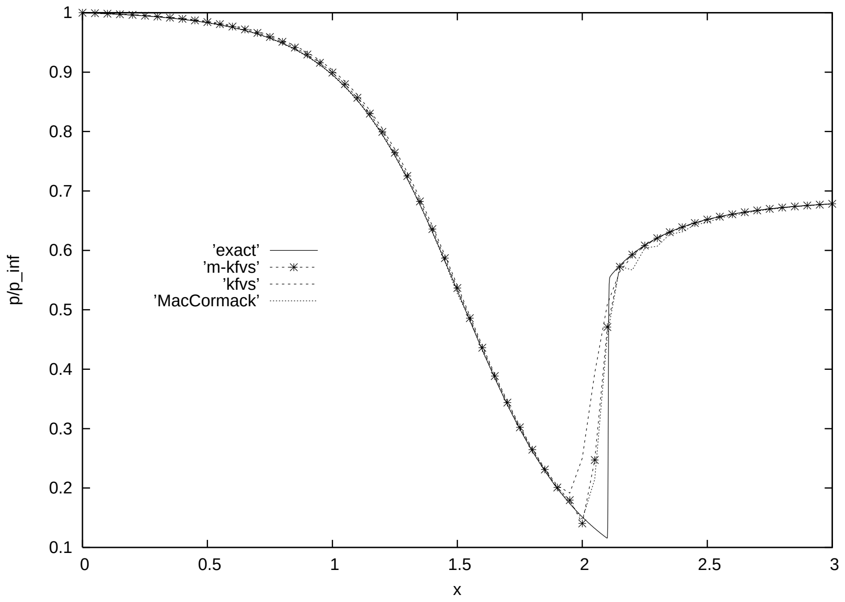


(a) Pressure distribution through the nozzle

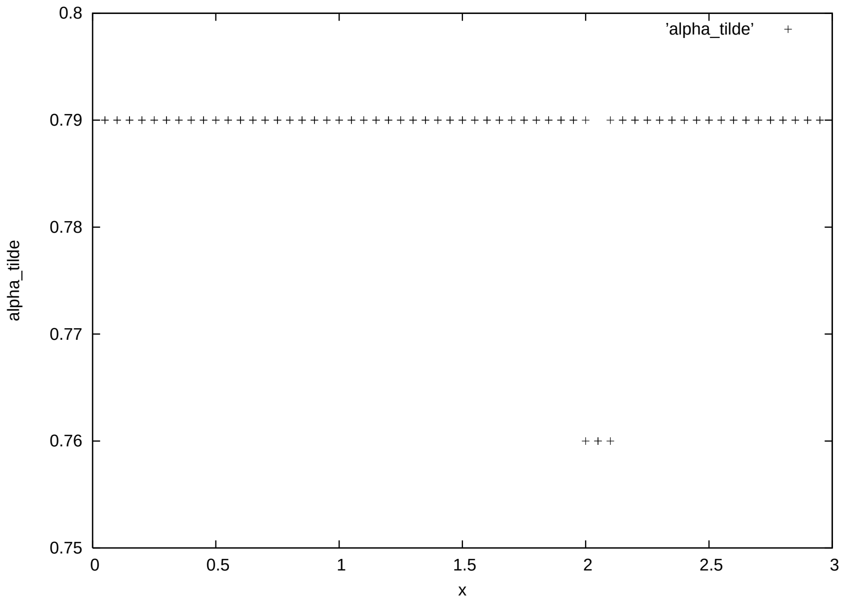


(c) Variation of $\tilde{\alpha}$

Figure 3: Convergent divergent nozzle problem using the model $\alpha = e^{-\frac{\tilde{\alpha}}{|v|}}$. Computed results are compared with first order *kfvs*, second order MacCormack scheme and exact solution.



(a) Pressure distribution through the nozzle



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

Figure 4: Convergent divergent nozzle problem using the model $\alpha = e^{-\alpha|v|}$. Computed results are compared with first order *kfvs*, second order MacCormack scheme and exact solution.