Adjoint based optimal control of dissipation in kinetic schemes

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Abstract

To resolve many flow features accurately, like accurate capture of suction peak in case of subsonic flows or crisp shocks in flows with discontinuities or to minimise the loss in stagnation pressure or even flow separation in viscous flows requires an accurate and low dissipative numerical scheme. It has been found that the first order Kinetic Flux Vector Split (KFVS) scheme is more dissipative. However, numerical dissipation can be reduced either by *h*-refinement or *p*-refinement or a combination of both, which requires more computational time and memory. In this paper we present a low dissipative modified KFVS (m-KFVS) method with molecular velocity dependent dissipation control function by still using the first order stencil. However, the dissipation generated by m-KFVS may not be minimal and hence the dissipation control vector is in general not optimal. The m-KFVS solver is then combined with discrete adjoint solver to find the optimal dissipation control vector, which results in minimal numerical dissipation. Numerical results are presented for standard inviscid test cases based on m-KFVS and m-KFVS-adjoint methods.

Keywords: Kinetic schemes, m-KFVS, MCIR splitting, optimal control of dissipation, discrete adjoint optimisation.

1 Modified KFVS (M-KFVS) Method

The kinetic schemes, also known as the Boltzmann schemes are based on the moment-methodstrategy [4] where upwinding is done at the Boltzmann level and after taking suitable moments we arrive at an upwind scheme for the governing Euler or Navier-Stokes equations. The Kinetic Flux Vector Split (KFVS) scheme [11, 5], which belongs to the family of kinetic schemes has been extensively used to compute inviscid as well as viscous flows around many complex configurations over the past two decades [11, 1, 12, 10]. In this paper we pursue yet another

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kinetic scheme known as modified KFVS (m-KFVS) method. We first briefly present the basic concepts of KFVS method w.r.t. 1D Euler equations. Consider the CIR split 1D Boltzmann equation

$$\frac{\partial F}{\partial t} + \frac{v + |v|}{2} \frac{\partial F}{\partial x} + \frac{v - |v|}{2} \frac{\partial F}{\partial x} = 0$$
(1)

where, F is the Maxwellian velocity distribution function. Replacing the spatial derivatives with respective finite difference approximations and using Taylor series expansion, we get the modified partial differential equation (*mpde*)

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

showing that the scheme is first order accurate and highly dissipative as the entire molecular velocity space, |v| contributes to the dissipation. However, higher order kinetic schemes [7, 1] have been developed but they require more points in the stencil and hence consume more computational time. To reduce the numerical dissipation in the first order scheme, a modified CIR (MCIR) splitting [13] has been introduced

$$v = v^{+} + v^{-} = \frac{v + |v|\phi}{2} + \frac{v - |v|\phi}{2}$$
(3)

where, ϕ is a dissipation control function. The MCIR split 1D Boltzmann equation is given by

$$\frac{\partial F}{\partial t} + \frac{v + |v|\phi}{2}\frac{\partial F}{\partial x} + \frac{v - |v|\phi}{2}\frac{\partial F}{\partial x} = 0$$
(4)

and the corresponding mpde is given by

$$\frac{\partial F}{\partial t} + v \frac{\partial F}{\partial x} = \frac{\Delta x}{2} |v| \phi \frac{\partial^2 F}{\partial x^2} + O\left(\Delta x\right)^2 \tag{5}$$

It can be noted that $\phi = 1$ gives the usual first order KFVS scheme while $\phi = 0$ leads to central differencing, which is unstable. Thus, by tuning ϕ such that $0 < \phi \leq 1$, we can control the numerical dissipation and hence can enhance the formal order of accuracy. We have considered two choices for ϕ , given by $\phi = e^{-\frac{\alpha}{|v|}}$ and $\phi = e^{-\alpha |v|}$ [2], where α is a mesh dependent function. For the first choice, the high velocity particles for which $|v| \gg \alpha \Rightarrow \phi \approx 1$ contribute maximum to the dissipation. For the second choice, the low velocity particles for which $\alpha |v| \ll 1 \Rightarrow \phi \approx 1$ contribute maximum to the numerical dissipation. Therefore, the first and second choices control the dissipation generated by low and high velocity particles respectively. However, with a suitable value of α , both these choices have the same overall effect at the Euler level. A detailed analysis of these choices and the underlying physical arguments are presented in [2]. Taking Ψ -moments [11] of eq. (4) we get the modified KFVS 1D Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial Gm^+}{\partial x} + \frac{\partial Gm^-}{\partial x} = 0$$
(6)

Here, Gm^{\pm} are the modified kinetic split fluxes and are given by $Gm^{\pm} = \langle \Psi, v^{\pm}F \rangle$. For the choice $\phi = e^{-\frac{\alpha}{|v|}}$, the split fluxes are found to be asymptotic series expansions [2] while the choice $\phi = e^{-\alpha|v|}$ has closed form expressions for the split fluxes, given by

$$Gm^{\pm} = \frac{G}{2} \pm \frac{1}{2} \left[e^{\left(\frac{\alpha^2}{4\beta} - \alpha u\right)} G^+ \left(u - \frac{\alpha}{2\beta} \right) - e^{\left(\frac{\alpha^2}{4\beta} + \alpha u\right)} G^- \left(u + \frac{\alpha}{2\beta} \right) \right]$$
(7)

where G is the unsplit flux, G^{\pm} are the usual KFVS fluxes and for the case of $\alpha = 0$ we get $Gm^{\pm} = G_{kfvs}^{\pm}$. Taking Ψ -moments of eq. (5), we get the *mpde* corresponding to 1D Euler equations

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = \frac{\partial}{\partial x} \left(D \frac{\partial U}{\partial x} \right) + O \left(\Delta x \right)^2 \tag{8}$$

Here, D is the dissipation matrix given by $D = \frac{\Delta x}{2} \frac{\partial}{\partial U} (Gm^+ - Gm^-)$. Fig. (1a) shows the plot of $max|\lambda(\alpha)|$ of D for different values of α . Here, $\lambda(\alpha)$ is an eigenvalue of D. It can be observed that large values of α implies $max|\lambda(\alpha)| \approx 0$. Thus, by choosing suitable α , it is possible to reduce the numerical dissipation and hence enhance the formal order of accuracy by still using the first order stencil. A detailed study on the mathematical properties of m-KFVS fluxes, its flux Jacobians and the dissipation analysis are presented in [3]. The cell centred finite volume method based on m-KFVS has been successfully applied to 1D, 2D and 3D inviscid test cases and some of the results are presented in Figs. (1b), (2), (3) and (4).

2 Minimising the numerical dissipation - A control theory problem

Although, the formal order of accuracy is of first order, the m-KFVS method resolves the discontinuties much more sharply compared to the first order KFVS method and near second order accuracy has been achieved in regions of smooth flow. However, the numerical dissipation generated by m-KFVS may not be minimal and hence the dissipation control vector α is in general not optimal. If we can find an optimal α distribution then we will be able to achieve minimum dissipation. One of the ways of attaining the above objective is by posing the minimisation of numerical dissipation as a control theory problem where the control variables are the dissipation control vector, α . The sensitivity gradients of the cost function w.r.t. the control variables are evaluated by solving the discrete adjoint equations [6]. These gradients are then used to get a direction of improvement and the process is repeated until minimum dissipation is achieved. It can be noted that this is different from the classical aerodynamic shape optimisation [9, 6] where shapes are optimised for say either to achieve the target pressure distribution or to minimise the drag or to maximise the lift or even to maximise the lift to drag ratio. Since we are minimising the dissipation generated by m-KFVS method by keeping the shape fixed, the present work can be called as scheme optimisation.

In the present work, the objective is to minimise the numerial dissipation generated and see how

much more improvement is possible in the solution compared to the above m-KFVS method. One natural choice for the cost function is a measure of change in entropy. The discrete form of the cost function, which is to be minimised is defined as the sum of the squares of change in entropy at all cells in the computational domain, that is,

$$I = I\left\{U\left(\alpha\right)\right\} = \sum_{i=1}^{N} \left(\frac{\Delta S}{R}\right)_{i}^{2}, \quad \text{where} \quad \left(\frac{\Delta S}{R}\right)_{i} = \ln\left(\frac{p}{\rho^{\gamma}}\right)_{i} - \ln\left(\frac{p}{\rho^{\gamma}}\right)_{\infty} \tag{9}$$

Here, U is the conserved vector, α is the dissipation control variable, N is the maximum number of cells in the computational domain, $\left(\frac{\Delta S}{R}\right)_i$ is the change in entropy at any cell i and the conditions at ∞ are given by freestream conditions.

Let us study more on the cost function. Entropy change in any cell is the sum of physical and numerical changes in entropy. In isentropic flows the only contribution to the cost function comes from the numerical change in entropy as the physical change in entropy is zero. Therefore, the cost function is driven to its minimal value on that grid using optimisation solver. In flows with discontinuties, both the physical and numerical entropy contribute to the cost function. Also, the numerical entropy cannot be driven to its minimal value as sufficient amount of numerical entropy is required to satisfy the stability conditions. Hence, the optimisation solver is driven to give optimally low dissipation, which yields wiggle free solution.

The cost function I has to satisfy the governing steady state equations as constraints. In the discrete form it can be written as

$$R_i(U,\alpha) = R_i(U_i, U_j, \alpha_i, \alpha_j) = 0, \quad j \in nbhd(i) \text{ and } i = 1 \text{ to } N.$$

$$(10)$$

where R_i is the cell centred finite volume residual at cell *i* based on m-KFVS method. The subscript *j* runs over the neighbouring cells which share a common face with the cell *i*. It is interesting to observe that the cost function *I* does not explicitly depend on α , but depends on α through the state equation. From the eq. (10) any perturbation in α results in a new conserved vector *U*, which in turn causes changes in the cost function *I*. Also, the number of control variables is equal to the number of cells in the computational domain, as each cell has a unique value of α .

Consider the discrete form of the first variation in the cost function

$$\delta I = \sum_{i=1}^{N} \left[\frac{\partial I}{\partial U_i} \delta U_i + \frac{\partial I}{\partial \alpha_i} \delta \alpha_i \right]$$
(11)

Here, the first term on the right hand side of the above equation represents the change in the cost function due to perturbation in the state vector, δU . The second term represents the direct effect of the perturbation $\delta \alpha$, which in the present case is zero as I is not an explicit function of α . Similarly, the first variation in the residual R_i is given by

$$\delta R_i = \frac{\partial R_i}{\partial U_i} \delta U_i + \frac{\partial R_i}{\partial \alpha_i} \delta \alpha_i + \sum_{j=1}^{nbhd(i)} \left[\frac{\partial R_i}{\partial U_j} \delta U_j + \frac{\partial R_i}{\partial \alpha_j} \delta \alpha_j \right] = 0, \quad i = 1 \text{ to } N.$$
(12)

Let V_i be the Lagrange multiplier or adjoint variable for cell *i*. We now premultiply the variation δR_i by the adjoint variable V_i and then taking the summation of this product over the entire computational domain, we get

$$\sum_{i=1}^{N} V_i^T \delta R_i = 0 \tag{13}$$

Since the above expression is zero, it can be subtracted from the cost function variation in eq. (11),

$$\delta I = \sum_{i=1}^{N} \frac{\partial I}{\partial U_i} \delta U_i - \sum_{i=1}^{N} V_i^T \delta R_i$$
(14)

Collecting all the terms that are coefficients of δU_i and then equating them to zero after applying transpose, we get the adjoint system of equations while terms that are coefficients of $\delta \alpha_i$ give the sensitivity gradients. The discrete adjoint equations which are linear in V_i are given by

$$\left(\frac{\partial R_i}{\partial U_i}\right)^T V_i + \sum_{j=1}^{nbhd(i)} \left(\frac{\partial R_j}{\partial U_i}\right)^T V_j - \left(\frac{\partial I}{\partial U_i}\right)^T = 0, \quad i = 1 \text{ to } N.$$
(15)

The above linear algebraic equations for adjoint vector V_i are then solved, which are then used to compute the sensitivity gradients

$$\frac{dI}{d\alpha_i} = -\left[V_i^T \left(\frac{\partial R_i}{\partial \alpha_i}\right) + \sum_{j=1}^{nbhd(i)} V_j^T \left(\frac{\partial R_j}{\partial \alpha_i}\right)\right], \quad i = 1 \text{ to } N.$$
(16)

The sensitivity gradients are then used to get a direction of descent and the above procedure is repeated until minimum dissipation is achieved. In the present work the sensitivity gradients are evaluated using TAPENADE [8]. The cell centred FVM based m-KFVS solver coupled with discrete adjoint solver has been applied to the standard test cases for 2D and 3D inviscid flows and the results are shown in Figs. (5) to (10). It can be observed that optimisation does reduce numerical dissipation, yields sharper shocks while still maintaining wiggle free smooth contours and in case of ONERA wing gives the famous Lambda shock.

References

- K. Anandhanarayanan. Development and applications of a gridfree kinetic upwind solver to multibody configurations. *Ph.D. Thesis*, Dept. of Aerospace Engg., IISc, Bangalore, India, 2003.
- [2] N. Anil and S.M. Deshpande. Low dissipative modified KFVS (m-KFVS) method. *Report 2004 FM 22*. Dept. of Aerospace Engg., IISc, Bangalore, India, 2004. http://eprints.iisc.ernet.in/archive/00009208/.
- [3] N. Anil, N.K.S. Rajan and S.M. Deshpande. Mathematical analysis of dissipation in m-KFVS method. *Report 2005 FM 1*. Dept. of Aerospace Engg., IISc, Bangalore, India, 2005.

- [4] S.M. Deshpande. A second order accurate kinetic theory based method for inviscid compressible flows. NASA Technical Paper 2613, NASA Langely Research Centre, Hampton, Virginia, 1986.
- [5] S. M. Deshpande. Kinetic flux splitting schemes. *Computational Fluid Dynamics Review* 1995. (Eds.) Hafez M and Oshima K, John Wiley & Sons Ltd., 161-181, 1995.
- [6] J. Elliott. Aerodynamic optimisation based on the Euler and Navier-Stokes equations using unstructured grids. *Ph.D. Thesis*, Dept. of Aero. and Astro., MIT, 1998.
- [7] A.K. Ghosh, J.S. Mathur and S.M. Deshpande. q-KFVS Scheme A New Higher Order Kinetic Method For Euler Equations, *16th ICNMFD*, Lecture Notes in Physics, Springer, 1999.
- [8] L. Hascoet and V. Pascual. TAPENADE 2.1 user's guide. *INRIA Project Report No. 0300*, September 2004.
- [9] A. Jameson. Aerodynamic design via control theory. J. Sci. Comp, Vol. 3, No. 3, 233-260, 1988.
- [10] A.K. Mahendra. Application of least squares kinetic upwind method to strongly rotating viscous flows. *M.Sc. (Engg.) Thesis*, Dept. of Aerospace Engg., IISc, Bangalore, India, 2003.
- [11] J.C. Mandal. Kinetic Upwind Method for Inviscid Compressible Flows. *Ph.D. Thesis*, Dept. of Aerospace Engg., IISc, Bangalore, India, 1989.
- [12] C. Praveen. Least Squares Based Kinetic Schemes for Euler Equations. *Ph.D. Thesis*, Dept. of Aerospace Engg., IISc, Bangalore, India, 2004.
- [13] V. Ramesh and S.M.Deshpande. Low dissipation grid free upwind kinetic scheme with modified CIR splitting. *Report 2004 FM 20*. Dept. of Aerospace Engg., IISc, Bangalore, India.



Figure 1: (a) Eigenvalues of the dissipation matrix w.r.t. Mach number. (b) 1D Convergentdivergent nozzle. Nozzle pressure obtained using m-KFVS is compared with first order KFVS and second order MacCormack schemes.



Figure 2: Subsonic flow past NACA 0012 aifoil, M = 0.63 and $aoa = 2^{\circ}$. (a) Entropy contours obtained using KFVS and m-KFVS methods. (b) C_p - distribution obtained using m-KFVS is compared with first order KFVS and second order q-KFVS methods.



Figure 3: Transonic flow past bi-NACA airofoil, M = 0.85 and $aoa = 0^{\circ}$. From left to right : Pressure contours obtained using KFVS, m-KFVS and second order accurate q-KFVS methods.



Figure 4: Subsonic flow past hemisphere-cylinder configuration, M = 0.7 and $aoa = 0^{\circ}$. From left to right : Entropy contours obtained using KFVS and m-KFVS methods are shown in the meridian plane.



Figure 5: Low subsonic flow past NACA 0012 aifoil, M = 0.1 and $aoa = 0^{\circ}$. From left to right : Entropy contours obtained using KFVS and m-KFVS-adjoint methods.



Figure 6: Transonic flow past NACA 0012 aifoil, M = 0.85 and $aoa = 1^{\circ}$. From left to right : Entropy contours obtained using m-KFVS, m-KFVS-adjoint and q-KFVS methods.



Figure 7: Transonic flow past NACA 0012 aifoil, M = 0.85 and $aoa = 1^{\circ}$. From left to right : Pressure contours obtained using KFVS, m-KFVS-adjoint and q-KFVS methods.



Figure 8: Supersonic flow past NACA 0012 aifoil, M = 1.2 and $aoa = 0^{\circ}$. From left to right : Entropy contours obtained using m-KFVS, m-KFVS-adjoint and q-KFVS methods.



Figure 9: Supersonic flow past NACA 0012 aifoil, M = 1.2 and $aoa = 0^{\circ}$. From left to right : Pressure contours obtained using KFVS, m-KFVS-adjoint and q-KFVS methods.



Figure 10: Transonic flow past Onera M6 wing, M = 0.84 and $aoa = 3.06^{\circ}$. From left to right : Pressure contours on the upper surface of the wing using KFVS and m-KFVS-adjoint methods.