Development and application of Kinetic Flux vector Splitting (KFVS) method to compressible flows

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1. Introduction

Kinetic flux based vector splitting (KFVS) method is based on the Boltzmann equation of kinetic theory of gases and is also called Boltzmann method. It uses the well known fact that suitable moments (called Ψ-moments to be explained later in this paper) of the Boltzmann equation are the Euler equations of gas dynamics when the velocity distribution function is a Maxwellian. The Euler equations are nonlinear vector conservation laws while the Boltzmann equation is for a scalar f called velocity distribution function and hence it is hoped that constructing a numerical method for Euler equations is easier by taking Ψ-moments of a numerical method for the Boltzmann equation.

2. Boltzmann Equation and Notation

The 1D Boltzmann equation without collision term is given by

$$\frac{\partial F}{\delta t} + v\,\frac{\partial F}{\partial x} = 0 \qquad (1)$$

where the Maxwellian is defined by

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

Here v is a particle or molecular velocity, I is the internal energy variable, I_0 is internal energy due to non translational degree of freedom and is given by

$$I_0 = \frac{(3-\gamma)}{4(\gamma-1)\beta} \qquad (3)$$

The internal energy Io is required to get the right amount of internal energy which for a given γ (Cp/Cv) is

$$e_{int} = \text{total internal energy per unit mass} = I_0 + \frac{RT}{2} = \frac{1}{2\beta(\gamma-1)} = \frac{p}{\rho(\gamma-1)} \qquad (4)$$

Further, u is fluid velocity, $\beta = \frac{1}{2RT}$, R = Gas constant and T the absolute temperature.
Define the moment function vector

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

which corresponds to mass, momentum and energy components. The Ψ-moments of the Boltzmann equation reduce to 1D Euler equations.

$$\frac{\partial U}{\partial t} + \frac{\partial G}{\partial x} = 0 \qquad (5)$$

$$\text{where } U = \text{conserved vector} = \begin{bmatrix} \rho \\ \rho u \\ e \end{bmatrix} \qquad (6)$$

$$G = \begin{bmatrix} \rho u \\ p + \rho u^2 \\ (p+e)u \end{bmatrix} \qquad (7)$$

And e = total energy per unit volume

$$= \rho e_{int} + \frac{1}{2}\rho u^2 = \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2 \qquad (8)$$

We have used the term molecule in a rather loose sense. Particles here loosely called molecules are in fact 1-D mass points with velocity (v, I) ~ F(v, I) i.e. v,I obey Maxwellian distribution.

3. Basic Theory of KFVS

We start with 1-D Boltzmann equation without collision term, i.e.

$$\frac{\partial F}{\partial t} + v\,\frac{\partial F}{\partial x} = 0 \qquad (9)$$

and following Courant, split the velocity as

$$v = \frac{v+|v|}{2} + \frac{v-|v|}{2}$$

which gives split Boltzmann equation as

$$\frac{\partial F}{\partial t} + \frac{v+|v|}{2}\frac{\partial F}{\partial x} + \frac{v-|v|}{2}\frac{\partial F}{\partial x} = 0 \qquad (10)$$

Taking Ψ-moments of (10) we obtain KFVS split Euler equation

$$\frac{\partial U}{\partial t} + \frac{\partial G^{+}}{\partial x} + \frac{\partial G^{-}}{\partial x} = 0 \qquad (11)$$

The split fluxes $G^{\pm}$ are given by

$$G^{\pm} = \int_0^{\infty} dI \int_{-\infty}^{\infty} \frac{v \pm |v|}{2} \psi \, F \, dv \qquad (12)$$

Performing integration we obtain (see Deshpande 1986, Mandal and Deshpande 1994)

$$G^{\pm} = \begin{bmatrix} \rho u \dfrac{A^{\pm}(s)}{2} \pm \dfrac{\rho}{2\sqrt{\pi}\beta} B(s) \\ (p + \rho u^2) \dfrac{A^{\pm}(s)}{2} \pm \dfrac{\rho}{2\sqrt{\pi}\beta} B(s) \\ u(e + p) \dfrac{A^{\pm}(s)}{2} \pm \dfrac{\rho}{2\sqrt{\pi}\beta} \left(e + \dfrac{p}{2}\right) B(s) \end{bmatrix} \qquad (13)$$

$$where\ s = u\sqrt{\beta},$$
$$A^{\pm}(s) = 1 \pm \mathrm{erf}(s)\ ,\ B(s) = \exp(-s^2) \qquad (14)$$

Defining the thermal flux vector

$$GT = \begin{bmatrix} \rho/\sqrt{(\pi\beta)} \\ \rho u/\sqrt{(\pi\beta)} \\ (e + p/2)\sqrt{(\pi\beta)} \end{bmatrix} \qquad (15)$$

The split flux can be written as

$$G^{\pm} = G \frac{A^{\pm}(s)}{2} \pm GT \frac{B(s)}{2} \qquad (16)$$

Using backward and forward differencing (BD/FD) for spatial derivatives in (11) we can easily write the semi-discrete conservation law as

$$\left(\frac{d\bar{U}}{dt}\right)_j^n + \frac{\left(G^n_{j+\frac{1}{2}} - G^n_{j-\frac{1}{2}}\right)}{\Delta x} = 0 \qquad (17)$$

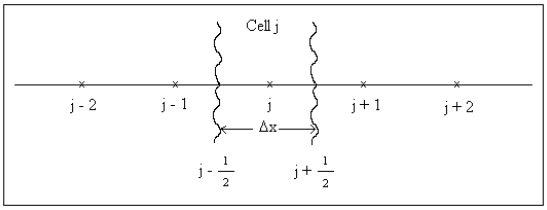

Fig 1 1-D cells of size Δx

Fig1 shows cells or finite volumes obtained from a uniform mesh for which the fluxes on the cell faces $j \pm \frac{1}{2}$ are given by

$$G^n_{j+\frac{1}{2}} = G^{+n}_j + G^{-n}_{j+1}, \qquad G^n_{j-\frac{1}{2}} = G^{+n}_{j-1} + G^{-n}_j \qquad (18)$$

We have used the well known upwind principle in constructing the numerical flux functions $G_{j\pm\frac{1}{2}}$. Using first order time marching in (17) we get the 1-D FVM-KFVS based state update formula

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}\left(G^n_{j+\frac{1}{2}} - G^n_{j-\frac{1}{2}}\right) \qquad (19)$$

We note that the above numerical scheme is first order accurate in space and time and for getting acceptable accuracy it is necessary to reduce numerical dissipation or diffusion inherently present in the above KFVS upwind method. It is very easy to develop a second order accurate KFVS state update by using second order finite differencing or by using linear variation within a cell in case of Finite Volume Method(FVM). We have followed this standard approach in writhing 2D and 3D FVM-KFVS codes (see Mathur 1992).

We will consider yet another modification called modified KFVS (MKFVS) method for reducing numerical dissipation.

4. Modified KFVS method

To develop MKFVS method we start with velocity split Boltzmann equation

$$\frac{\partial F}{\partial t} + \frac{v + |v|}{2} \frac{\partial F}{\partial x} + \frac{v - |v|}{2} \frac{\partial F}{\partial x} = 0 \qquad (20)$$

We now do mpde(modified pde) analysis for the upwind finite differenced equation

$$\left(\frac{\partial F}{\partial t}\right)_j + \frac{v + |v|}{2} \frac{F_j - F_{j-1}}{\Delta x} + \frac{v - |v|}{2} \frac{F_{j+1} - F_j}{\Delta x} = 0 \qquad (21)$$

This mpde analysis yields the mpde:

$$\frac{\partial F}{\partial t} + v \frac{\partial F}{\partial x} = \frac{\Delta x}{2} |v| \frac{\partial^2 F}{\partial x^2} + O(\Delta x^2) \qquad (22)$$

The mpde (22) clearly shows that the numerical scheme is first order accurate in space and has numerical kinematic viscosity

$$\nu_{NUM} = \frac{\Delta x}{2} |v| \qquad (23)$$

which is quite large due to velocity scale |v|. It is possible to modify the numerical scheme (21) by introducing a dissipation control junction Φ [See Anil (2008)]. We then obtain modified KFVS as

$$\frac{\partial F}{\partial t} + \frac{v + |v|\phi}{2} \frac{\partial F}{\partial x} + \frac{v - |v|\phi}{2} \frac{\partial F}{\partial x} = 0 \qquad (24)$$

Again using backward and forward differencing of spatial derivatives in (24) and thereafter doing mpde analysis yields the mpde

$$\frac{\partial F}{\partial t} + v \frac{\partial F}{\partial x} = \frac{\Delta x}{2} |v| \varphi \frac{\partial^2 F}{\partial x^2} + O(\Delta x^2) \qquad (25)$$

The choice Φ=1 gives the usual KFVS scheme with first order spatial accuracy while Φ =0 gived 2nd order spatial accuracy. Thus a suitable choice for Φ enables us to control numerical kinematic viscosity

$$v_{NUM}^{'} = \frac{\Delta x}{2}|v|\,\phi \qquad (26)$$

Taking Ψ moment of (25) and considering the mass component we obtain mpde at the Euler level as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = \frac{\partial^2(v_{NUM}^{''}\rho)}{\partial x^2} \qquad (27)$$

Where

$$v_{NUM}^{''} = \frac{\Delta x}{2}\sqrt{\beta/\pi}\int_{-\infty}^{+\infty}|v|\,\phi\,\exp[-\beta(v-u)^2]\,dv \quad (28)$$

which clearly shows that we can reduce numerical viscosity by suitable choosing Φ(v) . The choice [See Anil (2008)]

$$\phi(v) = \exp(-\alpha|v|) \qquad (29)$$

with α as dissipation control parameter has been found to be very good in that it can reduce the numerical dissipation as low as we please. It is interesting to note that α =0 leads to KFVS while α =∞ leads to a central differencing method. A certain amount of upwind bias is required for ensuring stability of MFKVS method. Defining non-dimensional $\tilde{\alpha}$ by

$$\tilde{\alpha} = \frac{\alpha}{\sqrt{\beta}} \qquad (30)$$

leads to

$$\phi(v) = \exp\left[-\tilde{\alpha}\sqrt{\beta}\,|v|\,\right] \qquad (31)$$

The modified KFVS fluxes are then given by

$$Gm^{\pm} = \int_{-\infty}^{\infty} dI \int_{-\infty}^{\infty} \frac{v \pm \phi|v|}{2}\,\psi\,F(v,I)\,dv \qquad (32)$$

Performing integration w.r.t v and I we obtain

$$Gm^{\pm} = \frac{G}{2} \pm \frac{1}{2}\left[\exp\left(\frac{\tilde{\alpha}^2}{4} - \tilde{\alpha}s\right)G_{kfvs}^{-}\left(u - \frac{\tilde{\alpha}}{2\sqrt{\beta}}\right) - \exp\left(\frac{\tilde{\alpha}^2}{4} + \tilde{\alpha}s\right)G_{kfvs}^{-}\left(u + \frac{\tilde{\alpha}}{2\sqrt{\beta}}\right)\right] \qquad (33)$$

Where $G_{kfvs}^{\pm}$ are usual KFVS fluxes evaluated for fluid variables ρ, $u \pm \frac{\tilde{\alpha}}{2\sqrt{\beta}}$ and p. It is very easy to modify computer program based on KFVS fluxes to one involving the modified split fluxes $Gm^{\pm}$.

The mpde for 1D Euler equations discretised using MKFVS is given by

$$\frac{\partial U}{\partial t} + A\frac{\partial U}{\partial x} = \frac{\delta}{\delta x}\left[\frac{\Delta x}{2}\frac{\partial}{\partial U}(Gm^{+} - Gm^{-})\frac{\partial U}{\partial x}\right] + \Delta(\Delta x^2) \qquad (34)$$

The dissipation matrix in (34) is easily seen to be

$$D = \frac{\Delta x}{2}\frac{\partial}{\partial u}(Gm^{+} - Gm^{-}) = \frac{\Delta x}{2}\left[Am^{+} - Am^{+}\right] \qquad (35)$$

where $= \frac{\partial G}{\partial u}$, $Am^{\pm} = \frac{\partial Gm^{\pm}}{\partial U}$ are Jacobians matrices corresponding to flux vectors G and $Gm^{\pm}$. The maximum numerical kinematic viscosity in the above mpde is

$$v_{NUM}^{''} = \frac{\Delta x}{2}max|\lambda(D)| \qquad (36)$$

Where $\lambda(D)$ are eigenvalues of matrix D. Fig. 2 shows plot of max| $\lambda(D)$| against $\tilde{\alpha}$ and it is obvious that

$$max|\lambda(D)| \to 0 \qquad as \quad \tilde{\alpha} \to \infty$$

thus demonstrating low dissipative nature of a numerical method based on MKFVS.

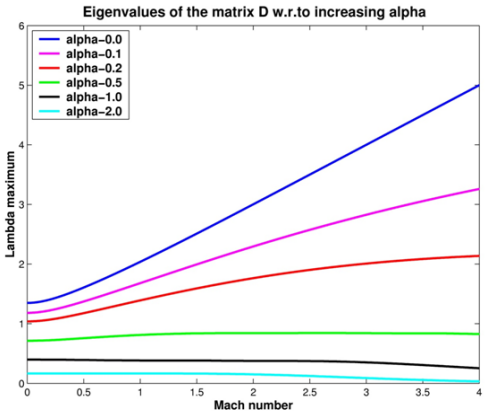

Fig 2: max $|\lambda(D)|$ variation with Mach No.

Anil [2008] has developed 2D and 3D FVM-MKFV computer program for obtaining numerical solution of inviscid compressible flows. For further reducing the numerical dissipation in the scheme Anil, Rajan, Omesh and Deshpande [2008] have solved optimal control problem. The values of α at grid points constitute a vector and the optimal problem is to minimize cost function $I(U,\alpha)$ subject to the pde

$$R(U,\alpha) = \frac{\partial}{\partial x}(G_1) + \frac{\partial}{\partial x}(G_2) = 0 \qquad (37)$$

as the constraint. These are 2D Euler equations of gas dynamics. Here U is the solution vector i.e. values of conserved vector U at all cell centers while α is the control vector. One choice for the cost function is

$$I(U,\alpha) = \sum_{i=1}^{N}\left(\frac{\Delta S}{R}\right)^2 \qquad (38)$$

$$\left(\frac{\Delta S}{R}\right)_i = change\ in\ entropy = \ln\left[\left(\frac{p}{\rho^{\gamma}}\right)_i \Big/ \left(\frac{p}{\rho^{\gamma}}\right)_{\infty}\right] \qquad (39)$$

where N is the total number of cell centers, i is the cell number and p_∞, ρ_∞ are values of pressure and density in the free stream. It may be noted that

$$\Delta s_{TOTAL} = \Delta s_{PHYS} + \Delta s_{NUM} \qquad (40)$$

where Δs_{TOTAL} = total entropy produced in the domain

Δs_{PHYS} = entropy produced due to physical processes such as shocks

Δs_{NUM} = entropy produced due to numerical dissipation

We note that Δs_{TOTAL} cannot be reduced by optimization routine below Δs_{PHYS} because governing equations are a constraint on optimization. The sensitivity gradients are obtained using discrete adjoint approach and automatic differentiation tool TAPENADE has been used to compute sensitivity gradients and values of α are updated using steepest descent method. We have used the simplest optimizer to test the idea. The m-KFVS adjoint solver (MKFVS-AD) has been applied to (i) low Mach number flow past NACA0012 airfoil, (ii) transonic flow past Onera M6 wing. We will consider only one example of computing supersonic flow at M = 1.2, A.O.A = 0 deg, past NACA 0012 airfoil. The Fig 3 shows pressure contours obtained using first order KFVS method, m-KFVS, m-KFVS-AD and q-KFVS (2nd order accurate KFVS method based on entropy variables) method.

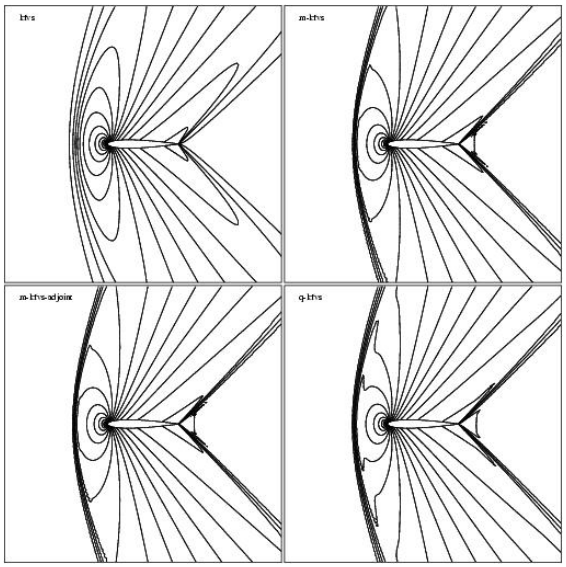

Fig 3: pressure contours for NACA 0012

It is clear that first order KFVS method is very dissipative and m-KFVS-AD method has less spurious wiggles in pressure contours compared to second order accurate q-KFVS method. Table 1 shows values of CL and CD obtained using using first order KFVS, m-KFVS-AD and q-KFVS methods. Exact value of CL is zero in the present case and the m-KFVS-AD method gives least value of CL(0.000040) as against 0.000063 for second order accurate q-KFVS method.

Table 1 comparison of Lift and Drag coefficient

Scheme	C_L	C_D
1st order KFVS	0.000168	0.1023
m-KFVS-AD	0.000040	0.0958
q-KFVS	0.000063	0.0968
AGARD	0.0	0.0946 to 0.0960

We will now study KFVS on moving grid (KFMG) which is very useful in dealing with problems involving moving bodies.

5. KFVS on moving grid (KFVS)

Consider a cell with boundaries a (t), b (t) which move with time as shown in fig (4)

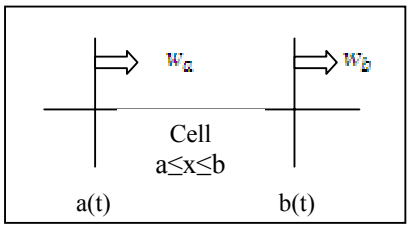

Fig 4 Moving cell

The velocities of boundaries are

$$w_a = \frac{da}{dt}, \qquad w_b = \frac{db}{dt} \tag{41}$$

The 1D Boltzmann equations without collision term is

$$\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} = 0 \tag{42}$$

Integral form of (42) is

$$\int_a^b \frac{\partial F}{\partial t}dx + \int_a^b \frac{\partial}{\partial x}(vF)\,dx = 0 \tag{43}$$

From elementary calculus we have

$$\frac{\partial}{\partial t}\int_a^b F dx = \int_a^b \frac{\partial F}{\partial t} + F(b)\frac{db}{dt} - F(a)\frac{da}{dt}$$

This gives the basic relation

$$\int_a^b \frac{\partial F}{\partial t}dx = \frac{\partial}{\partial t}\int_a^b F dx - \int_a^b \frac{\partial}{\partial x}(wF)dx \tag{44}$$

This relation is useful in deriving KFMG.

Combining (43) with (44) we get

$$\frac{\partial}{\partial t}\int_a^b F dx + \int_a^b \frac{\partial}{\partial x}[(v-w)F]dx = 0 \tag{45}$$

Let $\bar{v} = v - w$ velocity of a particle relative to a point moving with velocity $w = \frac{dx}{dt}$. We pass on to Euler

equation by taking ψ moment i.e.

$$\frac{\partial}{\partial t}\int_a^b \int F\,\psi dv dI dx + \int_a^b \int \bar{v}\,\psi F dv\, dI\, dx = 0 \qquad (46)$$

The flux G_{MG} on a moving surface is therefore given by

$$G_{MG} = \int_0^\infty dI \int_{-\infty}^{+\infty} \bar{v}\,\psi F dv \qquad (47)$$

$$= \begin{bmatrix} \rho\bar{u} \\ p + \rho\bar{u} \\ pw + e\bar{u} \end{bmatrix}$$

$$e = \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2, \quad \bar{u} = u - w \qquad (48)$$

The flux vector G_{MG} on a moving surface can now be split along lines similar to principle used in obtaining KFVS. Using $\bar{v}$ for splitting we get

$$G_{MG}^{\pm} = \begin{bmatrix} 1 & 0 & 0 \\ w & 1 & 0 \\ \frac{w^2}{2} & w & 1 \end{bmatrix} \begin{bmatrix} G_1^{\pm}(\bar{s}) \\ G_2^{\pm}(\bar{s}) \\ G_3^{\pm}(\bar{s}) \end{bmatrix} \qquad (49)$$

Where $G_{MG}^{\pm}$ The split fluxes $G_{MG}^{\pm}$ on a moving surface are related to the usual KFVS fluxes $G^{\pm}(s)$ except that these are now evaluated at $\bar{S}$ instead of S. The components of the column vector on RHS of (49) are given by

$$\left.\begin{aligned} G_1^{\pm}(\bar{s}) &= \rho\bar{u}\,\frac{A^{\pm}(\bar{s})}{2} \pm \frac{\rho}{2\sqrt{\pi\beta}}\,B(\bar{s}) \\ G_2^{\pm}(\bar{s}) &= (p + \rho\bar{u}^2)\frac{A^{\pm}(\bar{s})}{2} \pm \frac{\rho}{2\sqrt{\pi\beta}}\,B(\bar{s}) \\ G_3^{\pm}(\bar{s}) &= \bar{u}(\bar{e} + p)\frac{A^{\pm}(\bar{s})}{2} \pm \frac{\rho}{2\sqrt{\pi\beta}}\left(\bar{e} + \frac{p}{2}\right)B(\bar{s}) \end{aligned}\right\} \qquad (50)$$

Where $\bar{e} = \frac{p}{\gamma-1} + \frac{1}{2}\rho\bar{u}^2$

It can be easily verified that

$$G_{MG} = G_{MG}^{+} + G_{MG}^{-} \qquad (51)$$

Taking 1D moving mesh as shown in fig (5)

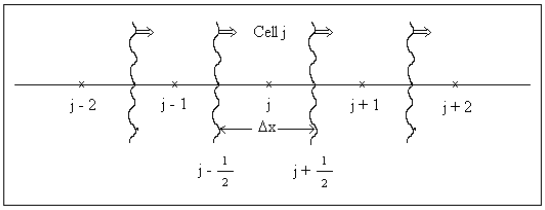

Fig 5 Cell j with moving boundaries

the semi discrete law for cell j corresponding to equation (46) is given by

$$\Delta x\left(\frac{d\bar{U}}{dt}\right)_j^n + \left(G_{MG\,j+\frac{1}{2}}^n - G_{MG\,j-\frac{1}{2}}^n\right) = 0 \qquad (52)$$

Here $\bar{u}_j^n$ is the cell- average defined by

$$\bar{U}_j^n = \frac{1}{\Delta x}\int_{x_{j-\frac{1}{2}}}^{x_{j-\frac{1}{2}}} U(t_n, x)dx$$

and it should not be confused with bar notation used in equations (47), (49) and (50). The numerical flux functions on moving boundaries are easily constructed from upwind principle as

$$\left.\begin{aligned} G_{MG\,j+\frac{1}{2}}^n &= G_{MG\,j}^{+n} + G_{MG\,j+1}^{-n} \\ G_{MG\,j-\frac{1}{2}}^n &= G_{MG\,j-1}^{+n} + G_{MG\,j}^{-n} \end{aligned}\right\} \qquad (53)$$

The update formula (52) reduces to Eulerian update formula for w = 0 and to Lagrangian update formula when w = u. For other values of w it is neither. Krishnamurthy (2002) and Krishnamurthy , Sarma & Deshpande (2004) have applied the KFMG method for computing unsteady transonic flow around NACA 0012 Oscillating airfoil. The parameters of calculation are:

(a) Angle of attack variation

$$\alpha(t) = \alpha_m + \alpha_0 \sin\left[\left(2\sqrt{\gamma}\,M_\infty\right)\omega t\right]$$

(b) Free stream Mach no. $M_\infty = 0.825$

(c) Mean angle of attack $\alpha_m = 0.016^0$, amplitude $\alpha_0 = 2.57^0$

(d) Reduced frequency k = ωc / 2 U_∞ = 0.0814, c =chord

(e) Airfoil oscillations are around quarter chord point

(f) Spring analogy method has been used to do regridding everytime body deforms. Translation and rotation of entire grid are used for rigid body motion.

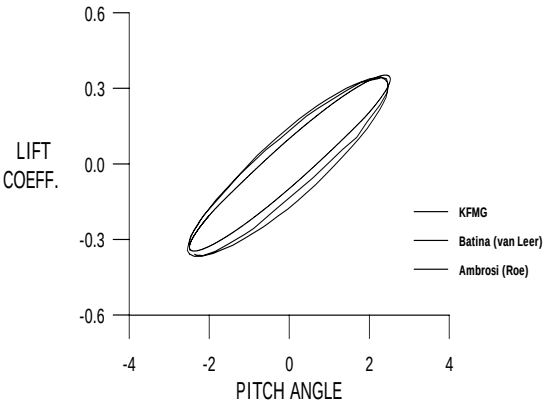

Fig 6: lift coefficient vs pitch angle

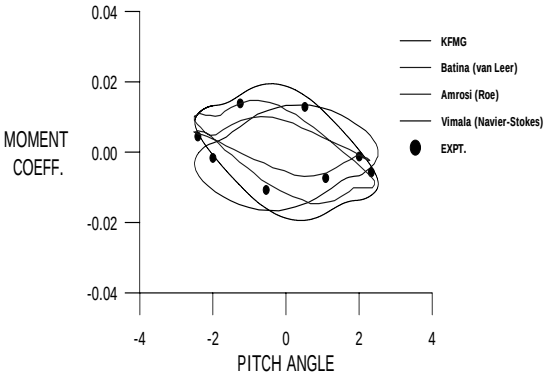

Fig 7: Moment coefficient vs pitch angle

Fig 6 shows variation of lift coefficient with pitch angle obtained by three numerical methods namely KFMG, Batina (based on Van Leer's flux vector splitting method) and Ambrosi (based on Roe's method).

Fig 7 shows C_m versus pitch angle. The solid dots are experimental points and results of other numerical methods are above shown. Large variation among values of C_m predicted by various numerical methods is very often noticed and reasons for this variation are not very clear.

6. Concluding Remarks

KFVS method and KFMG have been used exhaustively by Deshpande and scientists at NAL, Bangalore and DRDL, Hyderabad both in combination with Finite Volume and Least square kinetic upwind Meshfree (LSKUM) method. These codes have been used to compute flow past various oscillating and stationary bodies of interest in aerodynamic design of aerospace vehicles. Only a few results are presented in this paper. It is a great pleasure to dedicate this paper to my teacher and guide Prof. Satish Dhawan to whom I owe much.

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