ARDB Centre of Excellence for Aerospace CFD
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1 Introduction

Kinetic theory based methods enjoy certain advantages due to the fact that we deal with a scalar partial differential equation, the Boltzmann equation. In this report we compare a kinetic meshless method [1, 2] with another meshless method which is directly derived at the system conservation law (macroscopic or Euler) level [3, 4]. Both the methods use a least squares approximation for evaluating the flux divergence in the conservation law. The advantage of the kinetic formulation is that it leads to a much smaller least squares problem than the Euler formulation. This can have implications on the conditioning of the resulting system of equations particularly in 3-D.

2 Kinetic Meshless Method

Kinetic Meshless Method (KMM) is a grid-free scheme for numerical solution of conservation laws that can be derived from a Boltzmann equation by taking suitable moments. It has been applied to the solution of Euler equation of gas dynamics using the Boltzmann equation and the Maxwellian distribution function. The Boltzmann equation (without the collision term) which describes the evolution of the velocity distribution function is

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + v_z \frac{\partial f}{\partial z} = 0 \tag{1}$$

In kinetic schemes the Boltzmann equation is first discretized using an upwind scheme; taking moments will then give an update scheme for the Euler equations. In kinetic meshless method we discretize the Boltzmann equation using the (dual) least squares technique. Let us discretize the Boltzmann equation at node i given a set of neighbouring nodes or connectivity C_i as shown in fig. (1). Assume that we can define a consistent approximation to f at the mid-point of the line joining i and any neighbour $j \in C_i$. Using Taylor's formula we get

$$f_{ij} = f_i + \Delta x_{ij} \left(\frac{\partial f}{\partial x}\right)_i + \Delta y_{ij} \left(\frac{\partial f}{\partial y}\right)_i + \Delta z_{ij} \left(\frac{\partial f}{\partial z}\right)_i + HOT \tag{2}$$

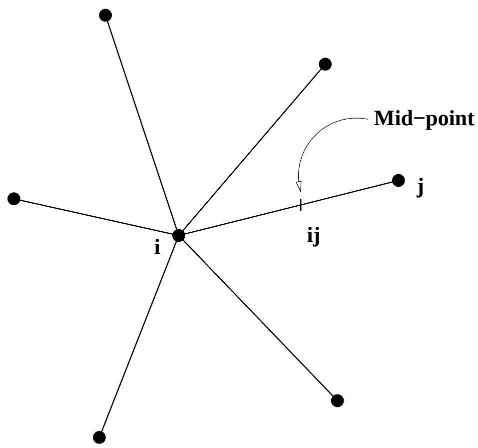

Figure 1: Connectivity for KMM

where $\Delta x_{ij} = (x_j - x_i)/2$, etc. In the least squares technique we determine the unknowns

$$X_k = \left[\left(\frac{\partial f}{\partial x}\right)_i, \quad \left(\frac{\partial f}{\partial y}\right)_i, \quad \left(\frac{\partial f}{\partial z}\right)_i \right]^\top$$

by minimizing the HOT in a least squares sense, i.e.,

$$\min \sum_{j \in C_i} \left[f_{ij} - f_i - \Delta x_{ij} \left(\frac{\partial f}{\partial x}\right)_i - \Delta y_{ij} \left(\frac{\partial f}{\partial y}\right)_i - \Delta z_{ij} \left(\frac{\partial f}{\partial z}\right)_i \right]^2 \tag{3}$$

with respect to the three unknowns. The minimization problem leads to the following equation

$$A_k X_k = b_k \tag{4}$$

where A_k is a 3×3 symmetric matrix given by

$$\left[\begin{array}{lll} \sum \Delta x_{ij}^2 & \sum \Delta x_{ij} \Delta y_{ij} & \sum \Delta x_{ij} \Delta z_{ij} \\ \sum \Delta x_{ij} \Delta y_{ij} & \sum \Delta y_{ij}^2 & \sum \Delta y_{ij} \Delta z_{ij} \\ \sum \Delta x_{ij} \Delta z_{ij} & \sum \Delta y_{ij} \Delta z_{ij} & \sum \Delta z_{ij}^2 \end{array} \right] \tag{5}$$

and all summations are over all $j \in C_i$. The solution can be written in compact form as

$$\left.\frac{\partial f}{\partial x}\right|_i = \sum_{j \in C_i} a_{ij}(f_{ij} - f_i), \quad \left.\frac{\partial f}{\partial y}\right|_i = \sum_{j \in C_i} b_{ij}(f_{ij} - f_i), \quad \left.\frac{\partial f}{\partial z}\right|_i = \sum_{j \in C_i} c_{ij}(f_{ij} - f_i) \tag{6}$$

where the coefficients (a, b, c) depend only on the set of all $(\Delta x, \Delta y, \Delta z)$ in the connectivity. The mid-point values f_{ij} are specified using an upwind-type definition

$$f_{ij} = \begin{cases} f_i & \text{if } \vec{v} \cdot \vec{\ell}_{ij} \geq 0 \\ f_j & \text{if } \vec{v} \cdot \vec{\ell}_{ij} \leq 0 \end{cases} \tag{7}$$

where $\vec{\ell}_{ij}$ is the unit vector directed from node i to node j. Substituting (6), (7) into the Boltzmann equation and taking moments leads to discrete update equations for the Euler equations,

$$\frac{\mathrm{d}U_i}{\mathrm{d}t} + \sum_{j\in C_i} [a_{ij}(F_{ij} - F_i) + b_{ij}(G_{ij} - G_i) + c_{ij}(H_{ij} - H_i)] = 0 \tag{8}$$

where F_{ij}, G_{ij}, H_{ij} are mid-point kinetic fluxes which naturally arise when the approximation (7) is used and are given in [5].

3 Meshless scheme at macroscopic level

Having seen how we can derive a full-stencil kinetic meshless scheme starting at the Boltzmann or kinetic level, let us try to do similar analysis directly at the Euler or macroscopic level [3, 4] without the use of Boltzmann equation. Consider a single conservation law in the divergence form

$$\frac{\partial u}{\partial t} + \mathrm{div}\ \vec{Q}(u) = 0 \tag{9}$$

where u is the conserved quantity and $\vec{Q}(u) = (F(u), G(u), H(u))$ is the flux vector. As in KMM we define mid-point states in an upwind manner and use a dual least squares approximation to approximate the flux derivatives required for calculating the divergence in the above equation. Assume that $\vec{Q}\cdot\vec{\ell}_{ij}$ is defined at the mid-point of the line segment $\bar{ij}$ using a suitable upwind flux formula, e.g., the KFVS flux [6], and denoted as $(\vec{Q}\cdot\vec{\ell}_{ij})_{ij}$. We expand this using Taylors formula about the state at node i,

$$\begin{aligned}
(\vec{Q}\cdot\vec{\ell}_{ij})_{ij} &= (\vec{Q}\cdot\vec{\ell}_{ij})_i + \Delta x_{ij}\frac{\partial}{\partial x}(\vec{Q}\cdot\vec{\ell}_{ij})_i + \Delta y_{ij}\frac{\partial}{\partial y}(\vec{Q}\cdot\vec{\ell}_{ij})_i \\
&\quad + \Delta z_{ij}\frac{\partial}{\partial z}(\vec{Q}\cdot\vec{\ell}_{ij})_i + HOT \\
&= (\vec{Q}\cdot\vec{\ell}_{ij})_i + \frac{\Delta x_{ij}^2}{\Delta r_{ij}}\left(\frac{\partial F}{\partial x}\right)_i + \frac{\Delta y_{ij}^2}{\Delta r_{ij}}\left(\frac{\partial G}{\partial y}\right)_i + \frac{\Delta z_{ij}^2}{\Delta r_{ij}}\left(\frac{\partial H}{\partial z}\right)_i \\
&\quad + \frac{\Delta x_{ij}\Delta y_{ij}}{\Delta r_{ij}}\left(\frac{\partial F}{\partial y} + \frac{\partial G}{\partial x}\right)_i \\
&\quad + \frac{\Delta y_{ij}\Delta z_{ij}}{\Delta r_{ij}}\left(\frac{\partial G}{\partial z} + \frac{\partial H}{\partial y}\right)_i \\
&\quad + \frac{\Delta z_{ij}\Delta x_{ij}}{\Delta r_{ij}}\left(\frac{\partial H}{\partial x} + \frac{\partial F}{\partial z}\right)_i \\
&\quad + HOT
\end{aligned}$$

where $\Delta r_{ij} = \sqrt{\Delta x_{ij}^2 + \Delta y_{ij}^2 + \Delta z_{ij}^2}$. There are six unknowns in the above expansion (neglecting the higher order terms) and these are determined by solving the least squares problem

$$\min \sum_{j\in C_i} [\Delta r_{ij}(LHS_{ij} - RHS_{ij})]^2 \tag{10}$$

where the higher order terms HOT, in the RHS are neglected. This leads to a linear system of six equations

$$A_e X_e = b_e$$

where A_e is a 6×6 symmetric matrix given by

$$\begin{bmatrix}
\sum \Delta x_{ij}^4 & \sum \Delta x_{ij}^2 \Delta y_{ij}^2 & \sum \Delta x_{ij}^2 \Delta z_{ij}^2 & \sum \Delta x_{ij}^3 \Delta y_{ij} & \sum \Delta x_{ij}^2 \Delta y_{ij} \Delta z_{ij} & \sum \Delta x_{ij}^3 \Delta z_{ij} \\
. & \sum \Delta y_{ij}^4 & \sum \Delta y_{ij}^2 \Delta z_{ij}^2 & \sum \Delta x_{ij} \Delta y_{ij}^3 & \sum \Delta y_{ij}^3 \Delta z_{ij} & \sum \Delta x_{ij} \Delta y_{ij}^2 \Delta z_{ij} \\
. & . & \sum \Delta z_{ij}^4 & \sum \Delta x_{ij} \Delta y_{ij} \Delta z_{ij}^2 & \sum \Delta y_{ij} \Delta z_{ij}^3 & \sum \Delta z_{ij}^3 \Delta x_{ij} \\
. & . & . & \sum \Delta x_{ij}^2 \Delta y_{ij}^2 & \sum \Delta x_{ij} \Delta y_{ij}^2 \Delta z_{ij} & \sum \Delta x_{ij}^2 \Delta y_{ij} \Delta z_{ij} \\
. & . & . & . & \sum \Delta y_{ij}^2 \Delta z_{ij}^2 & \sum \Delta x_{ij} \Delta y_{ij} \Delta z_{ij}^2 \\
. & . & . & . & . & \sum \Delta x_{ij}^2 \Delta z_{ij}^2
\end{bmatrix}$$

and X_e is the vector of unknowns

$$X_e = \begin{bmatrix} F_x \\ G_y \\ H_z \\ F_y + G_x \\ G_z + H_y \\ H_x + F_z \end{bmatrix}$$

Note that only the first three elements of X_e are required for the solution of the conservation law but we have to still solve a system of six equations involving a 6×6 matrix. In 2-D we get a system of 3 equations (having 3×3 matrix) of which only two variables (F_x and G_y) are required for the solution of the conservation law. In contrast to this, KMM, which is derived at the Boltzmann level always solves only for the required derivatives and there is no redundancy involved; in 3-D KMM we get a 3×3 system for the 3 unknowns and in 2-D we get a 2×2 system for 2 unknowns.

4 Why do we get 6 unknowns instead of 9 ?

Consider a vector

$$\vec{Q} = \hat{\imath}F + \hat{\jmath}G + \hat{k}H$$

and position vector $\vec{r} = \hat{\imath}x + \hat{\jmath}y + \hat{k}z$. Following the standard analysis in fluid mechanics we expand the vector at $\vec{r} + \Delta\vec{r}$ in terms of the field at $\vec{r}$. The Taylor expansion gives

$$\vec{Q}(\vec{r} + \Delta\vec{r}) = \vec{Q}(\vec{r}) + \begin{bmatrix} \frac{\partial F}{\partial x} & \frac{\partial F}{\partial y} & \frac{\partial F}{\partial z} \\ \frac{\partial G}{\partial x} & \frac{\partial G}{\partial y} & \frac{\partial G}{\partial z} \\ \frac{\partial H}{\partial x} & \frac{\partial H}{\partial y} & \frac{\partial H}{\partial z} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} + HOT$$

The gradient matrix is a Jacobian

$$A = \frac{\partial(F, G, H)}{\partial(x, y, z)}$$

We write

$$
\begin{aligned}
\vec{Q}(\vec{r}+\Delta\vec{r}) &= \vec{Q}(\vec{r}) + \frac{1}{2}(A+A^{\top})\begin{bmatrix}\Delta x\\ \Delta y\\ \Delta z\end{bmatrix} + \frac{1}{2}(A-A^{\top})\begin{bmatrix}\Delta x\\ \Delta y\\ \Delta z\end{bmatrix} + \ldots. \\
&= \vec{Q}(\vec{r}) + \begin{bmatrix} \frac{\partial F}{\partial x} & \frac{1}{2}(\frac{\partial F}{\partial y}+\frac{\partial G}{\partial x}) & \frac{1}{2}(\frac{\partial F}{\partial z}+\frac{\partial H}{\partial x}) \\ \frac{1}{2}(\frac{\partial F}{\partial y}+\frac{\partial G}{\partial x}) & \frac{\partial G}{\partial y} & \frac{1}{2}(\frac{\partial G}{\partial z}+\frac{\partial H}{\partial y}) \\ \frac{1}{2}(\frac{\partial F}{\partial z}+\frac{\partial H}{\partial x}) & \frac{1}{2}(\frac{\partial G}{\partial z}+\frac{\partial H}{\partial y}) & \frac{\partial H}{\partial z} \end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta y\\ \Delta z\end{bmatrix} \\
&\quad + \begin{bmatrix} 0 & \frac{1}{2}(\frac{\partial F}{\partial y}-\frac{\partial G}{\partial x}) & \frac{1}{2}(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}) \\ -\frac{1}{2}(\frac{\partial F}{\partial y}-\frac{\partial G}{\partial x}) & 0 & \frac{1}{2}(\frac{\partial G}{\partial z}-\frac{\partial H}{\partial y}) \\ -\frac{1}{2}(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}) & -\frac{1}{2}(\frac{\partial G}{\partial z}-\frac{\partial H}{\partial y}) & 0 \end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta y\\ \Delta z\end{bmatrix}
\end{aligned}
$$

The second term on the RHS of the above equation is the dot product of the deformation tensor (symmetric) and the vector

$$\Delta\vec{r} = \hat{\mathrm{i}}\Delta x + \hat{\mathrm{j}}\Delta y + \hat{\mathrm{k}}\Delta z \tag{11}$$

and the third term is a dot product of antisymmetric tensor and $\Delta\vec{r}$. Next take the curl of $\vec{Q}$, i.e,

$$
\begin{aligned}
\mathrm{curl}\ \vec{Q} &= \begin{vmatrix} \hat{\mathrm{i}} & \hat{\mathrm{j}} & \hat{\mathrm{k}} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F & G & H \end{vmatrix} \\
&= \hat{\mathrm{i}}\left(\frac{\partial H}{\partial y}-\frac{\partial G}{\partial z}\right) + \hat{\mathrm{j}}\left(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}\right) + \hat{\mathrm{k}}\left(\frac{\partial G}{\partial x}-\frac{\partial F}{\partial y}\right)
\end{aligned}
$$

Further

$$
\begin{aligned}
(\mathrm{curl}\ \vec{Q})\times\Delta\vec{r} &= \begin{vmatrix} \hat{\mathrm{i}} & \hat{\mathrm{j}} & \hat{\mathrm{k}} \\ \frac{\partial H}{\partial y}-\frac{\partial G}{\partial z} & \frac{\partial F}{\partial z}-\frac{\partial H}{\partial x} & \frac{\partial G}{\partial x}-\frac{\partial F}{\partial y} \\ \Delta x & \Delta y & \Delta z \end{vmatrix} \\
&= \hat{\mathrm{i}}\left[\left(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}\right)\Delta z - \left(\frac{\partial G}{\partial x}-\frac{\partial F}{\partial y}\right)\Delta y\right] \\
&\quad + \hat{\mathrm{j}}\left[\left(\frac{\partial G}{\partial x}-\frac{\partial F}{\partial y}\right)\Delta x - \left(\frac{\partial H}{\partial y}-\frac{\partial G}{\partial z}\right)\Delta z\right] \\
&\quad + \hat{\mathrm{k}}\left[\left(\frac{\partial H}{\partial y}-\frac{\partial G}{\partial z}\right)\Delta y - \left(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}\right)\Delta x\right] \\
&= \begin{bmatrix} 0 & \left(\frac{\partial F}{\partial y}-\frac{\partial G}{\partial x}\right) & \left(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}\right) \\ -\left(\frac{\partial F}{\partial y}-\frac{\partial G}{\partial x}\right) & 0 & \left(\frac{\partial G}{\partial z}-\frac{\partial H}{\partial y}\right) \\ -\left(\frac{\partial F}{\partial z}-\frac{\partial H}{\partial x}\right) & -\left(\frac{\partial G}{\partial z}-\frac{\partial H}{\partial y}\right) & 0 \end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta y\\ \Delta z\end{bmatrix}
\end{aligned}
$$

Hence the third term $= \frac{1}{2}(\text{curl } \vec{Q}) \times \Delta\vec{r}$

$$
\begin{aligned}
\vec{Q}(\vec{r}+\Delta\vec{r}) - \vec{Q}(\vec{r}) &= \begin{bmatrix} \frac{\partial F}{\partial x} & \frac{1}{2}(\frac{\partial F}{\partial y} + \frac{\partial G}{\partial x}) & \frac{1}{2}(\frac{\partial F}{\partial z} + \frac{\partial H}{\partial x}) \\ \frac{1}{2}(\frac{\partial F}{\partial y} + \frac{\partial G}{\partial x}) & \frac{\partial G}{\partial y} & \frac{1}{2}(\frac{\partial G}{\partial z} + \frac{\partial H}{\partial y}) \\ \frac{1}{2}(\frac{\partial F}{\partial z} + \frac{\partial H}{\partial x}) & \frac{1}{2}(\frac{\partial G}{\partial z} + \frac{\partial H}{\partial y}) & \frac{\partial H}{\partial z} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} \\
&\quad + \frac{1}{2}(\text{curl } \vec{Q}(\vec{r})) \times \Delta\vec{r}
\end{aligned}
$$

Taking dot product with $\Delta\vec{r}$ and using the identity

$$(\text{curl } \vec{Q} \times \Delta\vec{r}) \cdot \Delta\vec{r} = 0$$

we get

$$
\begin{aligned}
[\vec{Q}(\vec{r}+\Delta\vec{r}) - \vec{Q}(\vec{r})] \cdot \Delta\vec{r} &= \frac{\partial F}{\partial x}\Delta x^2 + \frac{\partial G}{\partial y}\Delta y^2 + \frac{\partial H}{\partial z}\Delta z^2 \\
&\quad + \left(\frac{\partial F}{\partial y} + \frac{\partial G}{\partial x}\right)\Delta x \Delta y \\
&\quad + \left(\frac{\partial G}{\partial z} + \frac{\partial H}{\partial y}\right)\Delta y \Delta z \\
&\quad + \left(\frac{\partial H}{\partial x} + \frac{\partial F}{\partial z}\right)\Delta z \Delta x
\end{aligned}
$$

which contains only six unknowns as seen before.

5 Reduction to FVM

In this section we look at how the meshless schemes at the kinetic and Euler level reduce on a standard uniform stencil as shown in figure (2). We have used two indices to number the points as is the practice with structured grids. Note that there are four points in the connectivity of node (i, j) which is sufficient for the least squares approximation to be over-determined. The mid-points will be denoted by fractional indices as is done in finite volume methods. We first calculate the terms in the KMM,

$$
\begin{aligned}
\sum \Delta f \Delta x &= (-h/2)(f_{i-1/2,j} - f_{i,j}) + (h/2)(f_{i+1/2,j} - f_{i,j}) \\
&= (h/2)(f_{i+1/2,j} - f_{i-1/2,j})
\end{aligned}
$$

$$
\begin{aligned}
\sum \Delta f \Delta y &= (-h/2)(f_{i,j-1/2} - f_{i,j}) + (h/2)(f_{i,j+1/2} - f_{i,j}) \\
&= (h/2)(f_{i,j+1/2} - f_{i,j-1/2})
\end{aligned}
$$

The 2×2 matrix of 2-D KMM reduces to

$$\begin{bmatrix} h^2/2 & 0 \\ 0 & h^2/2 \end{bmatrix}$$

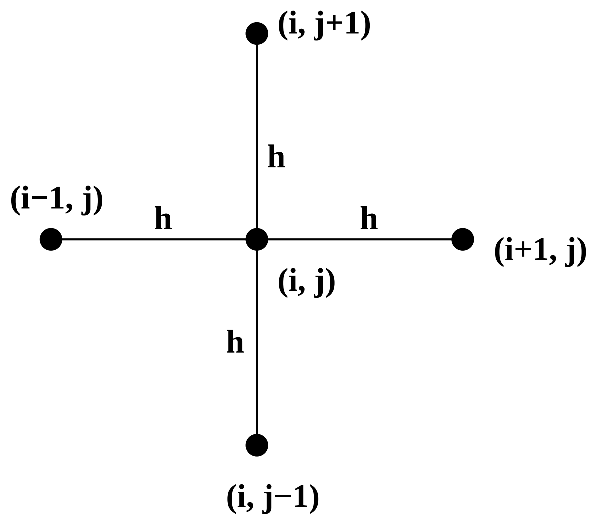

Figure 2:

so that the derivatives are given by

$$\frac{\partial f}{\partial x} = (f_{i+1/2,j} - f_{i-1/2,j})/h, \quad \frac{\partial f}{\partial y} = (f_{i,j+1/2} - f_{i,j-1/2})/h \tag{12}$$

Substituting these approximations in the Boltzmann equation and taking moments we obtain the standard finite volume KFVS method [6].

Now let us look at the scheme at the Euler level. The 3×3 least squares matrix for this stencil is given by

$$\begin{bmatrix} 2(h/2)^4 & 0 & 0 \\ 0 & 2(h/2)^4 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

which turns out to be singular. The reason is that the coefficient[1] multiplying the third unknown vanishes at all the points in the connectivity. One way to overcome this problem is to rotate the coordinate axes by some angle and solve in this new frame. Consider a rotation by 45^o. Then the 3×3 matrix is given by

$$\begin{bmatrix} (h/2)^4 & 0 & 0 \\ 0 & (h/2)^4 & 0 \\ 0 & 0 & (h/2)^4 \end{bmatrix}$$

which is non-singular. The other option is to increase the connectivity by adding points or by perturbing the coordinates of the nodes by some small random amount.

[1]These coefficients can be considered as shape functions. If any shape function vanishes identically then it leads to singularity of the type seen here.

In the case of KMM, the matrix is singular if and only if all the points lie on the same straight line. This corresponds to the fact that we cannot determine the gradient of a function, which is two-dimensional, when the given data is one-dimensional. Moreover KMM has been shown to be rotationally invariant [5], i.e., the update is independent of the coordinate system used. The macroscopic scheme on the special stencil shows that it is not rotationally invariant since the singularity vanishes upon a rotation of coordinates.

6 Results and Discussions

We have applied the KMM, and the LSFD-U [3, 4] which is based on the macroscopic formulation together with kinetic flux vector splitting, to a transonic flow over NACA-0012 airfoil. The flow conditions are $M_\infty = 0.85$ and $\alpha = 1^o$, and the total number of points is 4385, with 120 points on the airfoil surface. The points are obtained from an unstructured triangular grid and for this case we do not encounter any singularity for the Euler formulation which was discussed in the previous section. It may appear for other grids or point distributions.

Figure (3) shows the pressure distribution on the airfoil surface and there is no significant differences in the two solutions. The pressure and Mach number contours in figures (4), (5) also show similar results.

7 Summary

The least squares problem arising in the kinetic formulation involves only those variables which are required for updating the solution while the least squares method applied to Euler equations involves some redundant variables. The least squares matrix of the kinetic formulation is 2×2 in 2d and 3×3 in 3d, while for the Euler formulation they are 3×3 and 6×6 respectively. This combined with the fact that the matrix elements of kinetic formulation have units of $(\Delta x)^2$ while that of the Euler formulation has $(\Delta x)^4$, can lead to poor conditioning of the Euler formulation as compared to the kinetic formulation. Indeed on a standard Cartesian stencil the Euler formulation was seen to be ill-posed while the kinetic formulation leads to the finite volume method. In 3d, the Euler formulation requires the connectivity to have more than six points whereas for the kinetic formulation it is sufficient to have more than three points. Another important consideration in meshless methods is the solvability of the least squares problem on arbitrary point distributions. In 2d the least squares problem in the kinetic scheme is solvable if all the points in the connectivity do not lie on a line whereas no such geometric characterization is available for the Euler formulation. Comparison of results for a 2d transonic flow on a point distribution obtained from unstructured grid does not show any significant differences.

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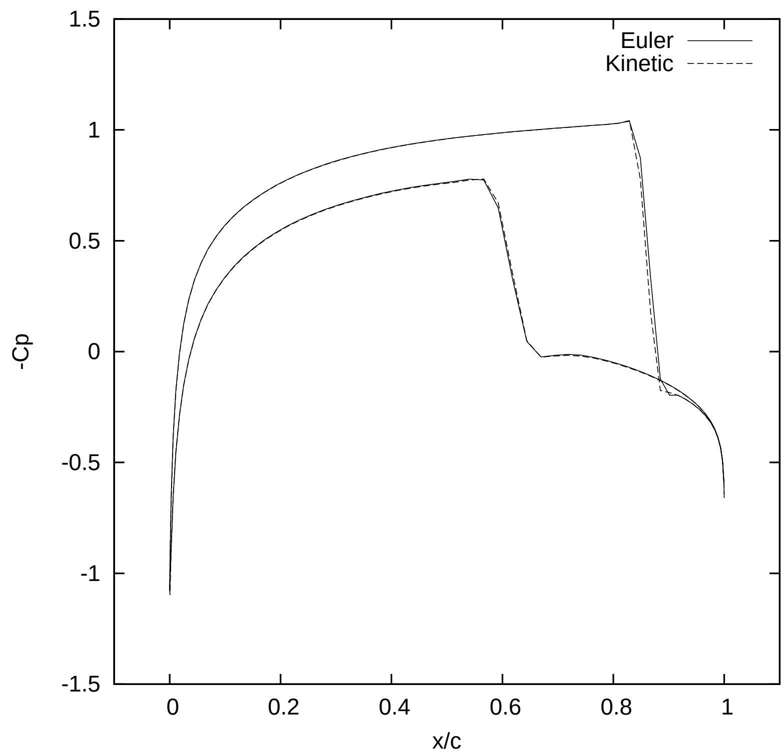

Figure 3: Pressure coefficient - Euler and Kinetic schemes

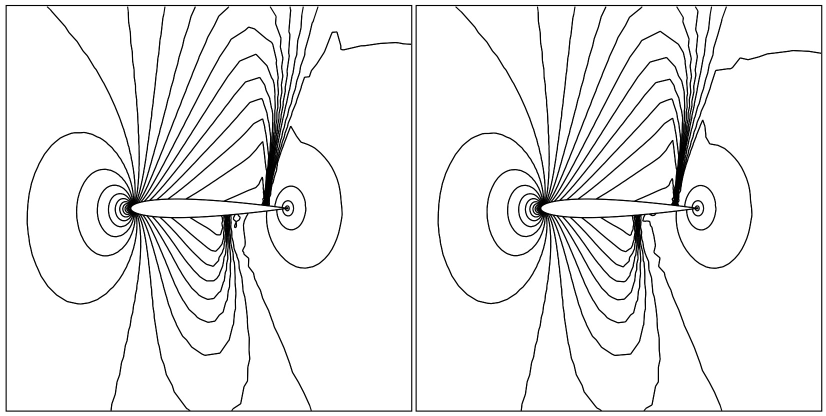

Figure 4: Pressure contours - Euler and Kinetic schemes

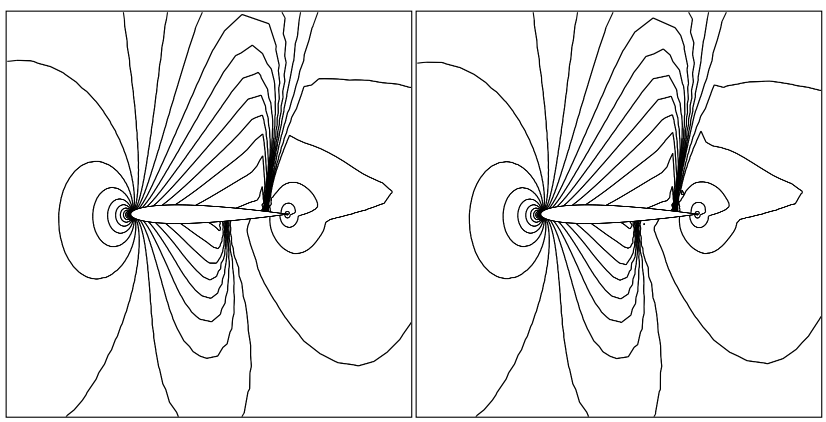

Figure 5: Mach number contours - Euler and Kinetic schemes